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Exact product forms for the simple cubic lattice Green function: I

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Abstract

The analytical properties of the lattice Green function

$$G(n,n,n;w)=\frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\frac{\cos n\theta_1\cos n\theta_2\cos n\theta_3}{w-\cos\theta_1-\cos\theta_2-\cos\theta_3}\,\mathrm{d}\theta_1\,\mathrm{d}\theta_2\,\mathrm{d}\theta_3$$

are investigated, where n is an integer and w is a complex variable. In particular, it is demonstrated that $G(n,n,n;w)$ is a solution of a fourth-order linear differential equation of the Fuchsian type. From this differential equation it is found that $G(n,n,n;w)$ can be evaluated in terms of a product of two Heun functions $\{H_j(n,v):j=1,2\}$, where

$$v\equiv v(w)=\frac{1}{w^2}\left(1+\sqrt{1-\frac{1}{w^2}}\right)^{-1}\left(1+\sqrt{1-\frac{9}{w^2}}\right)^{-1}.$$

A detailed discussion of the properties of $\{H_j(n,v):j=1,2\}$ is then given. The Heun function results are used to prove that the product form for $G(n,n,n;w)$ can be expressed in terms of complete elliptic integrals of the first and second kinds. It is also shown that $G(n,n,n;w)$ can be written in the hypergeometric form

$$wG(n,n,n;w)=\frac{(3n)!}{(3^n n!)^3}\left[\frac{w}{3}\left(1-\sqrt{1-\frac{9}{w^2}}\right)\right]^{3n}{}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\eta_+\right)\times{}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\eta_-\right)$$

where

$$\eta_\pm\equiv\eta_\pm(w)=\frac{1}{8w^2}\left[4w^2+(9-4w^2)\sqrt{1-\frac{9}{w^2}}\pm27\sqrt{1-\frac{1}{w^2}}\right].$$

This formula is valid for varying values of w in the neighbourhood of $w=\infty$, provided that the argument function $\eta_+(w)$ does not take real values in the interval $(1, +\infty)$. Finally, this ${}_2F_1$ product form is used to determine the asymptotic behaviour of $G(n, n, n; w)$ as $n \to \infty$.

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1. Introduction

The simple cubic lattice Green function

$$G(\ell, m, n; w) = \frac{1}{\pi^3} \int_0^{\pi}\int_0^{\pi}\int_0^{\pi} \frac{\cos \ell\theta_1 \cos m\theta_2 \cos n\theta_3}{w - \cos\theta_1 - \cos\theta_2 - \cos\theta_3} \, d\theta_1 \, d\theta_2 \, d\theta_3 \tag{1.1}$$

where $\{\ell, m, n\}$ is a set of integers and $w = w_1 + iw_2$ is a complex variable, defines a single-valued analytic function in a (w_1, w_2) plane which is cut along the real axis from $w = -3$ to $w = +3$. The set of points in this cut plane will be denoted by $\mathcal{C}^-$. We shall also assume, without loss of generality, that $\ell \geqslant m \geqslant n \geqslant 0$. It is readily found from (1.1) that $G(\ell, m, n; w)$ satisfies the symmetry relation

$$G(\ell, m, n; -w) = (-1)^{\ell+m+n+1} G(\ell, m, n; w). \tag{1.2}$$

We see, therefore, that it is only strictly necessary to analyse the properties of (1.1) for points $w \in \mathcal{C}^-$ which have $\mathrm{Re}(w) \geqslant 0$.

The function (1.1) plays an important role in many lattice statistical models which involve the simple cubic lattice with isotropic nearest-neighbour interactions (Berlin and Kac 1952, Duffin 1953, Maradudin *et al* 1960, Montroll and Weiss 1965, Joyce 1972, Kobelev and Kolomeisky 2002). For applications in solid-state physics one often requires the limiting behaviour of $G(\ell, m, n; w)$ as w approaches the upper and lower edges of the cut in the (w_1, w_2) plane (see Wolfram and Callaway 1963, Katsura *et al* 1971). It is convenient, therefore, to introduce the definitions

$$G^{\pm}(\ell, m, n; w_1) \equiv \lim_{\epsilon \to 0+} G(\ell, m, n; w_1 \pm i\epsilon) \equiv G_R(\ell, m, n; w_1) \mp iG_I(\ell, m, n; w_1) \tag{1.3}$$

where $-3 < w_1 < 3$. When $|w_1| \geqslant 3$ the imaginary part of $G^{\pm}(\ell, m, n; w_1)$ is always equal to zero.

A simple integral representation for (1.3) can be derived by first applying the formula

$$\mp i \int_0^{\infty} \exp[\pm i(\lambda \pm i\epsilon)t] dt = (\lambda \pm i\epsilon)^{-1} \tag{1.4}$$

to the denominator of the integrand in (1.1) with $w = w_1 \pm i\epsilon$, where λ is real and $\epsilon > 0$. The resulting multiple integral can then be simplified using the standard result

$$\frac{1}{\pi} \int_0^{\pi} \cos(n\theta) \exp(it\cos\theta) \, d\theta = i^n J_n(t) \tag{1.5}$$

where $J_n(t)$ denotes a Bessel function of the first kind of order n. Hence, we find (Wolfram and Callaway 1963)

$$G^{\pm}(\ell, m, n; w_1) = (\mp i)^{\ell+m+n+1} \int_0^{\infty} \exp(\pm iw_1 t) J_\ell(t) J_m(t) J_n(t) \, dt \tag{1.6}$$

where $-3 < w_1 < 3$. When $\ell + m + n$ is an even integer it follows from (1.3) and (1.6) that

$$G_R(\ell, m, n; w_1) = (-1)^{(\ell+m+n)/2} \int_0^{\infty} \sin(w_1 t) J_\ell(t) J_m(t) J_n(t) \, dt \tag{1.7}$$

$$G_{\text{I}}(\ell, m, n; w_1) = (-1)^{(\ell+m+n)/2} \int_0^\infty \cos(w_1 t) J_\ell(t) J_m(t) J_n(t)\, \mathrm{d}t. \tag{1.8}$$

Similar formulae can also be obtained when $\ell + m + n$ is an odd integer.

Recently, it has been shown by Joyce (2002) that $G(\ell, m, n; w)$ can be evaluated at a general lattice point $\{\ell, m, n\}$ in terms of complete elliptic integrals which only involve a single modulus k. In particular, it was found that the modified Green function

$$\overline{G}(\ell, m, n; w) \equiv (3/w)^{\ell+m+n} w G(\ell, m, n; w) \tag{1.9}$$

can be expressed in the ξ parametric form

$$\overline{G}(\ell, m, n; w) = R_0(\ell, m, n; \xi) + R_1(\ell, m, n; \xi) \left[\frac{2}{\pi} K(k)\right]^2 + R_2(\ell, m, n; \xi) \left[\frac{2}{\pi} K(k)\right] \left[\frac{2}{\pi} E(k)\right] + R_3(\ell, m, n; \xi) \left[\frac{2}{\pi} E(k)\right]^2 \tag{1.10}$$

where $K(k)$ and $E(k)$ are complete elliptic integrals of the first and second kind respectively, with a modulus

$$k \equiv k(\xi) = \frac{4\xi^{3/2}}{(1-\xi)^{3/2}(1+3\xi)^{1/2}}. \tag{1.11}$$

The connection between the parameter ξ and the variable w is given by

$$\xi \equiv \xi(w) = \frac{1}{w} \left(1 + \sqrt{1 - \frac{1}{w^2}}\right)^{-1/2} \left(1 + \sqrt{1 - \frac{9}{w^2}}\right)^{-1/2} \tag{1.12}$$

and $\{R_j(\ell, m, n; \xi) : j = 0, 1, 2, 3\}$ is a set of rational functions of ξ which can be obtained using recursion relations derived by Morita (1975). The formula (1.10) enables one to determine the value of $G(\ell, m, n; w)$ at *any* point w in the cut plane $\mathcal{C}^-$.

It was also noted by Joyce (2002) that the formula (1.10) for the Green functions $\{\overline{G}(n, n, n; w) : n = 1, 2, 3, 4\}$ and $\{\overline{G}(2n, n, n; w) : n = 1, 2, 3, 4\}$ could be factorized as a product of two linear forms in $K(k)$ and $E(k)$ whose coefficients are *polynomials* in the parameter ξ. For example, one finds that

$$\overline{G}(1, 1, 1; w) = \frac{81(1+3\xi)}{8(1-9\xi^4)^2} \left(\frac{2}{\pi}\right)^2 \left[(1+\xi)^2(1-3\xi)K(k) - (1-\xi)(1+3\xi^2)E(k)\right] \times \left[(1+\xi)(1-3\xi)(1+\xi^2)K(k) - (1-\xi)^2(1-3\xi^2)E(k)\right] \tag{1.13}$$

and

$$\overline{G}(2, 1, 1; w) = \frac{81(1-\xi)(1+3\xi)}{4(1-9\xi^4)^3} \left(\frac{2}{\pi}\right)^2 \left[(1+\xi)^3(1-3\xi)K(k) - (1-6\xi^2-3\xi^4)E(k)\right] \times \left[(1+\xi)(1-3\xi)(1+3\xi^2)^2 K(k) - (1-\xi)^2(1+18\xi^2-27\xi^4)E(k)\right]. \tag{1.14}$$

On the basis of these explicit formulae and similar results for $n = 2, 3, 4$ it was conjectured that the factorization property for $\overline{G}(n, n, n; w)$ and $\overline{G}(2n, n, n; w)$ is valid for *all* integer values of n.

Our main aim in paper I is to investigate the analytic properties of the *diagonal* lattice Green function $G(n, n, n; w)$. In particular, it will be proved in section 2 that $G(n, n, n; w)$ is a solution of a fourth-order differential equation of the Fuchsian type. In section 3 we shall use this differential equation to show that $G(n, n, n; w)$ can be written in terms of a *product* of two Heun functions $\{H_j(n, v) : j = 1, 2\}$, where

$$v \equiv v(w) = \xi^2(w) \tag{1.15}$$

and $\xi(w)$ is defined in (1.12). The properties of $\{H_j(n, v) : j = 1, 2\}$ are discussed in sections 4–6. In section 7 we shall use the Heun function results to *prove* the factorization conjecture for $G(n, n, n; w)$ which was proposed by Joyce (2002). Finally, the asymptotic behaviour of $G(n, n, n; w)$ as $n \to \infty$ will be established in section 8.

Similar methods have also been used to prove the factorization conjecture (Joyce 2002) for $G(2n, n, n; w)$. These results will be given in paper II.

2. Basic results for $G(n, n, n; w)$

In this section we shall establish a fourth-order differential equation for the diagonal Green function $G(n, n, n; w)$.

2.1. Series expansion for $G(n , n, n; w)$ about $w = \infty$

We begin by applying the formula

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

where $\mathrm{Re}(\alpha) > 0$, to the integrand denominator in (1.1). The resulting multiple integral can then be simplified using the standard result

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

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

$$G(n, n, n; w) = \int_0^\infty \exp(-wt)\,[I_n(t)]^3\, \mathrm{d}t \tag{2.3}$$

where $\mathrm{Re}(w) \geqslant 3$.

Next we consider the Taylor series expansion

$$[I_n(t)]^3 = \frac{t^{3n}}{(2^n n!)^3}\sum_{m=0}^{\infty} a_m(n)\left(\frac{t}{2}\right)^{2m} \tag{2.4}$$

where $|t| < \infty$ and $a_0(n) = 1$. Formulae for the coefficients $\{a_m(n) : m = 0, 1, 2, \ldots\}$ in (2.4) can be determined using the generating function identity

$$[{}_0F_1(-; n + 1; x)]^3 \equiv \sum_{m=0}^{\infty} a_m(n)x^m \tag{2.5}$$

where ${}_0F_1$ denotes a generalized hypergeometric series.

We now substitute (2.4) in the integral representation (2.3). This procedure yields the required series expansion

$$G(n, n, n; w) = \frac{(3n)!}{(2^n n!)^3}\frac{1}{w^{3n+1}}\sum_{m=0}^{\infty}\frac{\mu_m(n)}{w^{2m}} \tag{2.6}$$

where $|w| \geqslant 3$ and

$$\mu_m(n) = \frac{(3n + 2m)!}{2^{2m}(3n)!}a_m(n). \tag{2.7}$$

From the work of Jorna (1975) it can also be shown that

$$\mu_m(n) = \frac{(3n + 2m)!}{2^{2m}(3n)!(n + 1)_m m!}\,{}_3F_2\left[\begin{matrix} -m, & -m - n, & n + \frac{1}{2}; \\ & & & 4 \\ n + 1, & 2n + 1; & \end{matrix}\right] \tag{2.8}$$

where $(n+1)_m$ denotes a Pochhammer symbol and ${}_3F_2$ is a generalized hypergeometric series.

2.2. Differential equation for $[I_n(t)]^3$ and a recursion relation for $a_m(n)$

Appell (1880) has shown that if $\varphi(t)$ is a solution of the second-order differential equation

$$\frac{d^2\varphi}{dt^2} + f(t)\frac{d\varphi}{dt} + g(t)\varphi = 0 \tag{2.9}$$

then the function $\Omega(t) = [\varphi(t)]^3$ is a solution of the fourth-order differential equation

$$\begin{aligned}\frac{d^4\Omega}{dt^4} + 6f(t)\frac{d^3\Omega}{dt^3} &+ \left\{11[f(t)]^2 + 10g(t) + 4\frac{df}{dt}\right\}\frac{d^2\Omega}{dt^2}\\ &+ \left\{6[f(t)]^3 + 30f(t)g(t) + 7f(t)\frac{df}{dt} + 10\frac{dg}{dt} + \frac{d^2 f}{dt^2}\right\}\frac{d\Omega}{dt}\\ &+3\left\{6[f(t)]^2 g(t) + 3[g(t)]^2 + 2g(t)\frac{df}{dt} + 5f(t)\frac{dg}{dt} + \frac{d^2 g}{dt^2}\right\}\Omega = 0.\end{aligned} \tag{2.10}$$

If this result is applied to the function $\varphi(t) = I_n(t)$ it is found that

$$f(t) = \frac{1}{t} \tag{2.11}$$

$$g(t) = -\left(1 + \frac{n^2}{t^2}\right). \tag{2.12}$$

It readily follows from (2.10)–(2.12) that $\Omega(t) = [I_n(t)]^3$ is a solution of the differential equation

$$\begin{aligned}t^4\frac{d^4\Omega}{dt^4} + 6t^3\frac{d^3\Omega}{dt^3} &+ t^2\left[(7 - 10n^2) - 10t^2\right]\frac{d^2\Omega}{dt^2} + t\left[(1 - 10n^2) - 30t^2\right]\frac{d\Omega}{dt}\\ &+3\left[3n^4 - 2(2 - 3n^2)t^2 + 3t^4\right]\Omega = 0.\end{aligned} \tag{2.13}$$

We can now derive a recursion relation for the coefficients $\{a_m(n) : m = 0, 1, 2, \ldots\}$ by substituting the expansion (2.4) in (2.13). The final result is

$$\begin{aligned}&(m + 1)(m + n + 1)(m + 2n + 1)(m + 3n + 1)a_{m+1}(n)\\ &\quad - \left[3(2n + 1)(3n + 1) + 10(3n + 1)m + 10m^2\right]a_m(n) + 9a_{m-1}(n) = 0\end{aligned} \tag{2.14}$$

where $m = 0, 1, 2, \ldots,$ with the initial conditions $a_0(n) = 1$ and $a_{-1}(n) = 0$.

2.3. Recursion relation for $\mu_m(n)$ and a differential equation for $G(n, n, n; w)$

If the formula (2.7) is substituted in (2.14) we find that $\{\mu_m(n) : m = 0, 1, 2, \ldots\}$ satisfy the three-term recursion relation

$$\begin{aligned}&16(m + 1)(m + n + 1)(m + 2n + 1)(m + 3n + 1)\mu_{m+1}(n) - 4(2m + 3n + 1)(2m + 3n + 2)\\ &\quad\times\left[3(2n + 1)(3n + 1) + 10(3n + 1)m + 10m^2\right]\mu_m(n)\\ &\quad+9(2m + 3n - 1)(2m + 3n)(2m + 3n + 1)(2m + 3n + 2)\mu_{m-1}(n) = 0\end{aligned} \tag{2.15}$$

where $m = 0, 1, 2, \ldots,$ with the initial conditions $\mu_0(n) = 1$ and $\mu_{-1}(n) = 0$. From (2.15) and the expansion (2.6) we deduce that $G(n, n, n; w)$ is a solution of the fourth-order Fuchsian differential equation

$$\begin{aligned}(w^2 - 1)(w^2 - 9)\frac{d^4G}{dw^4} + 10w(w^2 - 5)\frac{d^3G}{dw^3} &- \left[5(2n^2 - 5)w^2 - 6(3n^2 - 7)\right]\frac{d^2G}{dw^2}\\ &- 15(2n^2 - 1)w\frac{dG}{dw} + (n^2 - 1)(9n^2 - 1)G = 0\end{aligned} \tag{2.16}$$

where $n = 0, 1, 2, \ldots$. For the special case $n = 0$ the recursion relation (2.15) has a common factor of $m + 1$ and it follows that $G(0, 0, 0; w)$ is also a solution of the third-order differential equation

$$(w^2 - 1)(w^2 - 9)\frac{d^3G}{dw^3} + 6w(w^2 - 5)\frac{d^2G}{dw^2} + (7w^2 - 12)\frac{dG}{dw} + wG = 0. \tag{2.17}$$

This result was first derived by Joyce (1973).

Finally, we shall find that it is useful to apply the transformation $z = 1/w^2$ to (2.16). In this manner we obtain the alternative differential equation

$$\mathbf{L}_{4,n}(G) = 0 \tag{2.18}$$

where the differential operator

$$\begin{aligned}\mathbf{L}_{4,n} = {} & 16z^4(z-1)(9z-1)\mathrm{D}_z^4 + 16z^3(81z^2 - 65z + 4)\mathrm{D}_z^3 \\ & + 4z^2\big[675z^2 + 18z(n^2 - 19) - 10(n^2 - 1)\big]\mathrm{D}_z^2 \\ & + 36z^2\big[30z + (3n^2 - 7)\big]\mathrm{D}_z + (n^2 - 1)(9n^2 - 1)\end{aligned} \tag{2.19}$$

and $\mathrm{D}_z = \mathrm{d}/\mathrm{d}z$.

3. Analysis of the differential equation $\mathbf{L}_{4,n}(G) = 0$

Our main aim in this section is to investigate the properties the differential equation (2.18). In particular, we shall show that the general solution of $\mathbf{L}_{4,n}(G) = 0$ can be expressed in terms of products of solutions of two second-order Heun differential equations. It follows from this result that $G(n, n, n; w)$ can be written in terms of a product of two Heun functions.

3.1. Singularity structure of the differential equation (2.18)

The basic differential equation (2.18) is of the Fuchsian type with four regular singular points at $z = 0, \frac{1}{9}, 1$ and ∞. The Riemann *P*-symbol (see Ince (1927), p 370) associated with equation (2.18) is given by

$$P\begin{bmatrix} 0 & \frac{1}{9} & 1 & \infty & \\ \frac{1}{2}(1+3n) & 0 & 0 & 0 & \\ \frac{1}{2}(1-3n) & 1 & 1 & 1 & z \\ \frac{1}{2}(1+n) & 2 & 2 & \frac{1}{2} & \\ \frac{1}{2}(1-n) & \frac{1}{2} & \frac{1}{2} & \frac{3}{2} & \end{bmatrix}. \tag{3.1}$$

In this scheme, the singular points are placed on the first row with the roots of the corresponding indicial equations beneath them. For an arbitrary *N*th order Fuchsian equation with ν regular singular points in the finite z plane and a regular singular point at $z = \infty$, 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 (3.1) that the differential equation (2.18) has the correct Fuchsian invariant of 12.

It is clear from (3.1) that the expansion (2.6) with $z = 1/w^2$ will give a series solution of (2.18) which is associated with the exponent $\frac{1}{2}(1+3n)$ at $z = 0$. Surprisingly, the series solution about $z = 0$ which is associated with the exponent $\frac{1}{2}(1-n)$ terminates after a finite number of terms and we obtain a simple *algebraic* solution of the type

$$G \equiv G^{(a)}(n, z) = z^{\frac{1}{2}(1-n)} \sum_{m=0}^{[\frac{1}{2}(n-1)]} g_m(n) z^m \tag{3.2}$$

where $\left[\frac{1}{2}(n-1)\right]$ denotes the largest integer less than or equal to $\frac{1}{2}(n-1)$, $g_0(n) = 1$ and $n = 1, 2, \ldots$. When $n \geqslant 3$ the higher-order coefficients $\{g_m(n) : m = 1, 2, \ldots\}$ in (3.2) can be generated using the three-term recursion relation

$$\begin{aligned}16(m+1)(m+n+1)(m-n+1)(m-2n+1)g_{m+1}(n) - 4(2m-n+1)(2m-n+2)\\ \times\left[(3+n)(1-2n) + 10(1-n)m + 10m^2\right]g_m(n)\\ +9(2m-n-1)(2m-n)(2m-n+1)(2m-n+2)g_{m-1}(n) = 0\end{aligned} \qquad (3.3)$$

where $m = 0, 1, 2, \ldots, \left[\frac{1}{2}(n-1)\right] - 1$, with the initial conditions $g_0(n) = 1$ and $g_{-1}(n) = 0$.

3.2. *Reduction of the order of* $\mathbf{L}_{4,n}(G) = 0$ *for* $n > 0$

If the series expansion (2.6) is substituted into a *general* third-order differential equation with polynomial coefficients we find by computer fitting that $G(n, n, n; w)$ is also a solution of a differential equation of the type

$$\mathbf{L}_{3,n}(G) = 0 \qquad (3.4)$$

where the differential operator

$$\mathbf{L}_{3,n} = z^3(z-1)(9z-1)A_3(n,z)\mathrm{D}_z^3 + z^2A_2(n,z)\mathrm{D}_z^2 + zA_1(n,z)\mathrm{D}_z + A_0(n,z) \qquad (3.5)$$

$\mathrm{D}_z = \mathrm{d}/\mathrm{d}z$ and $n = 1, 2, \ldots$. In this formula $\{A_j(n,z) : j = 0, 1, 2, 3\}$ are polynomials in z of degree $\left[\frac{1}{2}(n+1)\right]$, $\left[\frac{1}{2}(n+4)\right]$, $\left[\frac{1}{2}(n+4)\right]$ and $\left[\frac{1}{2}n\right]$ respectively. For the particular case $n = 4$ it is found that

$$A_0(4,z) = -2145(24 - 56z + 29z^2) \qquad (3.6)$$

$$A_1(4,z) = -6(5720 - 10\,520z - 1007z^2 + 7702z^3 - 1044z^4) \qquad (3.7)$$

$$A_2(4,z) = 12(280 - 4280z + 9189z^2 - 6124z^3 + 783z^4) \qquad (3.8)$$

$$A_3(4,z) = 8(120 - 168z + 29z^2). \qquad (3.9)$$

We see that a major disadvantage of the reduced equation (3.4) is that it becomes increasingly more complicated as n increases. It should be noted that all the zeros of the polynomial $A_3(n,z)$ are apparent singularities of the reduced differential equation (see Ince (1927), p 406).

The connection between (3.4) and the fourth-order differential equation (2.18) can be established by acting on $\mathbf{L}_{3,n}(G) = 0$ with the operator

$$\mathbf{L}_{1,n} = 8[2z\mathrm{D}_z - (n+1)]. \qquad (3.10)$$

We find that

$$\mathbf{L}_{1,n}\mathbf{L}_{3,n}(G) = A_3(n,z)\mathbf{L}_{4,n}(G) = 0 \qquad (3.11)$$

where $n = 1, 2, \ldots$. The possibility of reducing the order of $\mathbf{L}_{4,n}(G) = 0$ for $n > 0$ appears to be related to the existence of the algebraic solution (3.2).

3.3. *Product solutions for the differential equation (2.18)*

It can be proved by following a method recently described by Delves and Joyce (2001, pp 81–4) that any solution of the differential equation $\mathbf{L}_{4,n}(G) = 0$ can be expressed in the product form

$$G(z) = z^{-1/2}(1-z)^{-1/2}(1-9z)^{-1/2}Y_1(n,z)Y_2(n,z) \qquad (3.12)$$

where $Y_1(n,z)$ and $Y_2(n,z)$ are appropriate solutions of the second-order differential equations

$$\left[D_z^2 + U_+(n,z)\right]Y = 0 \tag{3.13}$$

and

$$\left[D_z^2 + U_-(n,z)\right]Y = 0 \tag{3.14}$$

respectively. The coefficients $U_\pm(n,z)$ in these equations are given by

$$\begin{aligned} U_\pm(n,z) = {}& \frac{(2-5n^2)}{8z^2} + \frac{(14-41n^2)}{8z} + \frac{3}{16(1-z)^2} + \frac{(35-8n^2)}{128(1-z)} \\ & + \frac{243}{16(1-9z)^2} + \frac{243(7-24n^2)}{128(1-9z)} \pm \frac{3n^2}{8z^2\sqrt{(1-z)(1-9z)}}. \end{aligned} \tag{3.15}$$

It is seen that the functions $U_\pm(n,z)$ involve the two branches of an algebraic function $f(z)$ which is defined by the polynomial equation

$$\psi(f,z) \equiv f^2 - (1-z)(1-9z) = 0. \tag{3.16}$$

Next we shall carry out a *direct* verification of the crucial results (3.13)–(3.15). In the first stage of the analysis we note that, if $Y_1(n,z)$ and $Y_2(n,z)$ are solutions of (3.13) and (3.14) respectively, then the product $Y_1(n,z)Y_2(n,z)$ is a solution of the fourth-order differential equation (Orr (1900), Watson (1944), p 146)

$$D_z\left[\frac{D_z^3 Y + 2(U_+ + U_-)D_z Y + Y D_z(U_+ + U_-)}{(U_+ - U_-)}\right] + (U_+ - U_-)Y = 0 \tag{3.17}$$

where $D_z = d/dz$, $U_\pm = U_\pm(n,z)$ and $U_+ \neq U_-$. We now use the particular formula (3.15) to evaluate and simplify the general equation (3.17). Finally, the transformation

$$Y = z^{1/2}(1-z)^{1/2}(1-9z)^{1/2}G \tag{3.18}$$

is applied to the dependent variable in the differential equation. In this manner, we obtain the expected equation $\mathbf{L}_{4,n}(G) = 0$.

3.4. Transformation of (3.13) and (3.14) to Heun differential equations

The set of points $\{(f,z) : \psi(f,z) = 0\}$ defines a complex curve which has a genus $g = 0$. It follows, therefore, that we can represent f and z as single-valued *rational* functions of a new parameter v. In particular, we find that

$$z = \frac{4v(1-v)(1-9v)}{(1-9v^2)^2} \tag{3.19}$$

$$f = \frac{(1-2v+9v^2)(1-18v+9v^2)}{(1-9v^2)^2} \tag{3.20}$$

are suitable representations. If (3.19) is used to transform the independent variable in (3.13) and (3.14) from z to v then it is found that $Y_1(n,v)$ and $Y_2(n,v)$ satisfy rather complicated differential equations of the type

$$\left[D_v^2 + p_+(n,v)D_v + q_+(n,v)\right]Y_1(n,v) = 0 \tag{3.21}$$

and

$$\left[D_v^2 + p_-(n,v)D_v + q_-(n,v)\right]Y_2(n,v) = 0 \tag{3.22}$$

respectively, where $p_\pm(n,v)$ and $q_\pm(n,v)$ are *rational* functions of v, and $D_v = d/dv$.

We can simplify (3.21) and reduce it to a standard form by applying the further transformation

$$Y_1(n, v) = v^{(n+1)/2}(1-v)^{(1-2n)/2}(1-9v)^{(1-2n)/2}(1-9v^2)^{-3/2} \times (1-2v+9v^2)^{1/2}(1-18v+9v^2)^{1/2} y_1(n, v). \tag{3.23}$$

In this manner, we deduce that $y_1(n, v)$ is a solution of the Heun differential equation (Snow 1952, Ronveaux 1995)

$$\frac{d^2 y}{dv^2} + \left(\frac{n+1}{v} + \frac{1-2n}{v-1} + \frac{1-2n}{v-\frac{1}{9}}\right)\frac{dy}{dv} + \frac{(2n-1)\left[(n-1)v + \frac{1}{9}(n+3)\right]}{v(v-1)\left(v-\frac{1}{9}\right)} y = 0. \tag{3.24}$$

The application of the transformation

$$Y_2(n, v) = v^{(2n+1)/2}(1-v)^{(1-n)/2}(1-9v)^{(1-n)/2}(1-9v^2)^{-3/2} \times (1-2v+9v^2)^{1/2}(1-18v+9v^2)^{1/2} y_2(n, v) \tag{3.25}$$

to (3.22) enables one to show that $y_2(n, v)$ is a solution of another Heun equation

$$\frac{d^2 y}{dv^2} + \left(\frac{2n+1}{v} + \frac{1-n}{v-1} + \frac{1-n}{v-\frac{1}{9}}\right)\frac{dy}{dv} + \frac{\left[(1-n^2)v + \frac{1}{9}(n-3)(2n+1)\right]}{v(v-1)\left(v-\frac{1}{9}\right)} y = 0. \tag{3.26}$$

3.5. Heun function product form for $G(n, n, n; w)$

The Heun differential equations (3.24) and (3.26) are of the Fuchsian type with four regular singular points at $v = 0, \frac{1}{9}, 1$ and ∞. The Riemann P-symbol (see Ince (1927), p 370) associated with equation (3.24) is given by

$$P\begin{bmatrix} 0 & \frac{1}{9} & 1 & \infty & \\ 0 & 0 & 0 & 1-n & v \\ -n & 2n & 2n & 1-2n & \end{bmatrix} \tag{3.27}$$

while the P-symbol for (3.26) is

$$P\begin{bmatrix} 0 & \frac{1}{9} & 1 & \infty & \\ 0 & 0 & 0 & 1-n & v \\ -2n & n & n & 1+n & \end{bmatrix}. \tag{3.28}$$

We see directly from these results that the Heun equations have the correct Fuchsian invariant of 2.

It is clear from the P-symbols that in the neighbourhood of the singularity $v = 0$ the Heun equations (3.24) and (3.26) will have series solutions of the type

$$y = H_j(n, v) \equiv \sum_{m=0}^{\infty} h_m^{(j)}(n) v^m \qquad (j = 1, 2) \tag{3.29}$$

respectively, where $|v| < \frac{1}{9}$ and $\left\{h_0^{(j)}(n) \equiv 1 : j = 1, 2\right\}$. We can generate the coefficients $\left\{h_m^{(1)}(n) : m = 1, 2, \ldots\right\}$ and $\left\{h_m^{(2)}(n) : m = 1, 2, \ldots\right\}$ using the recursion relations

$$(m+1)(m+n+1)h_{m+1}^{(1)}(n) - \left[(3+n)(1-2n) + 10(1-n)m + 10m^2\right]h_m^{(1)}(n) + 9(m-n)(m-2n)h_{m-1}^{(1)}(n) = 0 \tag{3.30}$$

and

$$(m+1)(m+2n+1)h_{m+1}^{(2)}(n) - \left[(3-n)(1+2n) + 10(1+n)m + 10m^2\right]h_m^{(2)}(n) + 9(m-n)(m+n)h_{m-1}^{(2)}(n) = 0 \tag{3.31}$$

respectively, where $m = 0, 1, 2, \ldots$, with the initial conditions $\{h_0^{(j)}(n) = 1 : j = 1, 2\}$ and $\{h_{-1}^{(j)}(n) = 0 : j = 1, 2\}$. If we adopt the notation used by Snow (1952) then we can write $H_1(n, v)$ and $H_2(n, v)$ in the form

$$H_1(n, v) = F\left[\tfrac{1}{9}, \tfrac{1}{9}(n+3)(2n-1); 1-n, 1-2n, n+1, 1-2n; v\right] \tag{3.32}$$

and

$$H_2(n, v) = F\left[\tfrac{1}{9}, \tfrac{1}{9}(n-3)(2n+1); 1-n, 1+n, 1+2n, 1-n; v\right] \tag{3.33}$$

respectively, where $F(a, b; \alpha, \beta, \gamma, \delta; v)$ denotes a Heun function. It should be noted that the second independent series solutions of the Heun equations (3.24) and (3.26) exhibit singularities at $v = 0$ which involve *logarithmic* terms.

We now take our solution of $\mathbf{L}_{4,n}(G) = 0$ to be the series expansion (2.6) for the Green function $G(n, n, n; w)$ in powers of $1/w$. For this particular case the solution of $\mathbf{L}_{4,n}(G) = 0$ does *not* have a logarithmic singularity at $w = \infty$ and it is clear, therefore, that the relevant solutions of the Heun equations (3.24) and (3.26) are constant multiples of $H_1(n, v)$ and $H_2(n, v)$ respectively. Finally, we combine equations (3.12), (3.19), (3.23), (3.25) and (3.29) in order to obtain the formula

$$w^{3n+1} G(n, n, n; w) = C_n \frac{(1-9v^2)^{3n+1}}{[(1-v)(1-9v)]^{3n}} H_1(n, v) H_2(n, v) \tag{3.34}$$

where C_n does not depend on the variable v. We can determine C_n by taking the limit $v \to 0$ in (3.34) and comparing the result with the leading-order term in (2.6), with $v \sim (2w)^{-2}$. Hence we obtain the required Heun function product form

$$w^{3n+1} G(n, n, n; w) = \frac{(3n)!}{(2^n n!)^3} \frac{(1-9v^2)^{3n+1}}{[(1-v)(1-9v)]^{3n}} H_1(n, v) H_2(n, v). \tag{3.35}$$

The general connection between the variables v and w can be established by finding the inverse of the transformation (3.19), with $z = 1/w^2$. This procedure gives

$$v(w) = \frac{1}{w^2} \left(1 + \sqrt{1 - \frac{1}{w^2}}\right)^{-1} \left(1 + \sqrt{1 - \frac{9}{w^2}}\right)^{-1}. \tag{3.36}$$

The final results were checked by using (3.36) to expand the product form (3.35) in powers of $1/w$, and agreement was found with the series expansion (2.6).

It is found that the transformation function $v(w)$ maps all the points $w \in \mathcal{C}^-$ into a region $\mathcal{R}_1$ in the v plane which forms part of the circle $|v| = \frac{1}{3}$. This image region is shown in figure 1. The points on the boundary of $\mathcal{R}_1$ are associated with the edges of the cut in the w plane.

4. Operator identities and recursion relations for $\{H_j(n, v) : j = 1, 2\}$

In this section, various operator identities are used to derive recursion relations for the Heun functions $\{H_1(n, v) : n = 0, 1, 2, \ldots\}$ and $\{H_2(n, v) : n = 0, 1, 2, \ldots\}$.

We begin by writing the Heun differential equation (3.24) in the alternative form

$$\widehat{\mathcal{H}}_{1,n}(y) = 0 \tag{4.1}$$

where

$$\widehat{\mathcal{H}}_{1,n} = v(v-1)(9v-1)\mathrm{D}_v^2 + \left[27(1-n)v^2 + 10(n-2)v + (n+1)\right]\mathrm{D}_v + (2n-1)\left[9(n-1)v + (n+3)\right] \tag{4.2}$$

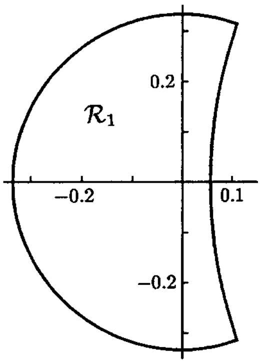

Figure 1. The region $\mathcal{R}_1$ in the v plane.

and $D_v = d/dv$. Next we consider the operator identity

$$\widehat{\mathcal{H}}_{1,n}\big[P_{1,1}(n,v)D_v + P_{1,0}(n,v)\big] = \big[Q_{1,1}(n,v)D_v + Q_{1,0}(n,v)\big]\widehat{\mathcal{H}}_{1,n-1} \qquad (4.3)$$

where

$$P_{1,1}(n,v) = Q_{1,1}(n,v) = \frac{n(v-1)(9v-1)(3v+1)}{3(3n-1)(3n-2)} \qquad (4.4)$$

$$P_{1,0}(n,v) = -\frac{n}{3(3n-1)(3n-2)}\big[27(n-2)v^2 + 6(11n-6)v - (29n-26)\big] \qquad (4.5)$$

$$Q_{1,0}(n,v) = -\frac{n}{3(3n-1)(3n-2)}\big[27(n-2)v^2 + 6(11n+2)v - (29n-10)\big]. \qquad (4.6)$$

We can prove this identity by allowing both sides of equation (4.3) to act on an arbitrary differentiable function $f(v)$.

If we now take the function $f(v)$ to be the Heun function $H_1(n-1,v)$ then it is clear from (4.3) that

$$\big[P_{1,1}(n,v)D_v + P_{1,0}(n,v)\big]H_1(n-1,v) = C_{1,n}H_1(n,v) \qquad (4.7)$$

where $C_{1,n}$ does not depend on the variable v. We can determine $C_{1,n}$ by using (3.29), (4.4) and (4.5) to expand both sides of (4.7) to leading-order in powers of v. In this manner we find that $C_{1,n} = 1$. Hence, we obtain the important relation

$$H_1(n,v) = \widehat{\mathcal{R}}_{1,n}H_1(n-1,v) \qquad (4.8)$$

where the raising operator $\widehat{\mathcal{R}}_{1,n}$ is defined as

$$\widehat{\mathcal{R}}_{1,n} = P_{1,1}(n,v)D_v + P_{1,0}(n,v). \qquad (4.9)$$

If we now make the substitution $n \to n+1$ in (4.8) and (4.9) it is found that

$$H_1(n+1,v) = P_{1,1}(n+1,v)D_v\big[P_{1,1}(n,v)D_vH_1(n-1,v) + P_{1,0}(n,v)H_1(n-1,v)\big] + P_{1,0}(n+1,v)H_1(n,v). \qquad (4.10)$$

The evaluation of the right-hand side of (4.10) can be simplified by using the Heun equation $\widehat{\mathcal{H}}_{1,n-1}(y) = 0$ to eliminate the second derivative $D_v^2H_1(n-1,v)$. We can then remove the remaining first derivative $D_vH_1(n-1,v)$ using (4.8). This procedure yields the required recursion relation

$$3(3n+1)(3n+2)vH_1(n+1,v) - n(n+1)\big[(3v-1)(9v^2-42v+1)H_1(n,v) + (v-1)^2(9v-1)^2H_1(n-1,v)\big] = 0 \qquad (4.11)$$

where $n = 1, 2, \ldots$.

A similar method will now be used to derive a recursion relation for $H_2(n, v)$. In the first stage of the analysis we express the Heun differential equation (3.26) in the form

$$\widehat{\mathcal{H}}_{2,n}(y) = 0 \tag{4.12}$$

where

$$\widehat{\mathcal{H}}_{2,n} = v(v-1)(9v-1)\mathrm{D}_v^2 + \left[27v^2 - 10(n+2)v + (2n+1)\right]\mathrm{D}_v + \left[9(1-n^2)v + (n-3)(2n+1)\right] \tag{4.13}$$

and introduce the further operator identity

$$\widehat{\mathcal{H}}_{2,n}\left[P_{2,1}(n,v)\mathrm{D}_v + P_{2,0}(n,v)\right] = \left[Q_{2,1}(n,v)\mathrm{D}_v + Q_{2,0}(n,v)\right]\widehat{\mathcal{H}}_{2,n-1} \tag{4.14}$$

where

$$P_{2,1}(n,v) = Q_{2,1}(n,v) = -\frac{n(v-1)(9v-1)(3v-1)}{6(3n-1)(3n-2)v} \tag{4.15}$$

$$P_{2,0}(n,v) = -\frac{n}{6(3n-1)(3n-2)v}\left[27nv^2 - 6(7n-2)v - (n-4)\right] \tag{4.16}$$

$$Q_{2,0}(n,v) = -\frac{n}{6(3n-1)(3n-2)v^2}\left[27(n+1)v^3 - 3(14n+3)v^2 - (n+3)v + 1\right]. \tag{4.17}$$

Next we allow both sides of the operator identity (4.14) to act on the Heun function $H_2(n-1, v)$. This procedure leads to the relation

$$H_2(n,v) = \widehat{\mathcal{R}}_{2,n} H_2(n-1,v) \tag{4.18}$$

where the raising operator $\widehat{\mathcal{R}}_{2,n}$ is given by

$$\widehat{\mathcal{R}}_{2,n} = P_{2,1}(n,v)\mathrm{D}_v + P_{2,0}(n,v). \tag{4.19}$$

Finally we make the substitution $n \to n+1$ in (4.18) and (4.19). In this manner it is found that

$$H_2(n+1,v) = P_{2,1}(n+1,v)\mathrm{D}_v\left[P_{2,1}(n,v)\mathrm{D}_v H_2(n-1,v) + P_{2,0}(n,v)H_2(n-1,v)\right] + P_{2,0}(n+1,v)H_2(n,v). \tag{4.20}$$

We simplify the evaluation of the right-hand side of (4.20) by using the Heun equation $\widehat{\mathcal{H}}_{2,n-1}(y) = 0$ to eliminate the second derivative $\mathrm{D}_v^2 H_2(n-1, v)$. It is then possible to remove the remaining first derivative $\mathrm{D}_v H_2(n-1, v)$ using (4.18). This procedure gives the second recursion relation

$$3(3n+1)(3n+2)v^2 H_2(n+1,v) + n(n+1)\left[(3v+1)(9v^2-12v+1)H_2(n,v) - (v-1)(9v-1)H_2(n-1,v)\right] = 0 \tag{4.21}$$

where $n = 1, 2, \ldots$.

We have also derived the further relation

$$H_j(n,v) = \widehat{\mathcal{L}}_{j,n} H_j(n+1,v) \tag{4.22}$$

where $j = 1, 2$ and $\{\widehat{\mathcal{L}}_{j,n} : j = 1, 2\}$ are *lowering* operators. In particular, we find that

$$\widehat{\mathcal{L}}_{1,n} = \frac{1}{(n+1)(v-1)(9v-1)}\left[v(3v+1)\mathrm{D}_v + (n+1) - 3(2n+1)v\right] \tag{4.23}$$

$$\widehat{\mathcal{L}}_{2,n} = \frac{1}{2(n+1)}\left[v(1-3v)\mathrm{D}_v + 2(n+1) + 3nv\right]. \tag{4.24}$$

The set of raising and lowering operators $\{\widehat{\mathcal{R}}_{j,n}, \widehat{\mathcal{L}}_{j,n} : n = 0, 1, 2, \ldots\}$, where $j = 1, 2$, is not closed under commutation. However, if the Heun functions $H_1(n, v)$ and $H_2(n, v)$ are scaled using (6.11) and (6.12), respectively, it can be shown (Miller (1968), p 199) that they form a realization of the Lie algebra $\mathcal{G}\{1, 0\}$.

5. Solutions of the Heun differential equations $\{\widehat{\mathcal{H}}_{j,n}(y) = 0 : j = 1, 2\}$ in terms of complete elliptic integrals

The main aim in this section is to show how the operator identities and recursion relations derived in section 4 can be used to express the solutions of the Heun equations (3.24) and (3.26) in terms of complete elliptic integrals of the first and second kind.

5.1. *Formulae for* $\{H_j(n, v) : j = 1, 2\}$

It has been shown by Joyce (1994, 1998) that $G(0, 0, 0; w)$ can be written in the ξ parametric form

$$G(0,0,0;w) = 2\xi\frac{(1+\xi)^{1/2}(1-3\xi)^{1/2}}{(1-\xi)^{5/2}(1+3\xi)^{1/2}}\left[\frac{2}{\pi}K(k)\right]^2 \tag{5.1}$$

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

$$k = \frac{4\xi^{3/2}}{(1-\xi)^{3/2}(1+3\xi)^{1/2}}. \tag{5.2}$$

The connection between the parameter ξ and the variable w is given by

$$\xi(z) = z^{1/2}\left(1+\sqrt{1-z}\right)^{-1/2}\left(1+\sqrt{1-9z}\right)^{-1/2} \tag{5.3}$$

with $z = 1/w^2$. If we compare (5.1) and (5.3) with the formulae (3.35) and (3.36), respectively, then it is seen that

$$H_1(0,v) = H_2(0,v) = \frac{1}{(1-\xi)^{3/2}(1+3\xi)^{1/2}}\left(\frac{2}{\pi}\right)K(k) \tag{5.4}$$

where $v = \xi^2$.

A similar formula for $H_1(1, v)$ can be derived by applying the raising operator $\widehat{\mathcal{R}}_{1,1}$ to (5.4). Hence we find that

$$\begin{aligned} H_1(1,v) = \frac{1}{v}\bigg[&B_1^{(1)}(1,v)(1-\xi)^{-3/2}(1+3\xi)^{-1/2}\left(\frac{2}{\pi}\right)K(k) \\ &+ B_1^{(2)}(1,v)(1-\xi)^{3/2}(1+3\xi)^{1/2}\left(\frac{2}{\pi}\right)E(k)\bigg] \end{aligned} \tag{5.5}$$

where

$$B_1^{(1)}(1,v) = -\tfrac{1}{8}(1-v)^2(1-9v) \tag{5.6}$$

$$B_1^{(2)}(1,v) = \tfrac{1}{8}(1+3v) \tag{5.7}$$

and $E(k)$ is the complete elliptic integral of the second kind.

It is now possible to use the recursion relation (4.11) to generate formulae for the higher-order Heun functions. In particular, it is found that

$$\begin{aligned} H_1(n,v) = \frac{1}{v^n}\bigg[&B_1^{(1)}(n,v)(1-\xi)^{-3/2}(1+3\xi)^{-1/2}\left(\frac{2}{\pi}\right)K(k) \\ &+ B_1^{(2)}(n,v)(1-\xi)^{3/2}(1+3\xi)^{1/2}\left(\frac{2}{\pi}\right)E(k)\bigg] \end{aligned} \tag{5.8}$$

where $\left\{B_1^{(j)}(n, v) : j = 1, 2\right\}$ satisfy the recursion relation

$$\begin{aligned} 3(3n+1)(3n+2)B_1^{(j)}(n+1,v) - n(n+1)\big[&(3v-1)(9v^2-42v+1)B_1^{(j)}(n,v) \\ &+ v(v-1)^2(9v-1)^2B_1^{(j)}(n-1,v)\big] = 0 \end{aligned} \tag{5.9}$$

with $n = 1, 2, \ldots$. The initial conditions for this relation are given for $j = 1$ and $j = 2$ by $B_1^{(1)}(0, v) = 1$, (5.6) and $B_1^{(2)}(0, v) = 0$, (5.7), respectively. In appendix A we list the polynomials $\left\{B_1^{(j)}(n, v) : j = 1, 2\right\}$ for $n \leqslant 4$.

In a similar manner we can use (4.18), (5.4) and (4.21) to express $H_2(n, v)$ in terms of $K(k)$ and $E(k)$. The final result is

$$H_2(n, v) = \frac{1}{v^{2n}}\left[B_2^{(1)}(n, v)(1-\xi)^{-3/2}(1+3\xi)^{-1/2}\left(\frac{2}{\pi}\right)K(k) + B_2^{(2)}(n, v)(1-\xi)^{3/2}(1+3\xi)^{1/2}\left(\frac{2}{\pi}\right)E(k)\right] \tag{5.10}$$

where $\left\{B_2^{(j)}(n, v) : j = 1, 2\right\}$ satisfy the recursion relation

$$3(3n+1)(3n+2)B_2^{(j)}(n+1, v) + n(n+1)\Big[(3v+1)(9v^2-12v+1)B_2^{(j)}(n, v) - v^2(v-1)(9v-1)B_2^{(j)}(n-1, v)\Big] = 0 \tag{5.11}$$

with $n = 1, 2, \ldots$. The initial conditions for relation (5.11) are given for $j = 1$ and $j = 2$ by

$$B_2^{(1)}(0, v) = 1 \tag{5.12}$$

$$B_2^{(1)}(1, v) = -\tfrac{1}{16}(1-v^2)(1-9v) \tag{5.13}$$

and

$$B_2^{(2)}(0, v) = 0 \tag{5.14}$$

$$B_2^{(2)}(1, v) = \tfrac{1}{16}(1-3v) \tag{5.15}$$

respectively. In appendix B we list the polynomials $\left\{B_2^{(j)}(n, v) : j = 1, 2\right\}$ for $n \leqslant 4$.

It is clear from the P-symbols (3.27) and (3.28) that the Heun series (3.29) and their analytic continuations define single-valued analytic functions $\{H_j(n, v) : j = 1, 2\}$ in the whole v plane, provided that a cut is made along the real axis from $v = \frac{1}{9}$ to $v = +\infty$. The elliptic integral formulae (5.8) and (5.10) give representations for these analytic functions provided that v lies in a certain finite region $\mathcal{R}_2$ of the cut plane. This region of validity is shown in figure 2, with the region $\mathcal{R}_1$. The points on the boundary of $\mathcal{R}_2$ are associated with values of $k^2 = k^2(v)$ which lie in the interval $2 \leqslant k^2 < \infty$.

We see from figure 2 that $\mathcal{R}_1$ lies entirely inside the region of validity $\mathcal{R}_2$. It follows, therefore, that the representations (5.8) and (5.10) can be used to analyse the properties of the product form (3.35) for *all* $w \in \mathcal{C}^-$.

5.2. *Formulae for independent second solutions of* $\{\widehat{\mathcal{H}}_{j,n}(y) = 0 : j = 1, 2\}$

Our aim now is to construct independent second solutions $\widetilde{H}_1(n, v)$ and $\widetilde{H}_2(n, v)$ of the Heun differential equations (3.24) and (3.26), respectively. We begin by noting that $K(k)$ and the complementary integral $K'(k)$ are both solutions of the differential equation (Borwein and Borwein 1987, p 9)

$$k(1-k^2)\frac{d^2y}{dk^2} + (1-3k^2)\frac{dy}{dk} - ky = 0. \tag{5.16}$$

It follows from this result and (5.4) that we can express $\{\widetilde{H}_j(0, v) : j = 1, 2\}$ in the form

$$\widetilde{H}_1(0, v) = \widetilde{H}_2(0, v) = \frac{1}{(1-\xi)^{3/2}(1+3\xi)^{1/2}}\left(\frac{2}{\pi}\right)K'(k) \tag{5.17}$$

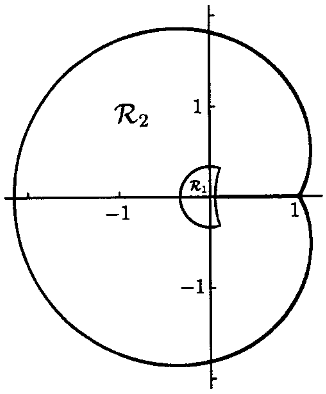

Figure 2. The regions $\mathcal{R}_1$ and $\mathcal{R}_2$ in the cut v plane.

where the modulus k is defined in (5.2). This non-physical second solution exhibits a *logarithmic* singularity at $v = 0$.

Next we apply the raising operators $\{\widehat{\mathcal{R}}_{j,1} : j = 1, 2\}$ to (5.17) and then make use of the recursion relations (4.11) and (4.21) with H formally replaced by $\widetilde{H}$. In this manner, we obtain the following particular form for the independent second solution,

$$\widetilde{H}_j(n, v) = \frac{1}{v^{jn}}\left[B_j^{(1)}(n, v)(1-\xi)^{-3/2}(1+3\xi)^{-1/2}\left(\frac{2}{\pi}\right)K'(k) - B_j^{(2)}(n, v)(1-\xi)^{3/2}(1+3\xi)^{1/2}\left(\frac{2}{\pi}\right)\widetilde{E}(k)\right] \tag{5.18}$$

where $j = 1, 2$ and

$$\widetilde{E}(k) \equiv E'(k) - K'(k). \tag{5.19}$$

The formula (5.18) gives single-valued analytic second solutions of the Heun equations (3.24) and (3.26) provided that v lies in a certain finite region of the v plane. It is found that this region is contained within the region $\mathcal{R}_2$ and includes the real interval $0 < v < 1$.

5.3. Connection with the algebraic solution $G^{(a)}(n, z)$

Next we express the general solutions of the Heun equations (3.24) and (3.26) as linear combinations of the functions $H_1(n, v)$, $\widetilde{H}_1(n, v)$ and $H_2(n, v)$, $\widetilde{H}_2(n, v)$ respectively, and then apply equations (3.23), (3.25) and (3.12). This procedure enables one to show that the *general* solution of $\mathbf{L}_{4,n}(G) = 0$ can be written in the form

$$G \equiv G(n, z) = v^{(1+3n)/2}[(1-v)(1-9v)]^{(1-3n)/2}\big[\lambda_1 H_1(n, v)H_2(n, v) + \lambda_2\widetilde{H}_1(n, v)H_2(n, v) + \lambda_3 H_1(n, v)\widetilde{H}_2(n, v) + \lambda_4\widetilde{H}_1(n, v)\widetilde{H}_2(n, v)\big] \tag{5.20}$$

provided $n \neq 0$, where $\{\lambda_i : i = 1, 2, 3, 4\}$ are constants and the connection between the variables v and z is given by (3.26).

If we use (5.8), (5.10) and (5.18) to evaluate (5.20) for the special case $\lambda_1 = \lambda_4 = 0$ and $\lambda_2 = -\lambda_3 = 1$ we find that *all* the elliptic integrals can be completely eliminated by making use of the Legendre relation (Borwein and Borwein 1987, p 24)

$$K(k)E'(k) + K'(k)E(k) - K(k)K'(k) = \frac{\pi}{2}. \tag{5.21}$$

Hence we obtain the identity

$$[v(1-v)(1-9v)]^{(1-3n)/2}\big[B_1^{(1)}(n,v)B_2^{(2)}(n,v)-B_1^{(2)}(n,v)B_2^{(1)}(n,v)\big]$$
$$= C_n^{(a)}G^{(a)}(n,z) \tag{5.22}$$

where $G^{(a)}(n,z)$ is the *algebraic* solution (3.2) and $C_n^{(a)}$ only depends on the variable n. It can be shown that

$$C_n^{(a)} = \frac{3}{8n}\frac{(n!)^3}{(3n)!}(-2)^{n-1} \tag{5.23}$$

with $n = 1, 2, \ldots$. We see that the Legendre relation provides an underlying mechanism for the existence of the algebraic solution $G^{(a)}(n,z)$.

Finally, we note that the solutions of the Heun differential equations (3.24) and (3.26) can also be defined for *non-integer* values of n. For the special case $n = N + \frac{1}{2}$, where $N = 0, 1, 2, \ldots$ it is found that *all* solutions of these differential equations are algebraic functions of v.

6. Hypergeometric representations for $\{H_j(n,v) : j = 1, 2\}$

In this section, we shall prove that the Heun functions $H_1(n,v)$ and $H_2(n,v)$ can be expressed in terms of a *single* ${}_2F_1$ hypergeometric function, provided that the variable v lies in a sufficiently small neighbourhood of the origin $v = 0$.

We begin the analysis by considering the hypergeometric function

$$\mathcal{Y} \equiv \mathcal{Y}(n,x) = {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; n+1; x\right). \tag{6.1}$$

It is known that this function is a solution of the differential equation

$$9x(1-x)\frac{d^2\mathcal{Y}}{dx^2} + 9[(n+1)-2x]\frac{d\mathcal{Y}}{dx} - 2\mathcal{Y} = 0. \tag{6.2}$$

We now apply the rational transformation

$$x \mapsto x_1(v) = \frac{27v(1-v)^2}{(1+3v)^3} \tag{6.3}$$

to (6.2). In this manner it is found that

$$v(1-v)(1-9v)(1+3v)^2\frac{d^2\mathcal{Y}}{dv^2} + (1+3v)\big[(n+1)+(9n-23)v+27(n+1)v^2$$
$$+27(n+1)v^3\big]\frac{d\mathcal{Y}}{dv} - 6(1-v)(1-9v)\mathcal{Y} = 0. \tag{6.4}$$

Next the further transformation

$$\mathcal{Y} = \frac{(1+3v)}{(1-v)^{2n}}y \tag{6.5}$$

is applied to (6.4). Hence we find that $y = y(n,v)$ is a solution of the Heun differential equation (3.24). It is readily seen from this result that

$$H_1(n,v) = \frac{(1-v)^{2n}}{(1+3v)}\,{}_2F_1\left[\frac{1}{3}, \frac{2}{3}; n+1; \frac{27v(1-v)^2}{(1+3v)^3}\right]. \tag{6.6}$$

The formula (6.6) gives a representation for the single-valued analytic function $H_1(n,v)$ provided that v lies in a certain finite region $\mathcal{R}_3$ of the cut plane. This region of validity is shown in figure 3, with the region $\mathcal{R}_1$. The points on the boundary of $\mathcal{R}_3$ are associated with values of $x = x_1(v)$ which have $1 \leqslant x < \infty$.

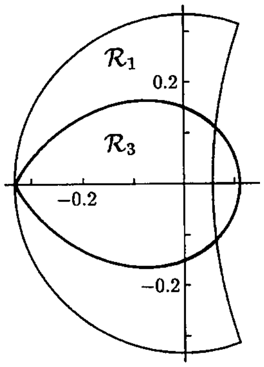

Figure 3. The regions $\mathcal{R}_1$ and $\mathcal{R}_3$ in the cut v plane.

From figure 3 we see that the points v in the upper-half plane that are in $\mathcal{R}_1$ and *outside* $\mathcal{R}_3$ form a finite region which we shall denote by $\mathcal{R}_4$. There is also a similar complex conjugate region $\mathcal{R}_4^*$ in the lower-half of the v plane. We can establish ${}_2F_1$ representations for $H_1(n, v)$ which are valid in $\mathcal{R}_4$ and $\mathcal{R}_4^*$ by using a standard formula (Erdélyi *et al* 1953, p 110, equation (12)) to construct the analytic continuation of (6.6) across the boundary of the region $\mathcal{R}_3$. The final result is

$$H_1(n, v) = \frac{(1-v)^{2n}}{(1+3v)}\,{}_2F_1\left[\frac{1}{3}, \frac{2}{3}; n+1; \frac{27v(1-v)^2}{(1+3v)^3}\right] \pm \frac{\mathrm{i}\sqrt{3}}{(1+3v)}\left[-\frac{(1-9v)^2}{27v}\right]^n {}_2F_1\left[\frac{1}{3}, \frac{2}{3}; n+1; \frac{(1-9v)^2}{(1+3v)^3}\right] \tag{6.7}$$

where the upper and lower signs are valid in $\mathcal{R}_4$ and $\mathcal{R}_4^*$, respectively.

It is possible to obtain similar ${}_2F_1$ results for $H_2(n, v)$ by applying the alternative transformations

$$x \mapsto x_2(v) = \frac{27v^2(1-v)}{(1-3v)^3} \tag{6.8}$$

and

$$\mathcal{Y} = \frac{(1-3v)}{(1-v)^n}y \tag{6.9}$$

to (6.2). In this case it is found that $y = y(n, v)$ is a solution of the second Heun differential equation (3.26). It follows, therefore, that $H_2(n, v)$ can be written in the form

$$H_2(n, v) = \frac{(1-v)^n}{(1-3v)}\,{}_2F_1\left[\frac{1}{3}, \frac{2}{3}; n+1; \frac{27v^2(1-v)}{(1-3v)^3}\right]. \tag{6.10}$$

The formula (6.10) gives a representation for the single-valued analytic function $H_2(n, v)$ provided that v lies in a certain semi-infinite region $\mathcal{R}_5$ of the cut plane. Fortunately, it is *not* necessary to construct the analytic continuation of (6.10) across the boundary of $\mathcal{R}_5$ because the region $\mathcal{R}_1$ of physical interest lies *entirely inside* $\mathcal{R}_5$.

The important formulae (6.6) and (6.10) can also be derived by making the substitutions

$$H_1(n, v) = \frac{n!}{\left(\frac{2}{3}\right)_n}E_1(n, v) \tag{6.11}$$

$$H_2(n, v) = \frac{n!}{\left(\frac{1}{3}\right)_n}E_2(n, v) \tag{6.12}$$

in (4.11) and (4.21), respectively. This procedure yields the following *simplified* Laplace recursion relations,

$$27(3n+1)vE_1(n+1,v) - 3n(3v-1)(9v^2-42v+1)E_1(n,v) - (3n-1)(v-1)^2(9v-1)^2E_1(n-1,v) = 0 \tag{6.13}$$

$$27(3n+2)v^2E_2(n+1,v) + 3n(3v+1)(9v^2-12v+1)E_2(n,v) - (3n-2)(v-1)(9v-1)E_2(n-1,v) = 0 \tag{6.14}$$

where $n = 1, 2, \ldots$. It is now possible to determine hypergeometric solutions of (6.13) and (6.14) by applying a standard method (see Milne-Thomson (1981), p 491).

It is interesting to note that we can use (5.4) and (6.6) with $v = \xi^2$ and $n = 0$ to derive the transformation formula

$${}_2F_1\left[\frac{1}{3},\frac{2}{3};1;\frac{27\xi^2(1-\xi^2)^2}{(1+3\xi^2)^3}\right] = \frac{(1+3\xi^2)}{(1-\xi)^{3/2}(1+3\xi)^{1/2}} \times {}_2F_1\left[\frac{1}{2},\frac{1}{2};1;\frac{16\xi^3}{(1-\xi)^3(1+3\xi)}\right]. \tag{6.15}$$

The substitution $\xi = p/(2+p)$ in (6.15) yields an identity given by Ramanujan (1957). In a similar manner we can use (5.4) and (6.10) to obtain the further transformation identity

$${}_2F_1\left[\frac{1}{3},\frac{2}{3};1;\frac{27\xi^4(1-\xi^2)}{(1-3\xi^2)^3}\right] = \frac{(1-3\xi^2)}{(1-\xi)^{3/2}(1+3\xi)^{1/2}} \times {}_2F_1\left[\frac{1}{2},\frac{1}{2};1;\frac{16\xi^3}{(1-\xi)^3(1+3\xi)}\right]. \tag{6.16}$$

7. Exact formulae for the Green function $G(n, n, n; w)$

Our main purpose in this section is to prove that $G(n, n, n; w)$ can be written in terms of a product of two linear forms in $K(k)$ and $E(k)$ whose coefficients are polynomials in the parameter ξ. It will also be shown that $G(n, n, n; w)$ is expressible in terms of a product of two ${}_2F_1$ hypergeometric functions.

7.1. Product form for $G(n, n, n; w)$ in terms of complete elliptic integrals

We begin by applying (5.8) and (5.10) to the Heun function product form (3.35). In this manner we obtain the ξ parametric formula

$$\overline{G}(n,n,n;w) \equiv (3/w)^{3n} wG(n,n,n;w) = 6^{3n}\frac{(3n)!}{(n!)^3}\frac{(1-9\xi^4)^{1-3n}}{(1-\xi)^3(1+3\xi)}\left(\frac{2}{\pi}\right)^2 \times \prod_{i=1}^{2}\left[B_i^{(1)}(n,v)K(k) + (1-\xi)^3(1+3\xi)B_i^{(2)}(n,v)E(k)\right] \tag{7.1}$$

where

$$k^2(\xi) = \frac{16\xi^3}{(1-\xi)^3(1+3\xi)} \tag{7.2}$$

$$\xi(w) = \frac{1}{w}\left(1+\sqrt{1-\frac{1}{w^2}}\right)^{-1/2}\left(1+\sqrt{1-\frac{9}{w^2}}\right)^{-1/2} \tag{7.3}$$

and $v = \xi^2$. The polynomials $\left\{B_1^{(j)}(n, v) : j = 1, 2\right\}$ and $\left\{B_2^{(j)}(n, v) : j = 1, 2\right\}$ in (7.1) can be determined using the recursion relations (5.9) and (5.11), respectively.

Explicit product forms of the type (7.1) were first obtained by Joyce (2002) for the special cases $n = 0, 1, 2, 3, 4$ by following methods developed by Morita (1975). We have derived these particular formulae by applying the polynomial expressions in appendices A and B to the *general* product form (7.1). In all cases agreement was found with the work of Joyce (2002). Further checks have also been carried out by expanding (7.1) in powers of $1/w$ for various integer values of $n \geqslant 0$ and comparing the results with the series (2.6). It should be noted that (7.1) enables one to calculate *extremely accurate* values for $G(n, n, n; w)$ at *any* point $w = w_1 + \mathrm{i}w_2$ in a complex (w_1, w_2) plane which is cut along the real axis from $w_1 = -3$ to $w_1 = +3$. For example, we find that

$$\begin{aligned} G(1000, 1000, 1000; 3) = 0.000\,091\,888\,144\,132\,067\,310\,942\,752\,976\,327\,816\,092 \\ 222\,748\,713\,302\,635\,909\,147\,604\,173\,686\,682\,252\,148 \\ 435\,124\,320\,431\,845\,557\,661\,224\,240\,623\,119\,351\ldots. \end{aligned} \tag{7.4}$$

If we make the substitution $w = w_1 - \mathrm{i}\epsilon$ in (7.1), where w_1 is real and $\epsilon > 0$, and then apply the definition (1.3) it is found that the right-hand side of (7.1) can be used to calculate $(3/w_1)^{3n} w_1 G^-(n, n, n; w_1)$ for $0 < w_1 < 3$, provided that $\xi = \xi(w)$ is replaced by

$$\begin{aligned} \widetilde{\xi} \equiv \widetilde{\xi}(w_1) &= \lim_{\epsilon \to 0+} \xi(w_1 - \mathrm{i}\epsilon) \\ &= \frac{1}{w_1}\left(1 - \mathrm{i}\sqrt{\frac{1}{w_1^2} - 1}\right)^{-1/2}\left(1 - \mathrm{i}\sqrt{\frac{9}{w_1^2} - 1}\right)^{-1/2}. \end{aligned} \tag{7.5}$$

For example, when $n = 10$ and $w_1 = 2$ the modified formula gives

$$G^-(10, 10, 10; 2) = G_{\mathrm{R}}(10, 10, 10; 2) + \mathrm{i}G_{\mathrm{I}}(10, 10, 10; 2) \tag{7.6}$$

where

$$\begin{aligned} G_{\mathrm{R}}(10, 10, 10; 2) = 0.013\,712\,569\,365\,260\,541\,486\,044\,864\,334\,171\,807\,911\,990 \\ 578\,266\,795\,397\,937\,108\,813\,161\,273\,018\,956\,326\,842\,010 \\ 597\,072\,115\,429\,438\,806\,103\,356\,325\,225\,528\,990\,206\ldots \end{aligned} \tag{7.7}$$

$$\begin{aligned} G_{\mathrm{I}}(10, 10, 10; 2) = 0.001\,521\,292\,642\,094\,924\,949\,875\,044\,972\,204\,457\,614\,030 \\ 831\,146\,470\,369\,909\,807\,579\,694\,240\,416\,378\,427\,589\,560 \\ 420\,719\,210\,783\,270\,381\,327\,209\,309\,277\,719\,264\,896\ldots. \end{aligned} \tag{7.8}$$

It would be very difficult to obtain such highly accurate values for $G_{\mathrm{R}}(10, 10, 10; 2)$ and $G_{\mathrm{I}}(10, 10, 10; 2)$ using the integral representations (1.7) and (1.8), respectively, because these integrals involve *oscillatory* integrands which have *slowly decreasing* amplitudes as $t \to \infty$.

7.2. Hypergeometric product forms for $G(n, n, n; w)$

We now substitute equations (6.6) and (6.10) in (3.35) and then use relation (3.36) to express the final result in terms of the variable w. Hence, we obtain the alternative product form

$$\begin{aligned} wG(n, n, n; w) = \frac{(3n)!}{(3^n n!)^3}\left[\frac{w}{3}\left(1 - \sqrt{1 - \frac{9}{w^2}}\right)\right]^{3n} {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; n + 1; \eta_+\right) \\ \times {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; n + 1; \eta_-\right) \end{aligned} \tag{7.9}$$

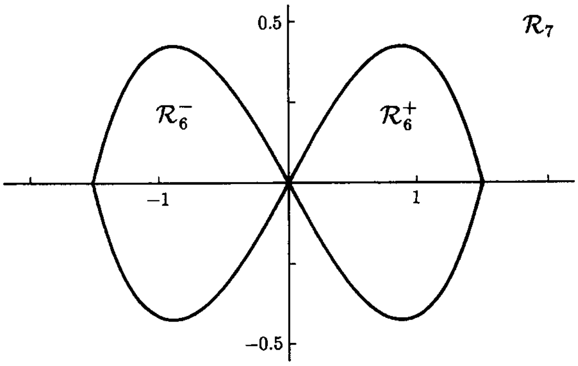

Figure 4. The regions $\mathcal{R}_6^{\pm}$ and $\mathcal{R}_7$ in the w plane.

where

$$\eta_{\pm} \equiv \eta_{\pm}(w) = \frac{1}{8w^2}\left[4w^2 + (9-4w^2)\sqrt{1-\frac{9}{w^2}} \pm 27\sqrt{1-\frac{1}{w^2}}\right]. \tag{7.10}$$

The formula (7.9) will remain valid for varying values of w in the neighbourhood of $w = \infty$, provided that the argument function $\eta_+(w)$ does not take real values in the interval $(1, +\infty)$.

In order to establish the precise region of validity for (7.9) we first determine the set of points $\mathcal{S}$ in the w plane which give real values of $\eta_+(w) \in \left(\frac{1}{2} + \frac{1}{2}\sqrt{5}, +\infty\right)$. It is found that the set $\mathcal{S}$ forms two closed paths which divide the w plane into three regions $\mathcal{R}_6^+$, $\mathcal{R}_6^-$ and $\mathcal{R}_7$, as shown in figure 4. From these results it follows that (7.9) is valid for all $w \in \mathcal{C}^-$ which are in the *outer* region $\mathcal{R}_7$.

When w is in one of the *inner* regions $\mathcal{R}_6^{\pm}$ it is necessary to modify the derivation of the ${}_2F_1$ product form by replacing (6.6) with the analytic continuation formula (6.7). This procedure yields the alternative representation

$$\begin{aligned} wG(n,n,n;w) = \frac{(3n)!}{(3^n n!)^3}\Bigg\{&\left[\frac{w}{3}\left(1-\sqrt{1-\frac{9}{w^2}}\right)\right]^{3n} {}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\eta_+\right) \\ &\pm \mathrm{i}\sqrt{3}(-1)^n\left[w\left(1-\sqrt{1-\frac{1}{w^2}}\right)\right]^n {}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;1-\eta_+\right)\Bigg\} \\ &\times {}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\eta_-\right) \end{aligned} \tag{7.11}$$

where the variable w lies in the region $\mathcal{R}_6^+ \cup \mathcal{R}_6^-$ with the real interval $\left[-\frac{3}{2}, \frac{3}{2}\right]$ deleted, and $\eta_{\pm} = \eta_{\pm}(w)$ is given by (7.10). The upper positive sign in (7.11) is valid when $\{\mathrm{Re}(w) > 0, \mathrm{Im}(w) < 0\}$ and $\{\mathrm{Re}(w) < 0, \mathrm{Im}(w) > 0\}$, while the lower negative sign is valid when $\{\mathrm{Re}(w) > 0, \mathrm{Im}(w) > 0\}$ and $\{\mathrm{Re}(w) < 0, \mathrm{Im}(w) < 0\}$.

Finally, we make the substitution $w = w_1 - \mathrm{i}\epsilon$ in (7.9), where w_1 is real and $\epsilon > 0$, and then apply the definition (1.3). This procedure gives

$$\begin{aligned} w_1 G^-(n,n,n;w_1) = \frac{(3n)!}{(3^n n!)^3}&\left[\frac{w_1}{3}\left(1+\mathrm{i}\sqrt{\frac{9}{w_1^2}-1}\right)\right]^{3n} {}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\tilde{\eta}_+\right) \\ &\times {}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\tilde{\eta}_-\right) \end{aligned} \tag{7.12}$$

where

$$\widetilde{\eta}_{\pm} \equiv \widetilde{\eta}_{\pm}(w_1) = \lim_{\epsilon\to 0+} \eta_{\pm}(w_1 - \mathrm{i}\epsilon)$$
$$= \frac{1}{8w_1^2}\left[4w_1^2 - \mathrm{i}\big(9-4w_1^2\big)\sqrt{\frac{9}{w_1^2}-1} \mp 27\mathrm{i}\sqrt{\frac{1}{w_1^2}-1}\right] \quad (7.13)$$

provided that $\frac{3}{2} < w_1 \leqslant 3$. In a similar manner we can use (7.11) to obtain the formula

$$w_1 G^-(n,n,n;w_1) = \frac{(3n)!}{(3^n n!)^3}\left\{\left[\frac{w_1}{3}\left(1+\mathrm{i}\sqrt{\frac{9}{w_1^2}-1}\right)\right]^{3n} {}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\widetilde{\eta}_+\right)\right.$$
$$\left. + \mathrm{i}\sqrt{3}(-1)^n\left[w_1\left(1+\mathrm{i}\sqrt{\frac{1}{w_1^2}-1}\right)\right]^{n} {}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;1-\widetilde{\eta}_+\right)\right\}$$
$$\times\, {}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\widetilde{\eta}_-\right). \quad (7.14)$$

This second result is valid when $0 < w_1 \leqslant \frac{3}{2}$.

7.3. Special cases $G(0,0,0;w)$, $G^{\pm}(n,n,n;0)$ *and* $G(n,n,n;3)$

When $n = 0$ we can achieve a considerable simplification of (7.9) by first using (6.15) and (6.16) to derive the transformation formula

$${}_2F_1\left[\frac{1}{3},\frac{2}{3};1;\frac{27v(1-v)^2}{(1+3v)^3}\right] = \left(\frac{1+3v}{1-3v}\right){}_2F_1\left[\frac{1}{3},\frac{2}{3};1;\frac{27v^2(1-v)}{(1-3v)^3}\right] \quad (7.15)$$

where $v = \xi^2$. If relation (3.36) is applied to (7.15) we find that

$${}_2F_1\left(\frac{1}{3},\frac{2}{3};1;\eta_+\right) = \frac{1}{2}\left(3\sqrt{1-\frac{1}{w^2}} - \sqrt{1-\frac{9}{w^2}}\right){}_2F_1\left(\frac{1}{3},\frac{2}{3};1;\eta_-\right) \quad (7.16)$$

where $\eta_{\pm} = \eta_{\pm}(w)$ are defined in (7.10). This formula is valid provided that w lies in the region $\mathcal{R}_7$ of the cut w plane. From (7.9) and (7.16) we see that

$$G(0,0,0;w) = \frac{1}{2w}\left(3\sqrt{1-\frac{1}{w^2}} - \sqrt{1-\frac{9}{w^2}}\right)\left[{}_2F_1\left(\frac{1}{3},\frac{2}{3};1;\eta_-\right)\right]^2. \quad (7.17)$$

It should be stressed that the *final* result (7.17) is valid for *all* $w \in \mathcal{C}^-$.

Next we make the substitution $w = \pm\mathrm{i}\epsilon$, where $\epsilon > 0$, in the formula (7.9) and then take the limit $\epsilon \to 0+$. This procedure gives

$$G^{\pm}(n,n,n;0) = (\mp\mathrm{i})^{3n+1}\frac{(3n)!}{(3^n n!)^3}\,{}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\frac{1}{2}\right)$$
$$\times \lim_{\epsilon\to 0+}\left(\frac{1}{\epsilon}\right){}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;-\frac{27}{4\epsilon^3}\right). \quad (7.18)$$

We now simplify (7.18) using standard ${}_2F_1$ formulae (see Erdélyi *et al* (1953)). In this manner it is found that

$$G^{\pm}(n,n,n;0) = \frac{(\mp\mathrm{i})^{3n+1}}{2^{2/3}\Gamma\left(\frac{5}{6}\right)\sqrt{3\pi}}\frac{\Gamma\left(\frac{n}{2}+\frac{1}{6}\right)}{\Gamma\left(\frac{n}{2}+\frac{5}{6}\right)} \quad (7.19)$$

where $\Gamma(z)$ denotes the gamma function and $n = 0, 1, 2, \ldots$. If this result is compared with (1.6), with $\ell = m = n$ and $w_1 = 0$, we obtain the integral formula

$$\int_0^\infty J_n^3(t)\,\mathrm{d}t = \frac{1}{2^{2/3}\Gamma\left(\frac{5}{6}\right)\sqrt{3}\pi}\frac{\Gamma\left(\frac{n}{2}+\frac{1}{6}\right)}{\Gamma\left(\frac{n}{2}+\frac{5}{6}\right)}. \tag{7.20}$$

It appears that (7.20) is also valid for non-integer and complex values of n.

When $w = 3$ we find that the general product formula (7.9) reduces to

$$G(n,n,n;3) = \frac{(3n)!}{3(3^n n!)^3}\,{}_2F_1\left[\frac{1}{3},\frac{2}{3};n+1;\frac{1}{4}\left(2-\sqrt{2}\right)\right] \times {}_2F_1\left[\frac{1}{3},\frac{2}{3};n+1;\frac{1}{4}\left(2+\sqrt{2}\right)\right]. \tag{7.21}$$

For the special case $n = 0$ we can also use (7.17) to obtain the reduced form

$$G(0,0,0;3) = \frac{\sqrt{2}}{3}\left\{{}_2F_1\left[\frac{1}{3},\frac{2}{3};1;\frac{1}{4}\left(2-\sqrt{2}\right)\right]\right\}^2. \tag{7.22}$$

8. Asymptotic behaviour of $G(n, n, n; w)$ as $n \to \infty$

A detailed investigation of the asymptotic form of the *general* lattice Green function $G(\ell, m, n; w)$ as $(\ell^2 + m^2 + n^2)^{1/2} \to \infty$ was carried out by Katsura and Inawashiro (1973) using stationary phase and saddle-point methods. Unfortunately, the work of these authors involved *complicated* calculations and the asymptotic representations for $G(\ell, m, n; w)$ were only given to *leading order*.

In this section, we shall show that the ${}_2F_1$ product forms obtained in section 7 can be used to derive uniform asymptotic *expansions* for $G(n, n, n; w)$, as $n \to \infty$, in a *very simple* manner.

8.1. General asymptotic representations

We begin by considering the standard asymptotic formula (Luke 1969, p 235)

$${}_2F_1\left(\frac{1}{3},\frac{2}{3};n+1;\eta\right) \sim \Lambda_M(n,\eta) \tag{8.1}$$

as $n \to \infty$, where

$$\Lambda_M(n,\eta) \equiv \sum_{m=0}^{M}\frac{\left(\frac{1}{3}\right)_m\left(\frac{2}{3}\right)_m}{(n+1)_m m!}\eta^m \tag{8.2}$$

and $M = 0, 1, 2, \ldots$. Next we apply (8.1) to the product form (7.9). This procedure yields the asymptotic representation

$$wG(n,n,n;w) \sim \frac{(3n)!}{(3^n n!)^3}\left[\frac{w}{3}\left(1-\sqrt{1-\frac{9}{w^2}}\right)\right]^{3n}\Lambda_M(n,\eta_+)\,\Lambda_M(n,\eta_-) \tag{8.3}$$

as $n \to \infty$, where M is *fixed* and $\eta_\pm = \eta_\pm(w)$ are defined in (7.10). We expect (8.3) to be valid provided that w lies in the region $\mathcal{R}_7$ of the cut w plane.

A uniform asymptotic expansion for $G(n, n, n; w)$ can now be derived by expanding the factorial multiplier and the Λ functions in (8.3) in powers of $1/n$. In particular, we find that

$$G(n,n,n;w) \sim \frac{\sqrt{3}}{2\pi wn}\left[\frac{w}{3}\left(1-\sqrt{1-\frac{9}{w^2}}\right)\right]^{3n}\sum_{m=0}^{\infty}\frac{b_m^{(1)}(w)}{n^m} \tag{8.4}$$

as $n \to \infty$, where $b_0^{(1)}(w) = 1$,

$$b_1^{(1)}(w) = \frac{1}{18w^2}(9 - 4w^2)\sqrt{1 - \frac{9}{w^2}} \tag{8.5}$$

$$b_2^{(1)}(w) = -\frac{1}{324w^6}(3645 - 3645w^2 + 594w^4 - 8w^6) \tag{8.6}$$

$$b_3^{(1)}(w) = -\frac{1}{8748w^8}(51\,030 - 51\,030w^2 + 4185w^4 + 14w^6)(9 - 4w^2)\sqrt{1 - \frac{9}{w^2}} \tag{8.7}$$

and $w \in \mathcal{R}_7$.

In a similar manner we can also apply (8.1) to the product form (7.11). Hence, we obtain

$$wG(n, n, n; w) \sim \frac{(3n)!}{(3^n n!)^3}\Lambda_M(n, \eta_-)\left\{\left[\frac{w}{3}\left(1 - \sqrt{1 - \frac{9}{w^2}}\right)\right]^{3n}\Lambda_M(n, \eta_+)\right.$$
$$\left. \pm\, \mathrm{i}\sqrt{3}(-1)^n\left[w\left(1 - \sqrt{1 - \frac{1}{w^2}}\right)\right]^n\Lambda_M(n, 1 - \eta_+)\right\} \tag{8.8}$$

as $n \to \infty$, with M *fixed*. We expect (8.8) to be valid provided that w lies in the region $\mathcal{R}_6^+ \cup \mathcal{R}_6^-$ with the real interval $\left[-\frac{3}{2}, \frac{3}{2}\right]$ deleted. If the factorial multiplier and the Λ functions in (8.8) are expanded in powers of $1/n$ it is found that

$$G(n, n, n; w) \sim \frac{\sqrt{3}}{2\pi wn}\left\{\left[\frac{w}{3}\left(1 - \sqrt{1 - \frac{9}{w^2}}\right)\right]^{3n}\sum_{m=0}^{\infty}\frac{b_m^{(1)}(w)}{n^m}\right.$$
$$\left. \pm\, \mathrm{i}\sqrt{3}(-1)^n\left[w\left(1 - \sqrt{1 - \frac{1}{w^2}}\right)\right]^n\sum_{m=0}^{\infty}\frac{b_m^{(2)}(w)}{n^m}\right\} \tag{8.9}$$

as $n \to \infty$, where $b_0^{(2)}(w) = 1$,

$$b_1^{(2)}(w) = -\frac{3}{2w^2}\sqrt{1 - \frac{1}{w^2}} \tag{8.10}$$

$$b_2^{(2)}(w) = -\frac{3}{4w^6}(15 - 15w^2 + 2w^4) \tag{8.11}$$

$$b_3^{(2)}(w) = \frac{3}{4w^8}(210 - 210w^2 + 45w^4 - 2w^6)\sqrt{1 - \frac{1}{w^2}} \tag{8.12}$$

and $w \in \mathcal{R}_6^+ \cup \mathcal{R}_6^-$ with the real interval $\left[-\frac{3}{2}, \frac{3}{2}\right]$ deleted. The role of the $\pm$ signs in equation (8.9) is explained in section 7.2. It should be noted that the coefficients $\{b_m^{(1)}(w), b_m^{(2)}(w) : m = 1, 2, \ldots\}$ in the expansions (8.4) and (8.9) all become infinite as $w \to 0$. The reasons for this breakdown at $w = 0$ will be discussed in section 8.3.

Next we let $w = w_1 - \mathrm{i}\epsilon$ in (8.4), where $\epsilon > 0$, and then apply the definition (1.3). In this manner, we find that

$$G^-(n, n, n; w_1) \sim \frac{\sqrt{3}}{2\pi w_1 n}\left[\frac{w_1}{3}\left(1 + \mathrm{i}\sqrt{\frac{9}{w_1^2} - 1}\right)\right]^{3n}\sum_{m=0}^{\infty}\frac{\widetilde{b}_m^{(1)}(w_1)}{n^m} \tag{8.13}$$

as $n \to \infty$, where $\frac{3}{2} < w_1 \leqslant 3$ and $\widetilde{b}_0^{(1)}(w_1) = 1$. Formulae for $\left\{\widetilde{b}_m^{(1)}(w_1) : m = 1, 2, 3\right\}$ can be readily obtained by making the formal replacements $w \mapsto w_1$ and

$$\sqrt{1-\frac{9}{w^2}} \mapsto -\mathrm{i}\sqrt{\frac{9}{w_1^2}-1} \tag{8.14}$$

in the right-hand sides of equations (8.5)–(8.7), respectively. When $0 < w_1 \leqslant \frac{3}{2}$ we can use (8.9) to derive the alternative asymptotic expansion

$$G^-(n,n,n;w_1) \sim \frac{\sqrt{3}}{2\pi w_1 n}\left\{\left[\frac{w_1}{3}\left(1+\mathrm{i}\sqrt{\frac{9}{w_1^2}-1}\right)\right]^{3n}\sum_{m=0}^{\infty}\frac{\widetilde{b}_m^{(1)}(w_1)}{n^m} + \mathrm{i}\sqrt{3}(-1)^n\left[w_1\left(1+\mathrm{i}\sqrt{\frac{1}{w_1^2}-1}\right)\right]^n\sum_{m=0}^{\infty}\frac{\widetilde{b}_m^{(2)}(w_1)}{n^m}\right\} \tag{8.15}$$

as $n \to \infty$, where $\widetilde{b}_0^{(2)}(w_1) = 1$. Formulae for $\left\{\widetilde{b}_m^{(2)}(w_1) : m = 1, 2, 3\right\}$ can be written down by making the formal replacements $w \mapsto w_1$ and

$$\sqrt{1-\frac{1}{w^2}} \mapsto -\mathrm{i}\sqrt{\frac{1}{w_1^2}-1} \tag{8.16}$$

in the right-hand sides of equations (8.10)–(8.12), respectively. It has been verified that the dominant leading-order terms in (8.13) and (8.15) are consistent with the work of Katsura and Inawashiro (1973).

8.2. Asymptotic expansions for $G^{\pm}(n,n,n;0)$ and $G(n,n,n;3)$

We begin by considering the standard expansion (Luke 1969, p 34)

$$\frac{\Gamma(z+a)}{\Gamma(z+b)} \sim (z+a-\rho)^{a-b}\sum_{m=0}^{\infty}\frac{(b-a)_{2m}B_{2m}^{(2\rho)}(\rho)}{(2m)!(z+a-\rho)^{2m}} \tag{8.17}$$

as $z \to \infty$, where $B_{2m}^{(2\rho)}(\rho)$ is a generalized Bernoulli polynomial and

$$\rho = \tfrac{1}{2}(1+a-b). \tag{8.18}$$

The application of (8.17) to the formula (7.19) gives the required asymptotic expansion

$$G^{\pm}(n,n,n;0) \sim \frac{(\mp\mathrm{i})^{3n+1}}{\Gamma\left(\frac{5}{6}\right)\sqrt{3\pi}}\frac{1}{n^{2/3}}\sum_{m=0}^{\infty}\frac{\left(\frac{2}{3}\right)_{2m}B_{2m}^{(1/3)}\left(\frac{1}{6}\right)}{(2m)!\left(\frac{n}{2}\right)^{2m}} \tag{8.19}$$

as $n \to \infty$. From this result it follows that

$$G^{\pm}(n,n,n;0) \sim \frac{(\mp\mathrm{i})^{3n+1}}{\Gamma\left(\frac{5}{6}\right)\sqrt{3\pi}}\frac{1}{n^{2/3}}\left(1-\frac{5}{81n^2}+\frac{242}{6561n^4}-\frac{114\,070}{1594\,323n^6} + \frac{38\,532\,659}{129\,140\,163n^8}-\frac{22\,574\,645\,015}{10\,460\,353\,203n^{10}}+\cdots\right) \tag{8.20}$$

as $n \to \infty$. A striking feature of this expansion is that the amplitude factor does *not* obey the expected $1/n$ decay law! In some respects the point $w = 0$ is similar to a *critical point* in the theory of phase transitions.

Next the behaviour of $G(n,n,n;3)$ as $n \to \infty$ is determined by making the substitution $w = 3$ in (8.3). Hence, we obtain

$$G(n,n,n;3) \sim \frac{(3n)!}{3(3^n n!)^3}\Lambda_M\left[n,\frac{1}{4}\left(2-\sqrt{2}\right)\right]\Lambda_M\left[n,\frac{1}{4}\left(2+\sqrt{2}\right)\right] \tag{8.21}$$

as $n \to \infty$. If the factorial factor and the Λ functions in (8.21) are expanded in powers of $1/n$ it is found that

$$G(n,n,n;3) \sim \frac{1}{2\pi\sqrt{3}n}\left(1 - \frac{1}{18n^2} - \frac{1}{108n^4} + \frac{163}{2\,916n^6} - \frac{12\,797}{104\,976n^8} - \frac{73\,589}{209\,952n^{10}} + \frac{50020\,687}{5\,668\,704n^{12}} - \frac{1861\,873\,501}{25\,509\,168n^{14}} - \frac{619\,957\,580\,233}{1224\,440\,064n^{16}} + \cdots\right) \tag{8.22}$$

as $n \to \infty$.

The asymptotic behaviour of $G(\ell, m, n; 3)$ as $R = (\ell^2 + m^2 + n^2)^{1/2} \to \infty$ was first determined by Duffin (1953) using completely different methods. In particular, it was proved that

$$G(\ell,m,n;3) \sim \frac{1}{2\pi R}\left\{1 + \frac{1}{8R^2}\left[-3 + \frac{5(\ell^4+m^4+n^4)}{R^4}\right] + O\left(\frac{1}{R^4}\right)\right\} \tag{8.23}$$

as $R \to \infty$. When $\ell = m = n$ this result is in agreement with the first two terms in the expansion (8.22). We have also used the expansion (8.22) to calculate an approximate value for $G(n, n, n; 3)$ when $n = 1000$. It is found from (7.4) that this asymptotic value has an error of $3.2927\ldots \times 10^{-54}$.

8.3. Multiple turning points

The main aim in this final subsection is to investigate why the asymptotic expansions (8.4) and (8.9) break down as $w \to 0$. We begin by applying the transformation

$$y = v^{-(n+1)/2}(1-v)^{(2n-1)/2}(1-9v)^{(2n-1)/2}Y \tag{8.24}$$

to the Heun equation (3.24), where Y is a new dependent variable. This procedure reduces (3.24) to the normal form

$$\frac{\mathrm{d}^2Y}{\mathrm{d}v^2} = [n^2 f(v) + g(v)]Y \tag{8.25}$$

where

$$f(v) = \frac{(1+3v)^4}{[2v(1-v)(1-9v)]^2} \tag{8.26}$$

$$g(v) = -\frac{(1-12v+102v^2-108v^3+81v^4)}{[2v(1-v)(1-9v)]^2}. \tag{8.27}$$

It is seen that the differential equation (8.25) has a turning point of multiplicity 4 (Olver 1977) at $v = -\frac{1}{3}$. We readily find from (3.36) that

$$\lim_{w\to 0} v(w) = -\tfrac{1}{3}. \tag{8.28}$$

It follows, therefore, that the expansions (8.4) and (8.9) break down as $w \to 0$ because the Heun equation (3.24) is associated with a *multiple turning point* at $v = -\frac{1}{3}$. Asymptotic solutions of (8.25) which are valid in the immediate neighbourhood of $v = -\frac{1}{3}$ can be constructed by following the sophisticated methods developed by Olver (1977, 1978). It is found that the leading-order terms in these solutions are expressible in terms of modified Bessel functions of order $\frac{1}{6}$.

In a similar manner it can be shown that the second Heun equation (3.26) also has a normal form of the type (8.25) with a turning point of multiplicity 4 at the point $v = \frac{1}{3}$. However, this turning point does not affect the asymptotic behaviour of $G(n, n, n; w)$ because the value of the function $v(w)$ is not equal to $\frac{1}{3}$ for any $w \in \mathcal{C}^-$.

Appendix A. Polynomials $\left\{B_1^{(j)}(n,v) : j = 1, 2\right\}$ for $n \leqslant 4$

$$B_1^{(1)}(0, v) = 1$$

$$B_1^{(1)}(1, v) = -\frac{1}{8}(1-v)^2(1-9v)$$

$$B_1^{(1)}(2, v) = \frac{1}{240}(1-v)^3(1-9v)(1-36v+27v^2)$$

$$B_1^{(1)}(3, v) = -\frac{1}{6720}(1-v)^3(1-9v)(1-51v+1212v^2-3132v^3+2187v^4-729v^5)$$

$$B_1^{(1)}(4, v) = \frac{1}{184\,800}(1-v)^3(1-9v)(1-68v+2074v^2-40\,364v^3 +169\,020v^4-281\,772v^5+194\,886v^6-96\,228v^7+19\,683v^8)$$

$$B_1^{(2)}(0, v) = 0$$

$$B_1^{(2)}(1, v) = \frac{1}{8}(1+3v)$$

$$B_1^{(2)}(2, v) = -\frac{1}{240}(1-9v^2)(1-42v+9v^2)$$

$$B_1^{(2)}(3, v) = \frac{1}{6720}(1+3v)(1-60v+1695v^2-8664v^3+15\,255v^4-4860v^5+729v^6)$$

$$B_1^{(2)}(4, v) = -\frac{1}{184\,800}(1-9v^2)(1-42v+9v^2)(1-32v+1135v^2 -5360v^3+10\,215v^4-2592v^5+729v^6)$$

Appendix B. Polynomials $\left\{B_2^{(j)}(n,v) : j = 1, 2\right\}$ for $n \leqslant 4$

$$B_2^{(1)}(0, v) = 1$$

$$B_2^{(1)}(1, v) = -\frac{1}{16}(1-v^2)(1-9v)$$

$$B_2^{(1)}(2, v) = \frac{1}{480}(1-v)^2(1-9v)(1-7v-27v^2-27v^3)$$

$$B_2^{(1)}(3, v) = -\frac{1}{13\,440}(1-v)^3(1-9v)(1-15v+24v^2+216v^3+729v^4+729v^5)$$

$$B_2^{(1)}(4, v) = \frac{1}{369\,600}(1-v)^3(1-9v)(1-24v+160v^2-16v^3 -1260v^4-4968v^5-13\,608v^6+19\,683v^8)$$

$$B_2^{(2)}(0, v) = 0$$

$$B_2^{(2)}(1, v) = \frac{1}{16}(1-3v)$$

$$B_2^{(2)}(2, v) = -\frac{1}{480}(1-9v^2)(1-12v+9v^2)$$

$$B_2^{(2)}(3, v) = \frac{1}{13\,440}(1-3v)(1-18v+57v^2+240v^3+513v^4-1458v^5+729v^6)$$

$$B_2^{(2)}(4, v) = -\frac{1}{369\,600}(1-9v^2)(1-12v+9v^2)(1-18v+85v^2 -40v^3+765v^4-1458v^5+729v^6).$$

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