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PII: S0305-4470(04)76144-2

Exact product forms for the simple cubic lattice Green function II

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Received 17 February 2004 Published 5 May 2004 Online at stacks.iop.org/JPhysA/37/5417 DOI: 10.1088/0305-4470/37/20/012

Abstract

The analytical properties of the lattice Green function

$$G(2n, n, n; w) = \frac{1}{\pi^3} \int_0^{\pi} \int_0^{\pi} \int_0^{\pi} \frac{\cos 2n\theta_1 \cos n\theta_2 \cos n\theta_3}{w - \cos \theta_1 - \cos \theta_2 - \cos \theta_3} \, \mathrm{d}\theta_1 \, \mathrm{d}\theta_2 \, \mathrm{d}\theta_3$$

are investigated, where *n* is an integer and *w* is a complex variable. In particular, it is shown that G(2n, 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(2n, n, n; w) can be evaluated in terms of a product of two Heun functions $\{H_i(n, v) : j = 1, 2\},$ 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 $\{H_i(n, v) : j = 1, 2\}$ is then given. The Heun function results are used to prove that the product form for G(2n, n, n; w) can be expressed in terms of complete elliptic integrals of the first and second kinds. It is also demonstrated that G(2n, n, n; w) can be written in the hypergeometric form

$$wG(2n, n, n; w) = \frac{\left(\frac{1}{4}\right)_{n} \left(\frac{3}{4}\right)_{n}}{(n!)^{2}} \left(\frac{w^{2}}{w^{2}+3}\right)^{1/2} \left[\frac{w^{2}}{8} \left(\sqrt{1-\frac{1}{w^{2}}} - \sqrt{1-\frac{9}{w^{2}}}\right)^{2}\right]^{2n} \times {}_{2}F_{1} \left(\frac{1}{4}, \frac{3}{4}; n+1; \eta_{+}\right) {}_{2}F_{1} \left(\frac{1}{4}, \frac{3}{4}; n+1; \eta_{-}\right)$$
where

where

$$\eta_{\pm} \equiv \eta_{\pm}(w) = \frac{1}{2} + \frac{w^2}{2(3+w^2)^2} \sqrt{1 - \frac{1}{w^2}} \left[\pm 16 + (5-w^2)\sqrt{1 - \frac{9}{w^2}} \right]$$

and $(a)_n$ denotes the Pochhammer symbol. 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,

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this ${}_{2}F_{1}$ product form is used to determine the asymptotic behaviour of G(2n, n, n; w) as $n \to \infty$.

PACS numbers: 02.30.Gp, 05.50.+q

1. Introduction

The simple cubic lattice Green function

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

where $\{\ell, m, n\}$ is a set of integers and $w = w_1 + iw_2$ is a complex variable, is of frequent occurrence in many lattice statistical problems 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 *et al* 2002). The triple integral (1.1) defines a single-valued analytic function $G(\ell, m, n; w)$ in a complex (w_1, w_2) plane which is cut along the real axis from w = -3 to w = +3. We shall denote the set of points (w_1, w_2) in this cut plane by C^- . It is readily found from (1.1) that $G(\ell, m, n; w)$ satisfies the symmetry relation

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

We see, therefore, that it is only strictly necessary to analyse the properties of (1.1) for points $w \in C^-$ which have $\operatorname{Re}(w) \ge 0$. It can also be assumed, without loss of generality, that $\ell \ge m \ge n \ge 0$.

For many applications in solid-state physics (Koster and Slater 1954, Wolfram and Callaway 1963, Katsura *et al* 1971b) one needs to know 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. It is convenient, therefore, to introduce the definitions

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

where $-3 < w_1 < 3$. When $|w_1| \ge 3$ the imaginary part of $G^{\pm}(\ell, m, n; w_1)$ is always equal to zero. Wolfram and Callaway (1963) have proved that (1.3) can be written in the single integral form

$$G^{\pm}(\ell, m, n; w_1) = (\mp i)^{\ell + m + n + 1} \int_0^\infty \exp(\pm i w_1 t) J_{\ell}(t) J_m(t) J_n(t) dt$$
(1.4)

where $-3 < w_1 < 3$ and $J_n(t)$ denotes a Bessel function of the first kind of order *n*. When $\ell + m + n$ is an even integer it follows from (1.3) and (1.4) that

$$G_{\rm R}(\ell, m, n; w_1) = (-1)^{(\ell+m+n)/2} \int_0^\infty \sin(w_1 t) J_\ell(t) J_m(t) J_n(t) \,\mathrm{d}t \tag{1.5}$$

$$G_{\rm I}(\ell, m, n; w_1) = (-1)^{(\ell+m+n)/2} \int_0^\infty \cos(w_1 t) J_\ell(t) J_m(t) J_n(t) \,\mathrm{d}t. \tag{1.6}$$

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

Joyce (2002) has used the recursion relation procedures developed by Morita (1975) to show that $G(\ell, m, n; w)$ can be evaluated exactly in the ξ parametric form

$$(3/w)^{\ell+m+n}wG(\ell, m, n; w) = R_0(\ell, m, n; \xi) + R_1(\ell, m, n; \xi) \left[\frac{2}{\pi}K(k)\right]^2 + R_2(\ell, m, n; \xi) \left[\frac{2}{\pi}K(k)\right] \left[\frac{2}{\pi}E(k)\right] + R_3(\ell, m, n; \xi) \left[\frac{2}{\pi}E(k)\right]^2$$
(1.7)

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

$$k \equiv k(\xi) = \frac{4\xi^{3/2}}{(1-\xi)^{3/2}(1+3\xi)^{1/2}}.$$
(1.8)

The parameter ξ and the variable w are connected by the relation

$$\xi \equiv \xi(w) = \frac{1}{w} \left(1 + \sqrt{1 - \frac{1}{w^2}} \right)^{-1/2} \left(1 + \sqrt{1 - \frac{9}{w^2}} \right)^{-1/2}$$
(1.9)

and $\{R_j(\ell, m, n; \xi) : j = 0, 1, 2, 3\}$ is a set of rational functions of ξ which are obtained recursively. It was also noted by Joyce (2002) that the formula (1.7) for $\{G(n, n, n; w) : n = 1, 2, 3, 4\}$ and $\{G(2n, n, n; w) : n = 1, 2, 3, 4\}$ could all be factorized in terms of a product of two linear forms in K(k) and E(k) whose coefficients are polynomials in the parameter ξ . On the basis of these limited results it was *conjectured* that the factorization property for G(n, n, n; w) and G(2n, n, n; w) is valid for *all* integer values of *n*.

Recently, Joyce and Delves (2004) in paper I have investigated the detailed analytical properties of the diagonal Green function G(n, n, n; w). In this work a *proof* of the factorization conjecture for G(n, n, n; w) was given. Our main aim in paper II is to carry out a similar analysis for the Green function G(2n, n, n; w). In particular, it will be proved in section 2 that G(2n, 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(2n, n, n; w) can be expressed in terms of a product of two Heun functions $\{H_j(n, v) : j = 1, 2\}$, where $v \equiv v(w) = \xi^2(w)$. The properties of $\{H_j(n, v) : j = 1, 2\}$ are discussed in sections 4 and 5, while in section 6 we shall use the Heun function results to prove the factorization conjecture for G(2n, n, n; w). The asymptotic behaviour of G(2n, n, n; w) as $n \to \infty$ will be determined in section 8.

2. Basic results for the Green function G(2n, n, n; w)

In this section we shall derive a fourth-order differential equation for G(2n, n, n; w).

2.1. Series expansion for G(2n, 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 $\text{Re}(\alpha) > 0$, to the integrand denominator in (1.1). The resulting multiple integral can then be simplified using the well-known 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

$$G(2n, n, n; w) = \int_0^\infty \exp(-wt) I_{2n}(t) [I_n(t)]^2 dt$$
(2.3)

where $\operatorname{Re}(w) \ge 3$.

We now consider the Taylor series expansion

$$I_{2n}(t)[I_n(t)]^2 = \frac{1}{(n!)^2(2n)!} \left(\frac{t}{2}\right)^{4n} \sum_{m=0}^{\infty} a_m(n) \left(\frac{t}{2}\right)^{2m}$$
(2.4)

where $|t| < \infty$ and $a_0(n) = 1$. A formula for the coefficient $a_m(n)$ in (2.4) can be determined by considering the generating function identity

$${}_{0}F_{1}(-;2n+1;x)[{}_{0}F_{1}(-;n+1;x)]^{2} \equiv \sum_{m=0}^{\infty} a_{m}(n)x^{m}$$
(2.5)

where ${}_{0}F_{1}$ denotes a generalized hypergeometric series. If the standard relation (see Erdélyi *et al* (1953), p 185)

$$\left[{}_{0}F_{1}(-;n+1;x)\right]^{2} = {}_{1}F_{2}\left(n+\frac{1}{2};n+1,2n+1;4x\right)$$
(2.6)

is applied to (2.5) it is readily found that

$$a_m(n) = \frac{1}{(2n+1)_m m!} \Phi_m(n)$$
(2.7)

where $(2n + 1)_m$ is a Pochhammer symbol and

$$\Phi_m(n) \equiv {}_3F_2 \begin{bmatrix} -m, & -m-2n, & n+\frac{1}{2}; \\ & & & 4 \\ n+1, & 2n+1; \end{bmatrix}$$
(2.8)

is a terminating generalized hypergeometric series.

We can determine a recursion relation for $\Phi_m(n)$ by using a REDUCE computer algebra package which involves an implementation of the method of Zeilberger (1990). Hence, we obtain

$$(m+n+1)(m+3n+1)(m+4n+1)\Phi_{m+1}(n) - \left[(3n+1)(4n+1)(5n+3) + (118n^2+80n+13)m+2(33n+10)m^2+11m^3\right]\Phi_m(n) + m\left[(67n^2-2n+3) + (76n-1)m+19m^2\right]\Phi_{m-1}(n) - 9m(m-1)(m+2n-1)\Phi_{m-2}(n) = 0$$
(2.9)

where m = 0, 1, 2, ..., with the initial conditions $\Phi_0(n) = 1$ and $\Phi_{-1}(n) = \Phi_{-2}(n) \equiv 0$.

Finally, we substitute (2.4) in the integral representation (2.3). This procedure yields the required series expansion

$$G(2n, n, n; w) = \frac{(4n)!}{2^{4n}(n!)^2(2n)!} \frac{1}{w^{4n+1}} \sum_{m=0}^{\infty} \frac{\mu_m(n)}{w^{2m}}$$
(2.10)

where $|w| \ge 3$ and

$$\mu_m(n) = \frac{(4n+2m)!}{2^{2m}(4n)!(2n+1)_m m!} \Phi_m(n)$$
(2.11)

with $\mu_0(n) = 1$.

2.2. Fourth-order differential equation for G(2n, n, n; w)

In order to derive a differential equation for G(2n, n, n; w) we first apply the formula (2.11) to (2.9). After carrying out some algebraic simplifications we find that the coefficients $\{\mu_m(n) : m = 0, 1, 2, ...\}$ satisfy the four-term recursion relation

$$16(m+1)(m+n+1)(m+3n+1)(m+4n+1)\mu_{m+1}(n) -8(2m+4n+1) [(3n+1)(4n+1)(5n+3) + (118n^2 + 80n + 13)m +2(33n+10)m^2 + 11m^3] \mu_m(n) + 4(2m+4n+1)(2m+4n-1) \times [(67n^2 - 2n+3) + (76n-1)m + 19m^2] \mu_{m-1} - 9(2m+4n+1) \times (2m+4n-1)(2m+4n-2)(2m+4n-3)\mu_{m-2} = 0$$
(2.12)

where $m = 0, 1, 2, \ldots$, with the initial conditions $\mu_0(n) = 1$ and $\mu_{-1}(n) = \mu_{-2}(n) \equiv 0$.

It follows from the relation (2.12) and the series (2.10) that the Green function G(2n, n, n; w) is a solution of the fourth-order differential equation

$$\mathbf{L}_{4,n}(G) = 0 \tag{2.13}$$

where the differential operator

$$\mathbf{L}_{4,n} = 16z^{4}(z-1)^{2}(9z-1) \mathbf{D}_{z}^{4} + 8z^{3}(z-1)(171z^{2} - 131z + 8) \mathbf{D}_{z}^{3} + 4z^{2} \left[756z^{3} + 3(12n^{2} - 359)z^{2} - (56n^{2} - 355)z + 10(2n^{2} - 1) \right] \mathbf{D}_{z}^{2} + 2z^{2} \left[648z^{2} + 12(12n^{2} - 59)z - (128n^{2} - 127) \right] \mathbf{D}_{z} - (4n^{2} - 1)(16n^{2} - 1)$$
(2.14)

and $D_z = d/dz$, with $z = 1/w^2$.

3. Analysis of the differential equation $L_{4,n}(G) = 0$

Our main aim in this section is to investigate the properties the differential equation (2.13). In particular, we shall show that the general solution of $L_{4,n}(G) = 0$ can be expressed in terms of products of solutions of two second-order Heun differential equations. It follows from this result that G(2n, n, n; w) can be written in terms of a product of two Heun functions.

3.1. Singularity structure of the differential equation (2.13)

The basic differential equation (2.13) 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 (2.13) is given by

$$P\begin{bmatrix} 0 & \frac{1}{9} & 1 & \infty \\ \frac{1}{2}(1+4n) & 0 & 0 & 0 \\ \frac{1}{2}(1-4n) & 1 & 1 & 1 & z \\ \frac{1}{2}(1+2n) & 2 & \frac{1}{2} & 2 \\ \frac{1}{2}(1-2n) & \frac{1}{2} & \frac{3}{2} & \frac{1}{2} \end{bmatrix}.$$
(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 v 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 (2.13) has the correct Fuchsian invariant of 12.

It is clear from (3.1) that the expansion (2.10) with $z = 1/w^2$ will give a series solution of (2.13) which is associated with the exponent $\frac{1}{2}(1 + 4n)$ at z = 0. We also find that (2.13) has a simple *algebraic* solution of the type

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

where $g_0(n) \equiv 1$ and n = 1, 2, ... When $n \ge 2$ the coefficients $\{g_m(n) : m = 1, 2, ...\}$ in (3.2) can be generated using the four-term recursion relation

$$2(m+1)(m+n+1)(m-2n+1)(m-3n+1)g_{m+1}(n) -(m-n+1)(2m-2n+1)\Big[(4+n)(1-3n)+11(1-2n)m+11m^2\Big]g_m(n) +2(m-n)(m-n+1)\Big[5(1+2n^2)-38nm+19m^2\Big]g_{m-1}(n) -9(m-n)(m-n+1)(m-n-1)(2m-2n-1)g_{m-2}(n) = 0$$
(3.3)

where m = 0, 1, 2, ..., n - 2, with the initial conditions $g_0(n) = 1$, $g_{-1}(n) \equiv 0$ and $g_{-2}(n) \equiv 0$. From this result we obtain the explicit formulae

$$G^{(a)}(2,z) = \frac{1}{z^{3/2}} (1-z)^{3/2}$$
(3.4)

$$G^{(a)}(3,z) = \frac{1}{16z^{5/2}}(1-z)^{1/2}(16-28z+15z^2)$$
(3.5)

$$G^{(a)}(4,z) = \frac{1}{10z^{7/2}}(1-z)^{3/2}(10-14z+9z^2).$$
(3.6)

3.2. Product solutions for the differential equation (2.13)

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 $L_{4,n}(G) = 0$ can be expressed in the product form

$$G(z) = z^{-1/2} (1-z)^{-1/2} (1-9z)^{-1/2} Y_1(n,z) Y_2(n,z)$$
(3.7)

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

$$\left[D_{z}^{2} + U_{+}(n, z)\right]Y = 0$$
(3.8)

and

$$\left[D_{z}^{2} + U_{-}(n, z)\right]Y = 0$$
(3.9)

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

$$U_{\pm}(n,z) = \frac{(1-5n^2)}{4z^2} + \frac{(7-41n^2)}{4z} + \frac{3}{16(1-z)^2} + \frac{(35-16n^2)}{128(1-z)} + \frac{243}{16(1-9z)^2} + \frac{243(7-48n^2)}{128(1-9z)} \pm \frac{n^2}{z^2(1-z)\sqrt{1-9z}}.$$
(3.10)

Next we shall carry out a *direct* verification of the important results (3.8)–(3.10). In the first stage of the analysis we note that, if $Y_1(n, z)$ and $Y_2(n, z)$ are solutions of (3.8) and (3.9)

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),

$$D_{z}\left[\frac{D_{z}^{3}Y + 2(U_{+} + U_{-})D_{z}Y + YD_{z}(U_{+} + U_{-})}{(U_{+} - U_{-})}\right] + (U_{+} - U_{-})Y = 0 \quad (3.11)$$

where $D_z = d/dz$, $U_{\pm} = U_{\pm}(n, z)$ and $U_{+} \neq U_{-}$. We now use the particular formula (3.10) to evaluate and simplify the general equation (3.11). Finally, the transformation

$$Y = z^{1/2} (1 - z)^{1/2} (1 - 9z)^{1/2} G$$
(3.12)

is applied to the dependent variable in the differential equation. This procedure yields the expected equation $L_{4,n}(G) = 0$.

3.3. Transformation of (3.8) and (3.9) to Heun differential equations

If the independent variable in the *algebraic* differential equations (3.8) and (3.9) is transformed from z to v using the formula (Joyce 1994, 1998)

$$z = \frac{4v(1-v)(1-9v)}{(1-9v^2)^2}$$
(3.13)

then we find that $Y_1(n, v)$ and $Y_2(n, v)$ satisfy rather complicated differential equations of the type

$$\left[D_{v}^{2} + p_{+}(n, v) D_{v} + q_{+}(n, v)\right] Y_{1}(n, v) = 0$$
(3.14)

and

$$\left[\mathbf{D}_{v}^{2} + p_{-}(n, v) \,\mathbf{D}_{v} + q_{-}(n, v) \right] Y_{2}(n, v) = 0 \tag{3.15}$$

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

It is possible to simplify (3.14) and reduce it to a standard form by applying the further transformation

$$Y_1(n,v) = v^{(n+1)/2} (1-v)^{(1-n)/2} (1-9v)^{(1-3n)/2} (1-9v^2)^{-3/2} \times (1-2v+9v^2)^{1/2} (1-18v+9v^2)^{1/2} y_1(n,v).$$
(3.16)

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

$$\frac{\mathrm{d}^2 y}{\mathrm{d}v^2} + \left(\frac{n+1}{v} + \frac{1-n}{v-1} + \frac{1-3n}{v-\frac{1}{9}}\right)\frac{\mathrm{d}y}{\mathrm{d}v} + \frac{\frac{1}{3}(1-3n)(3v-1)}{v(v-1)\left(v-\frac{1}{9}\right)}y = 0.$$
(3.17)

The application of the transformation

$$Y_2(n, v) = v^{(3n+1)/2} (1-v)^{(1-3n)/2} (1-9v)^{(1-n)/2} (1-9v^2)^{-3/2} \times (1-2v+9v^2)^{1/2} (1-18v+9v^2)^{1/2} y_2(n, v)$$
(3.18)

to (3.15) enables one to show that $y_2(n, v)$ is a solution of another Heun equation

$$\frac{d^2 y}{dv^2} + \left(\frac{3n+1}{v} + \frac{1-3n}{v-1} + \frac{1-n}{v-\frac{1}{9}}\right)\frac{dy}{dv} + \frac{\left[(1-n)v - \frac{1}{3}(3n+1)\right]}{v(v-1)\left(v-\frac{1}{9}\right)}y = 0.$$
(3.19)

If we make the substitutions $v = \frac{1}{9u}$ and $y = u\tilde{y}$ in (3.17) and (3.19) it is found that the two Heun equations are transformed into each other with $v \equiv u$ and $y \equiv \tilde{y}$.

3.4. Heun function product form for G(2n, n, n; w)

The Heun differential equations (3.17) and (3.19) 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 (3.17) is given by

$$P\begin{bmatrix} 0 & \frac{1}{9} & 1 & \infty \\ 0 & 0 & 0 & 1 & v \\ -n & 3n & n & 1 - 3n \end{bmatrix}$$
(3.20)

while the P-symbol for (3.19) is

$$P\begin{bmatrix} 0 & \frac{1}{9} & 1 & \infty \\ 0 & 0 & 0 & 1 & v \\ -3n & n & 3n & 1-n \end{bmatrix}.$$
(3.21)

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

It follows from the *P*-symbols that in the neighbourhood of the singularity v = 0 the Heun equations (3.17) and (3.19) will have series solutions of the type

$$y = H_j(n, v) \equiv \sum_{m=0}^{\infty} h_m^{(j)}(n) v^m \qquad (j = 1, 2)$$
 (3.22)

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

$$(m+1)(m+n+1)h_{m+1}^{(1)}(n) - \left[3(1-3n)+2(5-9n)m+10m^2\right]h_m^{(1)}(n) +9m(m-3n)h_{m-1}^{(1)}(n) = 0$$
(3.23)

and

$$(m+1)(m+3n+1)h_{m+1}^{(2)}(n) - \left[3(1+3n) + 2(5+9n)m + 10m^2\right]h_m^{(2)}(n) +9m(m-n)h_{m-1}^{(2)}(n) = 0$$
(3.24)

respectively, where m = 0, 1, 2, ..., with the initial conditions $\{h_0^{(j)}(n) = 1 : j = 1, 2\}$. 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

$$H_1(n,v) = F\left(\frac{1}{9}, -\frac{1}{3}+n; 1, 1-3n, 1+n, 1-3n; v\right)$$
(3.25)

and

$$H_2(n,v) = F\left(\frac{1}{9}, -\frac{1}{3} - n; 1, 1 - n, 1 + 3n, 1 - n; v\right)$$
(3.26)

respectively, where $F(a, b; \alpha, \beta, \gamma, \delta; v)$ denotes a general Heun function. We note that the second independent series solutions of the Heun equations (3.17) and (3.19) exhibit singularities at v = 0 which involve logarithmic terms. In the neighbourhood of the point $v = \infty$ the Heun differential equations for $H_1(n, v)$ and $H_2(n, v)$ also have series solutions $\frac{1}{v}H_2(n, \frac{1}{2v})$ and $\frac{1}{v}H_1(n, \frac{1}{9v})$, respectively.

We now take our solution of $L_{4,n}(G) = 0$ to be the series expansion (2.10) for the Green function G(2n, n, n; w) in powers of 1/w. For this particular case the solution of $L_{4,n}(G) = 0$ does *not* have a logarithmic singularity at $w = \infty$ and it is clear, therefore, that the relevant



Figure 1. The region \mathcal{D}_1 in the *v* plane.

solutions of the Heun equations (3.17) and (3.19) are constant multiples of $H_1(n, v)$ and $H_2(n, v)$ respectively. Finally, we combine equations (3.7), (3.13), (3.16), (3.18) and (3.22) in order to obtain the formula

$$wG(2n, n, n; w) = C_n(1 - 9v^2) \left[\frac{v}{(1 - v)(1 - 9v)}\right]^{2n} H_1(n, v) H_2(n, v)$$
(3.27)

where C_n does not depend on the variable v. We must determine C_n by taking the limit $v \to 0$ in (3.27) and comparing the result with the leading-order term in (2.10), with $v \sim (2w)^{-2}$. Hence we obtain the required Heun function product form

$$wG(2n, n, n; w) = \frac{(4n)!}{(n!)^2(2n)!} (1 - 9v^2) \left[\frac{v}{(1 - v)(1 - 9v)}\right]^{2n} H_1(n, v) H_2(n, v).$$
(3.28)

The general connection between the variables v and w can be established by finding the inverse of the transformation (3.13), with $z = 1/w^2$. This procedure gives

$$v(w) = \frac{1}{w^2} \left(1 + \sqrt{1 - \frac{1}{w^2}} \right)^{-1} \left(1 + \sqrt{1 - \frac{9}{w^2}} \right)^{-1}.$$
 (3.29)

We have checked the final results by using (3.29) to expand the product form (3.28) in powers of 1/w, and agreement was found with the series expansion (2.10).

The transformation function v(w) maps all the points $w \in C^-$ into a region D_1 in the v plane which forms part of the disc $|v| \leq \frac{1}{3}$. This image region is shown in figure 1. The boundary points of D_1 are associated with the edges of the cut in the w plane.

4. Hypergeometric representations, recursion relations and operator identities 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 $_2F_1$ hypergeometric functions, provided that the variable v lies in a sufficiently small neighbourhood of the origin v = 0. Recursion relations and operator identities are also derived for $H_1(n, v)$ and $H_2(n, v)$.



Figure 2. The regions D_1 and D_2 in the cut *v* plane.

4.1. Reduction of the Heun equations (3.17) and (3.19) to hypergeometric form

We begin the analysis by considering the hypergeometric function

$$\mathcal{Y} \equiv \mathcal{Y}(n, x) = {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; x\right).$$
 (4.1)

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

$$16x(1-x)\frac{d^{2}\mathcal{Y}}{dx^{2}} + 16[(n+1)-2x]\frac{d\mathcal{Y}}{dx} - 3\mathcal{Y} = 0.$$
(4.2)

We now apply the rational transformation

$$x \mapsto x_1(v) = \frac{64v}{(1+18v-27v^2)^2}$$
(4.3)

to (4.2). In this manner it is found that

$$v(1-v)(1-9v)(1+18v-27v^{2})^{2} \frac{d^{2}\mathcal{Y}}{dv^{2}} + (1+18v-27v^{2})$$

$$\times \left[(n+1) + 4(9n-5)v + 18(15n-7)v^{2} - 324(3n-1)v^{3} + 243(3n-1)v^{4} \right] \frac{d\mathcal{Y}}{dv} - 12(1-9v)^{2}\mathcal{Y} = 0.$$
(4.4)

Next, the further transformation

$$\mathcal{Y} = (1 + 18v - 27v^2)^{1/2}y \tag{4.5}$$

is applied to (4.4). Hence we find that y = y(n, v) is a solution of the Heun differential equation (3.17). It is readily seen from this result that

$$H_1(n,v) = (1+18v-27v^2)^{-1/2} {}_2F_1\left[\frac{1}{4},\frac{3}{4};n+1;\frac{64v}{(1+18v-27v^2)^2}\right].$$
(4.6)

The formula (4.6) gives a representation for the single-valued analytic function $H_1(n, v)$ provided that v lies in a certain finite region \mathcal{D}_2 of the cut plane. This region of validity is shown in figure 2, with the region \mathcal{D}_1 . The points on the boundary of \mathcal{D}_2 are associated with values of $x = x_1(v)$ which have $1 \le x < \infty$.

The points v in the upper-half plane Im(v) > 0 that are in \mathcal{D}_1 and *outside* \mathcal{D}_2 form a finite region which we shall denote by \mathcal{D}_3 . There is also a similar complex conjugate region \mathcal{D}_3^* in the lower-half plane Im(v) < 0. We can establish ${}_2F_1$ representations for $H_1(n, v)$ which are

valid in \mathcal{D}_3 and \mathcal{D}_3^* by using a standard formula (Erdélyi *et al* (1953), p 110, equation (12)) to construct the analytic continuation of (4.6) across the boundary of the region \mathcal{D}_2 . The final result is

$$H_{1}(n,v) = (1+18v-27v^{2})^{-1/2} \left\{ {}_{2}F_{1}\left[\frac{1}{4},\frac{3}{4};n+1;\frac{64v}{(1+18v-27v^{2})^{2}}\right] \\ \pm i\sqrt{2}\left[-\frac{(1-v)(1-9v)^{3}}{64v}\right]^{n} {}_{2}F_{1}\left[\frac{1}{4},\frac{3}{4};n+1;\frac{(1-v)(1-9v)^{3}}{(1+18v-27v^{2})^{2}}\right] \right\}$$
(4.7)

where the upper and lower signs are valid in \mathcal{D}_3 and \mathcal{D}_3^* , respectively. We can also use (4.7) to determine $H_1(n, v)$ for points v which lie on the *joint* boundary between \mathcal{D}_3 and \mathcal{D}_3^* provided that we first write $v = v_1 \pm i\epsilon$, where $v_1 \in \left[-\frac{1}{3}, -\frac{1}{9}(2\sqrt{3}-3)\right]$, and then take the limit $\epsilon \to 0+$.

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

$$x \mapsto x_2(v) = \frac{64v^3}{(1 - 6v - 3v^2)^2}$$
(4.8)

and

$$\mathcal{V} = (1 - 6v - 3v^2)^{1/2} y \tag{4.9}$$

to (4.2). In this case, it is found that y = y(n, v) is a solution of the second Heun differential equation (3.19). It follows, therefore, that $H_2(n, v)$ can be written in the form

$$H_2(n,v) = (1 - 6v - 3v^2)^{-1/2} {}_2F_1\left[\frac{1}{4}, \frac{3}{4}; n+1; \frac{64v^3}{(1 - 6v - 3v^2)^2}\right].$$
 (4.10)

The formula (4.10) gives a representation for the single-valued analytic function $H_2(n, v)$ provided that v lies in a certain closed region \mathcal{D}_4 of the cut plane. Fortunately, it is *not* necessary to construct the analytic continuation of (4.10) across the boundary of \mathcal{D}_4 because the region \mathcal{D}_1 of physical interest lies *entirely inside* \mathcal{D}_4 .

4.2. Recursion relations for $H_1(n, v)$ and $H_2(n, v)$

We now consider the Gauss contiguous relation (see Erdélyi et al (1953), p 104)

$$(c+1-a)(c+1-b)x {}_{2}F_{1}(a,b;c+2;x) + (c+1)[c-(2c-a-b+1)x] \times {}_{2}F_{1}(a,b;c+1;x) - c(c+1)(1-x) {}_{2}F_{1}(a,b;c;x) = 0.$$
(4.11)

If this result is applied to (4.6) with $a = \frac{1}{4}$, $b = \frac{3}{4}$, c = n and $x = x_1(v)$ we find that $H_1(n, v)$ satisfies the recursion relation

$$4(4n+1)(4n+3)vH_1(n+1,v) + n(n+1)\Big[(1-2v+9v^2)(1-90v+81v^2)H_1(n,v) - (1-v)(1-9v)^3H_1(n-1,v)\Big] = 0$$
(4.12)

where n = 1, 2, ... In a similar manner, the application of (4.11) to (4.10) leads to the further recursion relation

$$4(4n+1)(4n+3)v^{3}H_{2}(n+1,v) + n(n+1)\Big[(1-2v+9v^{2})(1-10v+v^{2})H_{2}(n,v) - (1-v)^{3}(1-9v)H_{2}(n-1,v)\Big] = 0$$
(4.13)

where n = 1, 2, ...

The important ${}_2F_1$ representations (4.6) and (4.10) were originally obtained by first using the Heun equations (3.17) and (3.19) to derive the recursion relations (4.12) and (4.13), respectively. These recursion relations were then reduced to Laplace form and solved in terms of hypergeometric functions by following a standard method (Milne-Thomson (1981), p 491). This alternative *deductive* approach, which is described in more detail in paper I (Joyce and Delves (2004)) for the case of the Green function G(n, n, n; w), provides one with the *motivation* for the direct analysis given in section 4.1.

4.3. Raising operators for $H_1(n, v)$ and $H_2(n, v)$

Next, the Heun function representation (4.6) is applied to the standard formula (see Erdélyi *et al* (1953), p 102)

$$(4n+1)(4n+3)(1-x)^{-n-1} {}_{2}F_{1}\left(\frac{1}{4},\frac{3}{4};n+2;x\right)$$

= $16(n+1)\frac{d}{dx}\left[(1-x)^{-n} {}_{2}F_{1}\left(\frac{1}{4},\frac{3}{4};n+1;x\right)\right]$ (4.14)

with $x = x_1(v)$. This procedure yields the relation

$$H_1(n+1,v) = \mathcal{R}_{1,n} H_1(n,v)$$
(4.15)

where

$$\widehat{\mathcal{R}}_{1,n} = \frac{(n+1)}{4(4n+1)(4n+3)} \Big\{ (1-v)(1-9v)(1+18v-27v^2) D_v \\ + \left[(9+64n) - 117v + 351v^2 - 243v^3 \right] \Big\}$$
(4.16)

is a differential raising operator with $D_v \equiv d/dv$.

Finally, it can also be shown using (4.10) and (4.14) that

$$H_2(n+1,v) = \widehat{\mathcal{R}}_{2,n} H_2(n,v)$$
(4.17)

where

$$\widehat{\mathcal{R}}_{2,n} = \frac{(n+1)}{12(4n+1)(4n+3)v^2} \Big\{ (1-v)(1-9v)(1-6v-3v^2) D_v \\ -3 \Big[1-9v - (1+64n)v^2 + 9v^3 \Big] \Big\}$$
(4.18)

and $n = 0, 1, 2 \dots$

4.4. Alternative $_2F_1$ representations for $H_1(n, v)$ and $H_2(n, v)$

We now apply the quadratic transformation formula (see Erdélyi et al (1953), p 112)

$${}_{2}F_{1}\left(a,a+\frac{1}{2};c;x\right) = \left(1-x\right)^{-a} {}_{2}F_{1}\left[2a,2c-2a-1;c;\frac{1}{2}-\frac{1}{2}\left(1-x\right)^{-1/2}\right]$$
(4.19)

with $a = \frac{1}{4}$ and c = n + 1, to equations (4.6) and (4.10). In this manner, we find that

$$H_1(n,v) = \frac{1}{(1-v)^{1/4}(1-9v)^{3/4}} \, {}_2F_1\left(\frac{1}{2}, 2n+\frac{1}{2}; n+1; k_1^2\right) \tag{4.20}$$

$$H_2(n,v) = \frac{1}{(1-v)^{3/4}(1-9v)^{1/4}} \, {}_2F_1\left(\frac{1}{2}, 2n+\frac{1}{2}; n+1; k_2^2\right) \tag{4.21}$$

where

$$k_1^2 \equiv k_1^2(v) = \frac{1}{2} - \frac{1}{2} \frac{(1+18v-27v^2)}{(1-v)^{1/2}(1-9v)^{3/2}}$$
(4.22)

$$k_2^2 \equiv k_2^2(v) = \frac{1}{2} - \frac{1}{2} \frac{(1 - 6v - 3v^2)}{(1 - v)^{3/2}(1 - 9v)^{1/2}}.$$
(4.23)

It can be shown that the formula (4.20) represents $H_1(n, v)$ provided that v lies in a semiinfinite region \mathcal{D}_5 of the cut plane which includes the real interval $\left(-\infty, \frac{1}{9}\right)$, while (4.21) gives a representation for $H_2(n, v)$ which is valid for all v in the cut plane.

Finally, we use the further transformation (see Erdélyi et al (1953), p 112)

$${}_{2}F_{1}\left(a,a+\frac{1}{2};c;x^{2}\right) = (1+x)^{-2a} {}_{2}F_{1}\left(2a,c-\frac{1}{2};2c-1;\frac{2x}{1+x}\right)$$
(4.24)

with $a = \frac{1}{4}$ and c = n + 1, to express (4.6) and (4.10) in the alternative forms

$$H_1(n,v) = \frac{1}{(1-\xi)^{1/2}(1+3\xi)^{3/2}} {}_2F_1\left(\frac{1}{2}, n+\frac{1}{2}; 2n+1; \widetilde{k}_1^2\right)$$
(4.25)

$$H_2(n,v) = \frac{1}{(1-\xi)^{3/2}(1+3\xi)^{1/2}} {}_2F_1\left(\frac{1}{2}, n+\frac{1}{2}; 2n+1; \widetilde{k}_2^2\right)$$
(4.26)

respectively, where

$$\widetilde{k}_1^2 \equiv \widetilde{k}_1^2(\xi) = \frac{16\xi}{(1-\xi)(1+3\xi)^3}$$
(4.27)

$$\widetilde{k}_2^2 \equiv \widetilde{k}_2^2(\xi) = \frac{16\xi^3}{(1-\xi)^3(1+3\xi)}$$
(4.28)

and $v = \xi^2$. It is found that (4.25) represents $H_1(n, v)$ provided that ξ lies in a certain finite region \mathcal{D}_6 of the ξ plane which includes the real interval $\left(-\frac{1}{3}, \frac{1}{3}\right)$. A diagram showing the region \mathcal{D}_6 has already been given by Joyce (1998, p 5112). The formula (4.26) is valid provided that $\xi \in \mathcal{D}_7$, where \mathcal{D}_7 is a finite region in the ξ plane which also includes the real interval $\left(-\frac{1}{3}, \frac{1}{3}\right)$ but is considerably *larger* than the region \mathcal{D}_6 . The region \mathcal{D}_7 has been illustrated by Joyce (1994, p 472).

5. Evaluation of $H_1(n, v)$ and $H_2(n, v)$ in terms of complete elliptic integrals

We shall now use the results derived in the previous section to obtain expressions for $\{H_j(n, v) : j = 1, 2\}$ in terms of complete elliptic integrals of the first and second kind. These formulae will play a crucial role in the proof of the Joyce (2002) conjecture for G(2n, n, n; w).

5.1. Formulae for $\{H_1(n, v), H_2(n, v) : n = 0, 1\}$

When n = 0 it follows from the formulae (4.25) and (4.26) that

$$H_1(0, v) = \frac{1}{(1-\xi)^{1/2}(1+3\xi)^{3/2}} \left(\frac{2}{\pi}\right) K(\widetilde{k}_1)$$
(5.1)

$$H_2(0,v) = \frac{1}{(1-\xi)^{3/2}(1+3\xi)^{1/2}} \left(\frac{2}{\pi}\right) K(\widetilde{k}_2)$$
(5.2)

where $v = \xi^2$ and $K(\tilde{k})$ denotes a complete elliptic integral of the first kind with a modulus $\tilde{k} \equiv \tilde{k}(\xi)$. We readily find using (4.27) and (4.28) that the modular functions $\tilde{k}_1^2(\xi)$ and $\tilde{k}_2^2(\xi)$ satisfy the cubic modular equation (see Borwein and Borwein (1987), p 125)

$$W_3\left[\tilde{k}_1^2(\xi), \tilde{k}_2^2(\xi)\right] = 0 \tag{5.3}$$

where $W_3(x, y)$ is a *polynomial* of degree 4 in the two variables x and y. It is also known that (see Joyce (1998), p 5111)

$$\frac{K\left[\tilde{k}_{1}(\xi)\right]}{K\left[\tilde{k}_{2}(\xi)\right]} = \frac{1+3\xi}{1-\xi}$$
(5.4)

where $\xi \in \mathcal{D}_6$. The application of (5.4) to (5.1) gives the relation

$$H_1(0,v) = H_2(0,v) = \frac{1}{(1-\xi)^{3/2}(1+3\xi)^{1/2}} \left(\frac{2}{\pi}\right) K(k)$$
(5.5)

where

$$k^{2} \equiv \widetilde{k}_{2}^{2}(\xi) = \frac{16\xi^{3}}{(1-\xi)^{3}(1+3\xi)}$$
(5.6)

and $\xi \in \mathcal{D}_7$. Particular attention has been focused on the modulus $\tilde{k}_2(\xi)$ in equation (5.5) because the region of validity \mathcal{D}_7 for the formula (5.2) is considerably *larger* than that for (5.1). It should be noted that the relation $H_1(0, v) = H_2(0, v)$ can also be obtained by making the substitution n = 0 in (3.25) and (3.26).

Next, we evaluate $H_1(1, v)$ in terms of complete elliptic integrals by applying the raising operator $\widehat{\mathcal{R}}_{1,0}$ to (5.5). Hence, we find that

$$H_{1}(1, v) = \frac{1}{v} \left[B_{1}^{(1)}(1, v)(1-\xi)^{-3/2}(1+3\xi)^{-1/2} \left(\frac{2}{\pi}\right) K(k) + B_{1}^{(2)}(1, v)(1-\xi)^{3/2}(1+3\xi)^{1/2} \left(\frac{2}{\pi}\right) E(k) \right]$$
(5.7)

where $\xi \in \mathcal{D}_7$,

$$B_1^{(1)}(1,v) = -\frac{1}{16}(1-v)(1-9v)(1+3v)^2$$
(5.8)

$$B_1^{(2)}(1,v) = \frac{1}{16}(1+18v-27v^2)$$
(5.9)

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

A similar formula for $H_2(1, v)$ can be derived by applying the operator $\widehat{\mathcal{R}}_{2,0}$ to (5.5). This procedure gives

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

where $\xi \in \mathcal{D}_7$ and

$$B_2^{(1)}(1,v) = -\frac{1}{48}(1-v)^3(1-9v)$$
(5.11)

$$B_2^{(2)}(1,v) = \frac{1}{48}(1-6v-3v^2).$$
(5.12)

5.2. General formulae for $H_1(n, v)$ and $H_2(n, v)$

Formulae for the higher-order Heun functions $\{H_1(n, v) : n = 2, 3, ...\}$ can be generated using the recursion relation (4.12) and equations (5.5) and (5.7). In particular, it is found that

$$H_{1}(n, v) = \frac{1}{v^{n}} \left[B_{1}^{(1)}(n, v)(1-\xi)^{-3/2}(1+3\xi)^{-1/2} \left(\frac{2}{\pi}\right) K(k) + B_{1}^{(2)}(n, v)(1-\xi)^{3/2}(1+3\xi)^{1/2} \left(\frac{2}{\pi}\right) E(k) \right]$$
(5.13)

where $\xi \in D_7$ and $\{B_1^{(j)}(n, v) : j = 1, 2\}$ satisfy the recursion relation

$$B_{1}^{(j)}(n+1,v) + \frac{n(n+1)}{4(4n+1)(4n+3)} \left[(1-2v+9v^{2})(1-90v+81v^{2})B_{1}^{(j)}(n,v) - v(1-v)(1-9v)^{3}B_{1}^{(j)}(n-1,v) \right] = 0$$
(5.14)

with n = 1, 2, ... The initial conditions for (5.14) are given for j = 1 and j = 2 by $\{B_1^{(1)}(0, v) = 1, (5.8)\}$ and $\{B_1^{(2)}(0, v) = 0, (5.9)\}$, respectively. In appendix A we list the polynomials $\{B_1^{(j)}(n, v) : j = 1, 2\}$ for $n \leq 4$.

In a similar manner, we can use (4.13) and equations (5.5) and (5.10) to express $H_2(n, v)$ in terms of K(k) and E(k). The final result is

$$H_{2}(n, v) = \frac{1}{v^{3n}} \left[B_{2}^{(1)}(n, v)(1-\xi)^{-3/2}(1+3\xi)^{-1/2} \left(\frac{2}{\pi}\right) K(k) + B_{2}^{(2)}(n, v)(1-\xi)^{3/2}(1+3\xi)^{1/2} \left(\frac{2}{\pi}\right) E(k) \right]$$
(5.15)

where $\xi \in D_7$ and $\{B_2^{(j)}(n, v) : j = 1, 2\}$ satisfy the recursion relation

$$B_{2}^{(j)}(n+1,v) + \frac{n(n+1)}{4(4n+1)(4n+3)} \left[(1-2v+9v^{2})(1-10v+v^{2})B_{2}^{(j)}(n,v) - v^{3}(1-v)^{3}(1-9v)B_{2}^{(j)}(n-1,v) \right] = 0$$
(5.16)

with n = 1, 2, ... The initial conditions for (5.16) are given for j = 1 and j = 2 by $\{B_2^{(1)}(0, v) = 1, (5.11)\}$ and $\{B_2^{(2)}(0, v) = 0, (5.12)\}$, respectively. In appendix B we list the polynomials $\{B_2^{(j)}(n, v) : j = 1, 2\}$ for $n \leq 4$.

It is possible to use (5.4), (5.13), (5.15) and the transformation properties of the Heun equations (3.17) and (3.19) to determine relations between $\{B_1^{(j)}(n, v) : j = 1, 2\}$ and $\{B_2^{(j)}(n, v) : j = 1, 2\}$. In particular, we find that

$$B_2^{(1)}(n,v) = \left(9v^4\right)^n \left[B_1^{(1)}\left(n,\frac{1}{9v}\right) + \frac{2}{27v^2}(1-v)(1-9v)B_1^{(2)}\left(n,\frac{1}{9v}\right) \right]$$
(5.17)

$$B_2^{(2)}(n,v) = -9^{n-1}v^{4n-2}B_1^{(2)}\left(n,\frac{1}{9v}\right).$$
(5.18)

5.3. Connection between $H_1(n, v)$ and $H_2(n, v)$

A connection between $H_1(n, v)$ and $H_2(n, v)$ can be established by first differentiating (5.13) with respect to v. We then eliminate K(k) and E(k) from the resulting expression using equations (5.13) and (5.15). This procedure eventually yields the relation

$$H_2(n, v) = \left[A_2^{(1)}(n, v) D_v + A_2^{(2)}(n, v)\right] H_1(n, v)$$
(5.19)

where

$$A_{2}^{(1)}(n,v) = (-1)^{n} \left(\frac{4}{3}\right) \frac{(4n)!}{(n!)^{2}(2n)!} v^{1-3n} (1-v)^{1-n} (1-9v)^{1-3n} \\ \times \left(B_{1}^{(1)} B_{2}^{(2)} - B_{1}^{(2)} B_{2}^{(1)}\right)$$
(5.20)

$$A_{2}^{(2)}(n,v) = (-1)^{n} \frac{(4n)!}{3(n!)^{2}(2n)!} v^{-3n} (1-v)^{-n} (1-9v)^{-3n} \\ \times \left\{ 3B_{1}^{(1)}B_{2}^{(1)} - (1-v)(1-9v) \left[(4n-3)B_{1}^{(2)}B_{2}^{(1)} - (4n+3)B_{1}^{(1)}B_{2}^{(2)} \right. \\ \left. - 3(1-v)^{2}B_{1}^{(2)}B_{2}^{(2)} + 4v \left(B_{2}^{(2)} \frac{dB_{1}^{(1)}}{dv} - B_{2}^{(1)} \frac{dB_{1}^{(2)}}{dv} \right) \right] \right\}$$
(5.21)

and $B_i^{(j)} \equiv B_i^{(j)}(n, v)$.

Finally, we note that the function $A_2^{(1)}(n, v)$ is closely related to the algebraic solution $G^{(a)}(n, z)$ which is defined in (3.2). In particular, it can be shown that

$$(1 - 9v^{2})^{2n-2} \sum_{m=0}^{n-1} g_{m}(n) z^{m} = (-1)^{n-1} \frac{4n(4n)!}{(n!)^{2}(2n)!} \frac{[v(1-v)(1-9v)]^{-n}}{(1-2v+9v^{2})} \\ \times \left[B_{1}^{(1)}(n,v) B_{2}^{(2)}(n,v) - B_{1}^{(2)}(n,v) B_{2}^{(1)}(n,v) \right]$$
(5.22)

where z = z(v) is defined in (3.13).

6. Exact product formulae for the Green function *G*(2*n*, *n*, *n*; *w*)

Our main purpose in this section is to prove that G(2n, 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(2n, n, n; w) is expressible in terms of a product of two $_2F_1$ hypergeometric functions.

6.1. Proof of the Joyce conjecture for G(2n, n, n; w)

We begin by applying (5.13) and (5.15) to the Heun function product form (3.28). In this manner, we obtain the ξ parametric formula

$$\overline{G}(2n, n, n; w) \equiv (3/w)^{4n} w G(2n, n, n; w) = (288)^{2n} \frac{\left(\frac{1}{4}\right)_n \left(\frac{3}{4}\right)_n}{(n!)^2} \frac{(1 - 9\xi^4)^{1 - 4n}}{(1 - \xi)^3 (1 + 3\xi)} \\ \times \left(\frac{2}{\pi}\right)^2 \prod_{i=1}^2 \left[B_i^{(1)}(n, v) K(k) + B_i^{(2)}(n, v) (1 - \xi)^3 (1 + 3\xi) E(k) \right]$$
(6.1)

where $k^2 \equiv \tilde{k}_2^2(\xi)$ is defined in (5.6),

$$\xi \equiv \xi(w) = \frac{1}{w} \left(1 + \sqrt{1 - \frac{1}{w^2}} \right)^{-1/2} \left(1 + \sqrt{1 - \frac{9}{w^2}} \right)^{-1/2}$$
(6.2)

and $v = \xi^2$. We can determine the polynomials $\{B_1^{(j)}(n, v) : j = 1, 2\}$ and $\{B_2^{(j)}(n, v): j = 1, 2\}$ in (6.1) using the recursion relations (5.14) and (5.16), respectively. The

transformation function $\xi(w)$ maps all the points $w \in C^-$ into a finite region \mathcal{D}_8 of the ξ plane which lies entirely within the region of validity \mathcal{D}_7 for (6.1). It follows, therefore, that the product form (6.1) can be used to represent G(2n, n, n; w) at *any* point $w = w_1 + iw_2$ in a complex (w_1, w_2) plane which is cut along the real axis from $w_1 = -3$ to $w_1 = +3$.

Explicit product forms of the type (6.1) 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 (6.1). In all cases agreement was found with the work of Joyce (2002). Further checks have also been carried out by expanding (6.1) in powers of 1/w for various integer values of $n \ge 0$ and comparing the results with the series (2.10). It should be noted that (6.1) enables one to calculate *extremely accurate* values for G(2n, n, n; w) at any point $w \in C^-$. For example, we find that

 $G(2000, 1000, 1000; 3) = 0.000\,064\,974\,732\,759\,318\,982\,257\,434\,824\,986\,095\,040$ $447\,836\,134\,237\,054\,824\,872\,894\,107\,567\,028\,537\,432$

$$075\,543\,202\,335\,400\,657\,259\,396\,774\,389\,797\,702\ldots$$
(6.3)

If we make the substitution $w = w_1 - i\epsilon$ in (6.1), where w_1 is real and $\epsilon > 0$, and then apply the definition (1.3) it is found that the right-hand side of (6.1) can be used to calculate $(3/w_1)^{4n}w_1G^-(2n, n, n; w_1)$ for $0 < w_1 < 3$, provided that $\xi = \xi(w)$ is replaced by

$$\widetilde{\xi} \equiv \widetilde{\xi}(w_1) = \lim_{\epsilon \to 0+} \xi(w_1 - i\epsilon) = \frac{1}{w_1} \left(1 - i\sqrt{\frac{1}{w_1^2} - 1} \right)^{-1/2} \left(1 - i\sqrt{\frac{9}{w_1^2} - 1} \right)^{-1/2}.$$
 (6.4)
For example, when $n = 10$ and $w_1 = 2$ the modified formula gives

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

 $G^{-}(20, 10, 10; 2) = G_{R}(20, 10, 10; 2) + iG_{I}(20, 10, 10; 2)$ (6.5)

where

$$G_{\rm R}(20, 10, 10; 2) = 0.002\,835\,466\,154\,520\,544\,442\,954\,939\,811\,909\,758\,470$$

$$618\,940\,267\,778\,655\,555\,353\,298\,266\,494\,520\,382\,665$$

$$921\,664\,380\,808\,874\,760\,169\,510\,161\,661\,424\,046\dots$$
(6.6)

$$G_{I}(20, 10, 10; 2) = -0.008\,023\,089\,279\,720\,478\,267\,990\,086\,421\,714\,426\,059$$

$$884\,706\,205\,832\,543\,996\,224\,125\,783\,704\,825\,653\,686$$

$$873\,277\,311\,394\,317\,013\,919\,288\,705\,627\,268\,880\ldots$$
(6.7)

It would be very difficult to obtain such highly accurate values for $G_R(20, 10, 10; 2)$ and $G_I(20, 10, 10; 2)$ using the integral representations (1.5) and (1.6), respectively, because these integrals involve *oscillatory* integrands which have *slowly decreasing* amplitudes as $t \to \infty$.

6.2. Hypergeometric product forms for G(2n, n, n; w)

We now substitute equations (4.6) and (4.10) in (3.28) and then use the relation (3.29) to express the final result in terms of the variable w. Hence, we obtain the alternative product form

$$wG(2n, n, n; w) = \frac{\left(\frac{1}{4}\right)_{n} \left(\frac{3}{4}\right)_{n}}{(n!)^{2}} \left(\frac{w^{2}}{w^{2}+3}\right)^{1/2} \left[\frac{w^{2}}{8} \left(\sqrt{1-\frac{1}{w^{2}}} - \sqrt{1-\frac{9}{w^{2}}}\right)^{2}\right]^{2n} \times {}_{2}F_{1} \left(\frac{1}{4}, \frac{3}{4}; n+1; \eta_{+}\right) {}_{2}F_{1} \left(\frac{1}{4}, \frac{3}{4}; n+1; \eta_{-}\right)$$
(6.8)



Figure 3. The regions D_9 and D_{10} in the *w* plane.

where

$$\eta_{\pm} \equiv \eta_{\pm}(w) = \frac{1}{2} + \frac{w^2}{2(3+w^2)^2} \sqrt{1 - \frac{1}{w^2}} \left[\pm 16 + (5-w^2) \sqrt{1 - \frac{9}{w^2}} \right].$$
(6.9)

The formula (6.8) 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 (6.8) we first determine the set of points S in the w plane which give real values of $\eta_+(w) \in (\frac{1}{2} + \frac{1}{4}\sqrt{5}, +\infty)$. It is found that the set S forms a closed path which divides the w plane into two regions \mathcal{D}_9 and \mathcal{D}_{10} , as shown in figure 3. From these results it follows that (6.8) is valid for all $w \in C^-$ which are in the *outer* region \mathcal{D}_{10} .

When *w* is in the *inner* region D_9 it is necessary to modify the derivation of the $_2F_1$ product form by replacing (4.6) with the analytic continuation formula (4.7). This procedure yields the alternative representation

$$wG(2n, n, n; w) = \frac{\left(\frac{1}{4}\right)_{n}\left(\frac{3}{4}\right)_{n}}{(n!)^{2}} \left(\frac{w^{2}}{w^{2}+3}\right)^{1/2} \\ \times \left\{ \left[\frac{w^{2}}{8} \left(\sqrt{1-\frac{1}{w^{2}}} - \sqrt{1-\frac{9}{w^{2}}} \right)^{2} \right]^{2n} {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; \eta_{+}\right) \right. \\ \left. \pm i\sqrt{2} \left[-w^{2} \left(1 - \sqrt{1-\frac{1}{w^{2}}} \right)^{2} \right]^{n} {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; 1-\eta_{+}\right) \right\} \\ \left. \times {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; \eta_{-}\right) \right.$$
(6.10)

where the variable w lies in the region \mathcal{D}_9 with the real interval $\left[-\sqrt{5}, \sqrt{5}\right]$ deleted, and $\eta_{\pm} \equiv \eta_{\pm}(w)$ are given by (6.9). The upper positive sign in (6.10) is valid when $\{\operatorname{Re}(w) > 0, \operatorname{Im}(w) < 0\}$ and $\{\operatorname{Re}(w) < 0, \operatorname{Im}(w) > 0\}$, while the lower negative sign is valid when $\{\operatorname{Re}(w) \ge 0, \operatorname{Im}(w) > 0\}$ and $\{\operatorname{Re}(w) \le 0, \operatorname{Im}(w) < 0\}$.

Next we make the substitution $w = w_1 - i\epsilon$ in (6.8), where w_1 is real and $\epsilon > 0$, and then apply the definition (1.3). This procedure gives

Exact product forms for the simple cubic lattice Green function II

$$w_{1}G^{-}(2n, n, n; w_{1}) = \frac{\left(\frac{1}{4}\right)_{n}\left(\frac{3}{4}\right)_{n}}{(n!)^{2}} \left(\frac{w_{1}^{2}}{w_{1}^{2}+3}\right)^{1/2} \left[\frac{w_{1}^{2}}{8}\left(\sqrt{\frac{1}{w_{1}^{2}}-1}-\sqrt{\frac{9}{w_{1}^{2}}-1}\right)^{2}\right]^{2n} \times {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; \widetilde{\eta}_{+}\right) {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; \widetilde{\eta}_{-}\right)$$
(6.11)

where

 $\widetilde{\eta}_{\pm} \equiv \widetilde{\eta}_{\pm}(w_1) = \lim_{\epsilon \to 0^+} \eta_{\pm}(w_1 - i\epsilon)$ $= \frac{1}{2} - \frac{w_1^2}{2(3+w_1^2)^2} \sqrt{\frac{1}{w_1^2} - 1} \left[\pm 16i + (5-w_1^2)\sqrt{\frac{9}{w_1^2} - 1} \right]$ (6.12)

provided that $\sqrt{5} < w_1 \leq 3$. In a similar manner we can use (6.10) to obtain the formula

$$w_{1}G^{-}(2n, n, n; w_{1}) = \frac{\left(\frac{1}{4}\right)_{n}\left(\frac{3}{4}\right)_{n}}{(n!)^{2}} \left(\frac{w_{1}^{2}}{w_{1}^{2}+3}\right)^{1/2} \\ \times \left\{ \left[\frac{w_{1}^{2}}{8} \left(\sqrt{\frac{1}{w_{1}^{2}}-1} - \sqrt{\frac{9}{w_{1}^{2}}-1}\right)^{2}\right]^{2n} {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; \tilde{\eta}_{+}\right) \right. \\ \left. + i\sqrt{2} \left[-w_{1}^{2} \left(1 + i\sqrt{\frac{1}{w_{1}^{2}}-1}\right)^{2}\right]^{n} {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; 1-\tilde{\eta}_{+}\right) \right\} \\ \left. \times {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; \tilde{\eta}_{-}\right) \right.$$

$$(6.13)$$

where $\tilde{\eta}_{\pm} \equiv \tilde{\eta}_{\pm}(w_1)$ are defined in (6.12). This second result is valid when $0 < w_1 \leq \sqrt{5}$.

When n = 0 we can simplify (6.8) by first using (4.6), (4.10) and the relation $H_1(0, v) = H_2(0, v)$ to obtain the transformation formula

$${}_{2}F_{1}\left[\frac{1}{4},\frac{3}{4};1;x_{1}(v)\right] = \left(\frac{1+18v-27v^{2}}{1-6v-3v^{2}}\right)^{1/2} {}_{2}F_{1}\left[\frac{1}{4},\frac{3}{4};1;x_{2}(v)\right]$$
(6.14)

where $v \in D_2$ and $\{x_i(v) : i = 1, 2\}$ are defined in (4.3) and (4.8), respectively. Next (3.29) is applied to (6.14). Hence, we find that

$${}_{2}F_{1}\left(\frac{1}{4},\frac{3}{4};1;\eta_{+}\right) = \left(\frac{w^{2}}{w^{2}+3}\right)^{1/2} \left(2-\sqrt{1-\frac{9}{w^{2}}}\right) {}_{2}F_{1}\left(\frac{1}{4},\frac{3}{4};1;\eta_{-}\right)$$
(6.15)

where $\eta_{\pm} \equiv \eta_{\pm}(w)$ are defined in (6.9) and $w \in \mathcal{D}_{10} \cap \mathcal{C}^-$. From (6.8) and (6.15) we obtain the required result

$$G(0,0,0;w) = \frac{w}{w^2 + 3} \left(2 - \sqrt{1 - \frac{9}{w^2}} \right) \left[{}_2F_1\left(\frac{1}{4},\frac{3}{4};1;\eta_-\right) \right]^2.$$
(6.16)

It should be stressed that the *final* result (6.16) is valid for all $w \in C^-$, even though the formula (6.15) is only valid in a *restricted* region of the cut w plane.

6.3. Alternative $_2F_1$ product formulae for G(2n, n, n; w)

It is possible to obtain an alternative $_2F_1$ product formula by applying (4.25) and (4.26) to (3.28). This procedure yields the ξ parametric representation

$$wG(2n, n, n; w) = \frac{\left(\frac{1}{4}\right)_{n} \left(\frac{3}{4}\right)_{n}}{(n!)^{2}} \frac{(1 - 9\xi^{4})}{(1 - \xi)^{2} (1 + 3\xi)^{2}} \left[\frac{8\xi^{2}}{(1 - \xi^{2})(1 - 9\xi^{2})}\right]^{2n} \\ \times {}_{2}F_{1}\left(\frac{1}{2}, n + \frac{1}{2}; 2n + 1; \widetilde{k}_{1}^{2}\right) {}_{2}F_{1}\left(\frac{1}{2}, n + \frac{1}{2}; 2n + 1; \widetilde{k}_{2}^{2}\right)$$
(6.17)

where $\xi \equiv \xi(w)$ is defined in (6.2), and $\{\tilde{k}_i^2 \equiv \tilde{k}_i^2(\xi) : i = 1, 2\}$ are given by (4.27) and (4.28), respectively. This closed-form expression clearly has a simpler structure than the complete elliptic integral formula (6.1). However, it should be noted that (6.1) is valid for *all* $w \in C^-$, while (6.17) only has a *limited* region of validity in the cut w plane.

Fortunately, we can improve this situation by substituting (4.20) and (4.21) in the product form (3.28) and then using (3.29) to express the final result in terms of the variable w. In this manner, we find that

$$wG(2n, n, n; w) = \frac{\left(\frac{1}{4}\right)_{n} \left(\frac{3}{4}\right)_{n}}{(n!)^{2}} \left(\frac{2}{w^{2}}\right)^{2n} \left(\frac{1}{2}\sqrt{1 - \frac{1}{w^{2}}} + \frac{1}{2}\sqrt{1 - \frac{9}{w^{2}}}\right)^{-4n-1} \times {}_{2}F_{1}\left(\frac{1}{2}, 2n + \frac{1}{2}; n+1; k_{+}^{2}\right) {}_{2}F_{1}\left(\frac{1}{2}, 2n + \frac{1}{2}; n+1; k_{-}^{2}\right)$$
(6.18)

where

$$k_{\pm}^{2} \equiv k_{\pm}^{2}(w) = \frac{1}{2} + \left(\sqrt{1 - \frac{1}{w^{2}}} + \sqrt{1 - \frac{9}{w^{2}}}\right)^{-3} \\ \times \left(\sqrt{1 + \frac{1}{w}}\sqrt{1 - \frac{3}{w}} + \sqrt{1 - \frac{1}{w}}\sqrt{1 + \frac{3}{w}}\right) \\ \times \left[\pm \frac{8}{w^{2}} - \left(1 + \frac{3}{w^{2}}\right)\sqrt{1 - \frac{1}{w^{2}}} - \left(1 - \frac{1}{w^{2}}\right)\sqrt{1 - \frac{9}{w^{2}}}\right].$$
(6.19)
The combinit product form (6.18) is of particular importance because it can be used to determine

The explicit product form (6.18) is of particular importance because it can be used to determine the Green function G(2n, n, n; w) at *any* point $w \in C^-$.

7. Evaluation of G(2n, n, n; w) and $G^{-}(2n, n, n; w_1)$ for special values of w and w_1

We shall now show that the product forms for G(2n, n, n; w) and $G^{-}(2n, n, n; w_1)$ can be simplified when w and w_1 take certain special values.

7.1. Evaluation of G(2n, n, n; 3)

When w = 3 it is known from the work of Watson (1939) that

$$G(0, 0, 0; 3) = \left(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}\right) \left\{\frac{2}{\pi} K(k[6])\right\}^2$$
(7.1)

where the modulus

$$k[6] = \left(2 - \sqrt{3}\right) \left(\sqrt{3} - \sqrt{2}\right) \tag{7.2}$$

is the *singular value* of order 6 (Borwein and Borwein 1987, p 139). For any positive integer N the singular value k[N] satisfies the equation

$$\frac{K'(k[N])}{K(k[N])} = \sqrt{N}$$
(7.3)

where $K'(k) \equiv K(k')$ and $k' \equiv \sqrt{1-k^2}$ is the complementary modulus.

More generally it can be shown, by applying singular value theory of the second kind (Borwein and Borwein 1987, p 152) to the product form (6.1) with w = 3, that

$$G(2n, n, n; 3) = (-1)^n \frac{\left(\frac{1}{4}\right)_n \left(\frac{3}{4}\right)_n}{(n!)^2} \left\{ G(0, 0, 0; 3)[r_1(n)]^2 - \frac{32[r_2(n)]^2}{3\pi^2 G(0, 0, 0; 3)} \right\}$$
(7.4)

where $\{r_j(n) : j = 1, 2\}$ satisfy the recursion relation

$$(4n+1)(4n+3)r_j(n+1) - 16n(n+1)\left[4\sqrt{2}r_j(n) + r_j(n-1)\right] = 0 \quad (7.5)$$

with n = 1, 2, ... The initial conditions for (7.5) are given for j = 1 and j = 2 by $\{r_1(0) = 1, r_1(1) = \frac{4}{3}\sqrt{2}\}$ and $\{r_2(0) = 0, r_2(1) = 1\}$, respectively. For the particular cases n = 1 and n = 2, the formula (7.4) gives

$$G(2, 1, 1; 3) = \frac{2}{3} \left[\frac{3}{\pi^2 G(0, 0, 0; 3)} - G(0, 0, 0; 3) \right]$$
(7.6)

$$G(4, 2, 2; 3) = \frac{1}{105} \left[1225G(0, 0, 0; 3) - \frac{3072}{\pi^2 G(0, 0, 0; 3)} \right]$$
(7.7)

respectively. The formulae (7.6) and (7.7) are in agreement with the work of Glasser and Boersma (2000).

It is also possible to use (6.8) to obtain the simplified closed-form result

$$G(2n, n, n; 3) = \frac{\left(\frac{1}{4}\right)_{n} \left(\frac{3}{4}\right)_{n}}{2\sqrt{3}(n!)^{2}} {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; \frac{1}{2} + \frac{\sqrt{2}}{3}\right) {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; \frac{1}{2} - \frac{\sqrt{2}}{3}\right).$$
(7.8)

In section 8 we shall use (7.8) to investigate the asymptotic behaviour of G(2n, n, n; 3) as $n \to \infty$.

7.2. Evaluation of $G^{-}(2n, n, n; 1)$

If we make the substitution $w_1 = 1$ in (6.13) we obtain the simplified result

$$G^{-}(2n, n, n; 1) = G_{R}(2n, n, n; 1) + iG_{I}(2n, n, n; 1)$$
(7.9)

where

$$G_{\rm R}(2n,n,n;1) = \frac{\left(\frac{1}{4}\right)_n \left(\frac{3}{4}\right)_n}{2(n!)^2} \left[{}_2F_1\left(\frac{1}{4},\frac{3}{4};n+1;\frac{1}{2}\right)\right]^2$$
(7.10)

$$G_{\rm I}(2n, n, n; 1) = (-1)^n \sqrt{2} G_{\rm R}(2n, n, n; 1).$$
(7.11)

It is now possible to use the standard formula (Erdélyi et al 1953, p 104)

$${}_{2}F_{1}\left(\frac{1}{4},\frac{3}{4};n+1;\frac{1}{2}\right) = \frac{\sqrt{\pi}n!}{2^{n}\Gamma\left(\frac{n}{2}+\frac{5}{8}\right)\Gamma\left(\frac{n}{2}+\frac{7}{8}\right)}$$
(7.12)

to express (7.10) in the form

$$G_{\rm R}(2n,n,n;1) = \frac{\sqrt{2}}{8\pi} \frac{\Gamma(\frac{n}{2} + \frac{1}{8})\Gamma(\frac{n}{2} + \frac{3}{8})}{\Gamma(\frac{n}{2} + \frac{5}{8})\Gamma(\frac{n}{2} + \frac{7}{8})}$$
(7.13)

where $\Gamma(z)$ denotes the gamma function.

For the special case n = 0 the formula (7.13) can be written as

$$G_{\rm R}(0,0,0;1) = \frac{\left[\Gamma\left(\frac{1}{8}\right)\Gamma\left(\frac{3}{8}\right)\right]^2}{16\pi^3}.$$
(7.14)

Next, we consider the relation (see Borwein and Borwein (1987), p 298)

$$K(k[2]) = \frac{\left(\sqrt{2}+1\right)^{1/2} \Gamma\left(\frac{1}{8}\right) \Gamma\left(\frac{3}{8}\right)}{2^{13/4} \pi^{1/2}}$$
(7.15)

where the modulus $k[2] = \sqrt{2} - 1$ is the singular value of order 2. If (7.15) is applied to (7.14) we obtain the alternative formula

$$G_{\rm R}(0,0,0;1) = \sqrt{2} \left(\sqrt{2} - 1\right) \left\{\frac{2}{\pi} K(k[2])\right\}^2.$$
(7.16)

The results (7.14) and (7.16) are consistent with the earlier work of Katsura *et al* (1971a) and Joyce (1973).

Finally, we note that the formula (7.13) can be used to show that

$$G_{\rm R}(4N, 2N, 2N; 1) = G_{\rm R}(0, 0, 0; 1) \frac{\left(\frac{1}{8}\right)_N \left(\frac{3}{8}\right)_N}{\left(\frac{5}{8}\right)_N \left(\frac{7}{8}\right)_N}$$
(7.17)

$$G_{\rm R}(4N+2,2N+1,2N+1;1) = \frac{2}{3\pi^2 G_{\rm R}(0,0,0;1)} \frac{\binom{5}{8}_N \binom{7}{8}_N}{\binom{9}{8}_N \binom{11}{8}_N}$$
(7.18)

where N = 0, 1, 2...

7.3. Evaluation of $G^{-}(2n, n, n; 0)$

If we make the substitution $w = -i\epsilon$ in (3.28) and take the limit $\epsilon \to 0+$, it is found that

$$G^{-}(2n, n, n; 0) = \frac{8i}{3} \frac{\left(\frac{1}{4}\right)_n \left(\frac{3}{4}\right)_n}{2^{2n} (n!)^2} H_1\left(n, -\frac{1}{3}\right) H_2\left(n, -\frac{1}{3}\right).$$
(7.19)

We now use the formula (4.21) to write

$$H_2\left(0, -\frac{1}{3}\right) = H_1\left(0, -\frac{1}{3}\right) = \frac{3^{3/4}}{2\pi}K(k[3])$$
(7.20)

where $k[3] = \frac{1}{4}\sqrt{2}(\sqrt{3}-1)$ is the singular value of order 3. Next, the raising operators $\widehat{\mathcal{R}}_{1,0}$ and $\widehat{\mathcal{R}}_{2,0}$ are applied to (4.21) with n = 0. This procedure gives

$$H_1\left(1, -\frac{1}{3}\right) = -3^{1/4}\left(\frac{4}{\pi}\right) \left\{ K(k[3]) - 2E(k[3]) \right\}$$
(7.21)

and

$$H_2\left(1, -\frac{1}{3}\right) = \frac{1}{3^{1/4}} \left(\frac{4}{\pi}\right) \left\{ \left(\sqrt{3} + 2\right) K(k[3]) - 2\sqrt{3}E(k[3]) \right\}$$
(7.22)

respectively.

From singular value theory of the second kind (Borwein and Borwein 1987, p 152) it is known that

$$4\sqrt{3}E(k[3]) = \frac{\pi}{K(k[3])} + 2\left(\sqrt{3} + 1\right)K(k[3]).$$
(7.23)

This result enables one to express (7.21) and (7.22) in the alternative forms

$$H_1\left(1, -\frac{1}{3}\right) = \frac{4}{\pi 3^{1/4}} \left\{ K(k[3]) + \frac{\pi}{2K(k[3])} \right\}$$
(7.24)

and

$$H_2\left(1, -\frac{1}{3}\right) = \frac{4}{\pi 3^{1/4}} \left\{ K(k[3]) - \frac{\pi}{2K(k[3])} \right\}$$
(7.25)

respectively.

Formulae for $\{H_1(n, -\frac{1}{3}) : n = 2, 3, ...\}$ and $\{H_2(n, -\frac{1}{3}) : n = 2, 3, ...\}$ can now be generated using the recursion relations (4.12) and (4.13), respectively. In particular, we find that

$$H_1\left(n, -\frac{1}{3}\right) = \frac{3^{3/4}}{2\pi} 2^n \left\{ K(k[3])s_1(n) + \frac{2\pi}{3K(k[3])}s_2(n) \right\}$$
(7.26)

$$H_2\left(n, -\frac{1}{3}\right) = \frac{3^{3/4}}{2\pi} 2^n \left\{ K(k[3])s_1(n) - \frac{2\pi}{3K(k[3])}s_2(n) \right\}$$
(7.27)

where $\{s_j(n) : j = 1, 2\}$ satisfies the recursion relation

$$(4n+1)(4n+3)s_j(n+1) - 8n(n+1)\left[5s_j(n) - 2s_j(n-1)\right] = 0$$
(7.28)

with n = 1, 2, ... The initial conditions for (7.28) are given for j = 1 and j = 2 by $\{s_1(0) = 1, s_1(1) = \frac{4}{3}\}$ and $\{s_2(0) = 0, s_2(1) = 1\}$, respectively. Finally, we apply (7.26) and (7.27) to the formula (7.19). Hence, we find that

$$G_{1}(2n, n, n; 0) = \frac{\left(\frac{1}{4}\right)_{n} \left(\frac{3}{4}\right)_{n}}{(n!)^{2}} \left\{ G_{1}(0, 0, 0; 0)[s_{1}(n)]^{2} - \frac{16}{3\pi^{2}G_{1}(0, 0, 0; 0)}[s_{2}(n)]^{2} \right\}$$
(7.29)

where

$$G_{\rm I}(0,0,0;0) = \frac{2\sqrt{3}}{\pi^2} \left\{ K(k[3]) \right\}^2.$$
(7.30)

It should be noted that $G_{R}(2n, n, n; 0) = 0$ for n = 0, 1, 2, ...

An alternative closed-form expression for $G_I(2n, n, n; 0)$ can be obtained by taking the limit $w_1 \rightarrow 0+$ in (6.13). This procedure yields

$$G_{1}(2n, n, n; 0) = \sqrt{\frac{2}{3}} \frac{\left(\frac{1}{4}\right)_{n} \left(\frac{3}{4}\right)_{n}}{(n!)^{2}} {}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; -\frac{1}{3}\right) \operatorname{Re}\left[{}_{2}F_{1}\left(\frac{1}{4}, \frac{3}{4}; n+1; \frac{4}{3}\right)\right].$$
(7.31)

In section 8 we shall use (7.31) to investigate the asymptotic behaviour of $G_1(2n, n, n; 0)$ as $n \to \infty$.

7.4. Evaluation of $G\left(2n, n, n; \pm i\sqrt{3}\right)$

In this final subsection we begin by making the substitution $w = \pm i\sqrt{3}$ in (3.28). This procedure yields

$$G\left(2n, n, n; \pm i\sqrt{3}\right) = \mp \frac{4i}{3^{3/2}} \frac{\left(\frac{1}{4}\right)_n \left(\frac{3}{4}\right)_n}{2^{2n} (n!)^2} \left(\sqrt{3} - 1\right)^{4n+1} H_1(n, v_c) H_2(n, v_c)$$
(7.32)

where

$$v_c \equiv v\left(\pm i\sqrt{3}\right) = -\frac{\sqrt{3}}{9}\left(2-\sqrt{3}\right). \tag{7.33}$$

Next, we use (4.20) with $v = v_c$ to obtain the formula

$$H_1(n, v_c) = \frac{3^{3/8}}{2^{7/4}} \left(\sqrt{3} + 1\right)^{1/2} {}_2F_1\left(\frac{1}{2}, 2n + \frac{1}{2}; n + 1; \frac{1}{2}\right).$$
(7.34)

The application of the standard result (Erdélyi et al 1953, p 104)

$${}_{2}F_{1}\left(\frac{1}{2}, 2n+\frac{1}{2}; n+1; \frac{1}{2}\right) = \frac{\left[\Gamma\left(\frac{1}{4}\right)\right]^{2}}{2\pi^{3/2}} \frac{n!}{\left(\frac{3}{4}\right)_{n}}$$
(7.35)

to (7.34) gives

$$H_1(n, v_c) = \frac{3^{3/8}}{\pi 2^{3/4}} \left(\sqrt{3} + 1\right)^{1/2} \frac{n!}{\left(\frac{3}{4}\right)_n} K(k[1])$$
(7.36)

where

$$K(k[1]) = \frac{\left[\Gamma\left(\frac{1}{4}\right)\right]^2}{4\sqrt{\pi}}$$
(7.37)

and $k[1] = 1/\sqrt{2}$ is the singular value of order 1.

We can use the relation $H_2(0, v) = H_1(0, v)$ and equation (7.36) to obtain the formula

$$H_2(0, v_c) = \frac{3^{3/8}}{\pi 2^{3/4}} \left(\sqrt{3} + 1\right)^{1/2} K(k[1]).$$
(7.38)

If the raising operator $\widehat{\mathcal{R}}_{2,0}$ is applied to (4.20) with n = 0 it is also found that

$$H_2(1, v_c) = \frac{3^{1/8}}{\pi 2^{3/4}} \left(\sqrt{3} + 1\right)^{9/2} \left[\left(2\sqrt{2} + 3^{1/4}\right) K(k[1]) - 4\sqrt{2}E(k[1]) \right].$$
(7.39)

From singular value theory of the second kind (Borwein and Borwein 1987, p 152) it is known that

$$4E(k[1]) = 2K(k[1]) + \frac{\pi}{K(k[1])}.$$
(7.40)

This result enables one to write (7.39) in the alternative form

$$H_2(1, v_c) = \frac{3^{1/8}}{\pi 2^{3/4}} \left(\sqrt{3} + 1\right)^{9/2} \left[3^{1/4} K(k[1]) - \frac{\pi \sqrt{2}}{K(k[1])} \right].$$
(7.41)

Formulae for $\{H_2(n, v_c) : n = 2, 3, ...\}$ can now be generated using (7.38), (7.41) and the recursion relation (4.13). In particular, we find that

$$H_2(n, v_c) = \frac{3^{1/8}}{\pi 2^{3/4}} \frac{n!}{2^{2n} \left(\frac{1}{4}\right)_n} \left(\sqrt{3} + 1\right)^{4n + \frac{1}{2}} \left\{ 3^{1/4} K(k[1]) t_1(n) - \frac{\pi \sqrt{2}}{K(k[1])} t_2(n) \right\}$$
(7.42)

where $\{t_i(n) : j = 1, 2\}$ satisfies the recursion relation

$$(4n+3)t_j(n+1) - 56nt_j(n) + (4n-3)t_j(n-1) = 0$$
(7.43)

with n = 1, 2, ... The initial conditions for (7.43) are given for j = 1 and j = 2 by $\{t_1(0) = 1, t_1(1) = 1\}$ and $\{t_2(0) = 0, t_2(1) = 1\}$, respectively. If the formulae (7.36) and (7.42) are applied to (7.32) we obtain the required result

$$G\left(2n, n, n; \pm i\sqrt{3}\right) = G\left(0, 0, 0; \pm i\sqrt{3}\right)t_1(n) \pm \frac{4i}{3\pi}t_2(n)$$
(7.44)

where

$$G\left(0,0,0;\pm i\sqrt{3}\right) = \mp i \frac{2^{3/2}}{\pi^2 3^{3/4}} \left\{ K(k[1]) \right\}^2.$$
(7.45)

An alternative ${}_2F_1$ formula for $H_2(n, v_c)$ can also be derived by substituting $v = v_c$ in (4.10). Hence, we find that

$$H_2(n, v_c) = \frac{3}{2^{5/2}} \left(\sqrt{3} + 1\right)^{\frac{1}{2}} {}_2F_1\left(\frac{1}{4}, \frac{3}{4}; n+1; \frac{1}{2} - \frac{7}{24}\sqrt{3}\right).$$
(7.46)

From equations (7.32), (7.36) and (7.46) we obtain the closed-form expression

$$G\left(2n,n,n;\pm i\sqrt{3}\right) = \mp i \frac{K(k[1])}{\pi 2^{1/4} 3^{1/8}} \frac{\left(\frac{1}{4}\right)_n}{n!} \left(\frac{\sqrt{3}-1}{\sqrt{2}}\right)^{4n} {}_2F_1\left(\frac{1}{4},\frac{3}{4};n+1;\frac{1}{2}-\frac{7}{24}\sqrt{3}\right).$$
(7.47)

In section 8 we shall use (7.47) to investigate the behaviour of $G(2n, n, n; \pm i\sqrt{3})$ as $n \to \infty$.

5440

8. Asymptotic behaviour of G(2n, n, n; w) and $G^{-}(2n, n, n; w_1)$ as $n \to \infty$

The asymptotic behaviour of $G(\ell, m, n; w)$ as $(\ell^2 + m^2 + n^2)^{1/2} \to \infty$ has been investigated by Katsura and Inawashiro (1973) using stationary phase and saddle-point methods. This work 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 given in section 6.2 enable one to derive uniform asymptotic *expansions* for G(2n, n, n; w), as $n \to \infty$, in a very *direct* and *simple* manner.

8.1. General asymptotic representations

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

$${}_{2}F_{1}\left(\frac{1}{4},\frac{3}{4};n+1;\eta\right) \sim \Lambda_{M}(n,\eta)$$

$$(8.1)$$

as $n \to \infty$, where

$$\Lambda_M(n,\eta) \equiv \sum_{m=0}^M \frac{\left(\frac{1}{4}\right)_m \left(\frac{3}{4}\right)_m}{(n+1)_m m!} \eta^m$$
(8.2)

and M = 0, 1, 2, ... Next we apply (8.1) to the product form (6.8). This procedure yields the asymptotic representation

$$G(2n, n, n; w) \sim \frac{1}{w\pi\sqrt{2}} \frac{\Gamma(n + \frac{1}{4})\Gamma(n + \frac{3}{4})}{[\Gamma(n+1)]^2} \left[\frac{w^2}{8} \left(\sqrt{1 - \frac{1}{w^2}} - \sqrt{1 - \frac{9}{w^2}} \right)^2 \right]^{2n} \times \left(\frac{w^2}{w^2 + 3} \right)^{1/2} \Lambda_M(n, \eta_+) \Lambda_M(n, \eta_-)$$
(8.3)

as $n \to \infty$, where *M* is *fixed* and $\eta_{\pm} = \eta_{\pm}(w)$ are defined in (6.9). We expect (8.3) to be valid provided that *w* lies in the region \mathcal{D}_{10} of the cut *w* plane.

A uniform asymptotic expansion for G(2n, n, n; w) can now be derived by expanding the ratio of gamma functions and the Λ functions in (8.3) in powers of 1/n. In particular, we find that

$$G(2n, n, n; w) \sim \frac{1}{\pi\sqrt{2}wn} \left[\frac{w^2}{8} \left(\sqrt{1 - \frac{1}{w^2}} - \sqrt{1 - \frac{9}{w^2}} \right)^2 \right]^{2n} \left(\frac{w^2}{w^2 + 3} \right)^{1/2} \sum_{m=0}^{\infty} \frac{b_m^{(1)}(w)}{n^m}$$
(8.4)

as
$$n \to \infty$$
, where $b_0^{(1)}(w) = 1$,
 $b_1^{(1)}(w) = \frac{3w^2(5-w^2)}{16(w^2+3)^2} \sqrt{1-\frac{1}{w^2}} \sqrt{1-\frac{9}{w^2}}$
(8.5)

$$b_2^{(1)}(w) = \frac{3}{512(w^2+3)^4} \left(2979 - 12\,284w^2 + 5778w^4 - 572w^6 + 3w^8\right) \tag{8.6}$$

$$b_{3}^{(1)}(w) = \frac{3w^{2}(5-w^{2})}{8192(w^{2}+3)^{6}}\sqrt{1-\frac{1}{w^{2}}}\sqrt{1-\frac{9}{w^{2}}}\left(44\,307-357\,564w^{2}+239\,538w^{4}-10\,236w^{6}-13w^{8}\right)$$
(8.7)

$$b_{4}^{(1)}(w) = \frac{3}{524288(w^{2}+3)^{8}} \left(857417481 - 13228000488w^{2} + 32434085628w^{4} - 27205809624w^{6} + 8960294070w^{8} - 1187975768w^{10} + 58488444w^{12} - 633704w^{14} - 183w^{16}\right)$$
(8.8)

and $w \in \mathcal{D}_{10}$.

In a similar manner we can also apply (8.1) to the product form (6.10). Hence, we obtain

$$G(2n, n, n; w) \sim \frac{1}{w\pi\sqrt{2}} \frac{\Gamma(n + \frac{1}{4})\Gamma(n + \frac{3}{4})}{[\Gamma(n+1)]^2} \left(\frac{w^2}{w^2 + 3}\right)^{1/2} \Lambda_M(n, \eta_-) \\ \times \left\{ \left[\frac{w^2}{8} \left(\sqrt{1 - \frac{1}{w^2}} - \sqrt{1 - \frac{9}{w^2}} \right)^2 \right]^{2n} \Lambda_M(n, \eta_+) \right. \\ \left. \pm i\sqrt{2} \left[-w^2 \left(1 - \sqrt{1 - \frac{1}{w^2}} \right)^2 \right]^n \Lambda_M(n, 1 - \eta_+) \right\}$$
(8.9)

as $n \to \infty$, with *M* fixed. We expect (8.9) to be valid provided that *w* lies in the region \mathcal{D}_9 with the real interval $\left[-\sqrt{5}, \sqrt{5}\right]$ deleted. The role of the \pm signs in equation (8.9) is explained in section 6.2. If the ratio of gamma functions and the Λ functions in (8.9) are expanded in powers of 1/n it is found that

$$G(2n, n, n; w) \sim \frac{1}{\pi \sqrt{2}wn} \left\{ \left[\frac{w^2}{8} \left(\sqrt{1 - \frac{1}{w^2}} - \sqrt{1 - \frac{9}{w^2}} \right)^2 \right]^{2n} \sum_{m=0}^{\infty} \frac{b_m^{(1)}(w)}{n^m} \\ \pm i\sqrt{2} \left[-w^2 \left(1 - \sqrt{1 - \frac{1}{w^2}} \right)^2 \right]^n \sum_{m=0}^{\infty} \frac{b_m^{(2)}(w)}{n^m} \right\} \left(\frac{w^2}{w^2 + 3} \right)^{1/2}$$
(8.10)

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

$$b_1^{(2)}(w) = -\frac{3w^2}{(w^2+3)^2} \sqrt{1-\frac{1}{w^2}}$$
(8.11)

$$b_2^{(2)}(w) = \frac{3}{2(w^2+3)^4} \left(9 - 47w^2 + 24w^4 - 2w^6\right)$$
(8.12)

$$b_{3}^{(2)}(w) = -\frac{3w^{2}}{4(w^{2}+3)^{6}}\sqrt{1-\frac{1}{w^{2}}}\left(1269-3138w^{2}+1371w^{4}-162w^{6}+4w^{8}\right)$$
(8.13)

$$b_{4}^{(2)}(w) = \frac{3}{8(w^{2}+3)^{8}} \left(11\,421 - 192\,780w^{2} + 488\,691w^{4} - 417\,690w^{6} + 137\,970w^{8} - 17\,948w^{10} + 840w^{12} - 8w^{14} \right)$$
(8.14)

and $w \in \mathcal{D}_9$ with the real interval $\left[-\sqrt{5}, \sqrt{5}\right]$ deleted. It should be noted that the coefficients $\left\{b_m^{(1)}(w), b_m^{(2)}(w) : m = 1, 2, \ldots\right\}$ in the expansions (8.4) and (8.10) all become infinite as $w \to \pm i\sqrt{3}$. The reasons for this breakdown at $w = \pm i\sqrt{3}$ will be discussed in section 8.3.

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

$$G^{-}(2n, n, n; w_1) \sim \frac{1}{\pi\sqrt{2}n} \left[\frac{w_1^2}{8} \left(\sqrt{1 - \frac{1}{w_1^2}} + i\sqrt{\frac{9}{w_1^2} - 1} \right)^2 \right]^{2n} \left(\frac{1}{w_1^2 + 3} \right)^{1/2} \sum_{m=0}^{\infty} \frac{\widetilde{b}_m^{(1)}(w_1)}{n^m}$$
(8.15)

as $n \to \infty$, where $\sqrt{5} < w_1 \leq 3$ and $\widetilde{b}_0^{(1)}(w_1) = 1$. Formulae for $\{\widetilde{b}_m^{(1)}(w_1) : m = 1, 2, 3, 4\}$ can be readily obtained by making the formal replacements $w \mapsto w_1$ and

$$\sqrt{1 - \frac{9}{w^2}} \mapsto -i\sqrt{\frac{9}{w_1^2} - 1} \tag{8.16}$$

in the right-hand sides of equations (8.5)–(8.8), respectively. When $0 < w_1 \leq \sqrt{5}$ we can use (8.10) to derive the alternative asymptotic expansion

$$G^{-}(2n, n, n; w_{1}) \sim \frac{1}{\pi\sqrt{2}n} \left\{ \left[\frac{w_{1}^{2}}{8} \left(\sqrt{\frac{1}{w_{1}^{2}} - 1} - \sqrt{\frac{9}{w_{1}^{2}} - 1} \right)^{2} \right]^{2n} \sum_{m=0}^{\infty} \frac{\widetilde{b}_{m}^{(1)}(w_{1})}{n^{m}} + i\sqrt{2} \left[-w_{1}^{2} \left(1 + i\sqrt{\frac{1}{w_{1}^{2}} - 1} \right)^{2} \right]^{n} \sum_{m=0}^{\infty} \frac{\widetilde{b}_{m}^{(2)}(w_{1})}{n^{m}} \right\} \left(\frac{1}{w_{1}^{2} + 3} \right)^{1/2}$$
(8.17)

as $n \to \infty$, where $\tilde{b}_0^{(2)}(w_1) = 1$. Formulae for $\{\tilde{b}_m^{(2)}(w_1) : m = 1, 2, 3, 4\}$ can be written down by making the formal replacements $w \mapsto w_1$ and

$$\sqrt{1 - \frac{1}{w^2}} \mapsto -i\sqrt{\frac{1}{w_1^2} - 1} \tag{8.18}$$

in the right-hand sides of equations (8.11)-(8.14), respectively.

8.2. Some special cases

We shall now derive expansions for G(2n, n, n; 3), $G^{-}(2n, n, n; 1)$ and $G^{-}(2n, n, n; 0)$ in powers of 1/n using results given in section 7.

We begin the analysis by applying (8.1) to the formula (7.8). Hence, we obtain the asymptotic representation

$$G(2n, n, n; 3) \sim \frac{1}{2\pi\sqrt{6}} \frac{\Gamma\left(n + \frac{1}{4}\right)\Gamma\left(n + \frac{3}{4}\right)}{[\Gamma(n+1)]^2} \Lambda_M\left(n, \frac{1}{2} + \frac{\sqrt{2}}{3}\right) \Lambda_M\left(n, \frac{1}{2} - \frac{\sqrt{2}}{3}\right)$$
(8.19)

as $n \to \infty$. If the ratio of gamma functions and the Λ functions in (8.19) are expanded in powers of 1/n we find that

$$G(2n, n, n; 3) \sim \frac{1}{2\pi\sqrt{6n}} \left(1 - \frac{1}{96n^2} - \frac{157}{18\,432n^4} - \frac{3557}{1769\,472n^6} + \frac{10\,544\,227}{679\,477\,248n^8} + \frac{590\,022\,059}{21\,743\,271\,936n^{10}} - \frac{2774\,734\,887\,161}{12\,524\,124\,635\,136n^{12}} - \frac{539\,053\,078\,139\,887}{400\,771\,988\,324\,352n^{14}} + \frac{44\,569\,070\,631\,361\,169}{3799\,912\,185\,593\,856n^{16}} + \frac{16\,912\,634\,548\,105\,896\,634\,117}{88\,644\,351\,465\,533\,472\,768n^{18}} + \cdots \right)$$
(8.20)

as $n \to \infty$. It has been verified that (8.20) is consistent with the general expansion (8.4). Duffin (1953) has used completely different methods to prove that

$$G(\ell, m, n; 3) \sim \frac{1}{2\pi R} \left\{ 1 + \frac{1}{8R^2} \left[-3 + \frac{5(\ell^4 + m^4 + n^4)}{R^4} \right] + O\left(\frac{1}{R^4}\right) \right\}$$
(8.21)

as $R = (\ell^2 + m^2 + n^2)^{1/2} \to \infty$. When $\ell = 2n$ and m = n this result is in agreement with the first two terms in the expansion (8.20). We have also used (8.20) to calculate an approximate value for G(2n, n, n; 3) when n = 1000. It is found from (6.3) that this asymptotic value has an error of $-9.8545 \cdots \times 10^{-62}$.

Next we expand the exact formula (7.13) in powers of 1/n. This procedure yields

$$G^{-}(2n, n, n; 1) = \left[1 + i\sqrt{2}(-1)^{n}\right]G_{R}(2n, n, n; 1)$$
(8.22)

where

$$G_{\rm R}(2n,n,n;1) \sim \frac{1}{2\pi\sqrt{2}n} \left(1 - \frac{3}{32n^2} + \frac{123}{2048n^4} - \frac{7719}{65\,536n^6} + \frac{4\,115\,283}{8\,388\,608n^8} - \frac{950\,375\,949}{268\,435\,456n^{10}} + \frac{674\,225\,797\,359}{17\,179\,869\,184n^{12}} - \frac{340\,018\,590\,242\,127}{549\,755\,813\,888n^{14}} + \frac{1848\,888\,327\,048\,988\,803}{140\,737\,488\,355\,328n^{16}} - \frac{1628\,742\,598\,405\,608\,165\,009}{4503\,599\,627\,370\,496n^{18}} + \cdots \right)$$
(8.23)

as $n \to \infty$. If we compare this result with the general expansion (8.17) it is found that the coefficient of $1/n^{2m}$ in (8.23) is given by $\tilde{b}_{2m}^{(1)}(1) = \tilde{b}_{2m}^{(2)}(1)$, where m = 0, 1, 2, ... Finally, we use (7.31) and (8.1) to obtain the asymptotic representation

use (7.51) and (8.1) to obtain the asymptotic representation = (1, 2, 3)

$$G_{I}(2n, n, n; 0) \sim \frac{1}{\pi\sqrt{3}} \frac{\Gamma(n + \frac{1}{4})\Gamma(n + \frac{3}{4})}{[\Gamma(n+1)]^{2}} \Lambda_{M}\left(n, -\frac{1}{3}\right) \Lambda_{M}\left(n, \frac{4}{3}\right)$$
(8.24)

as $n \to \infty$, with *M* fixed. It follows from this result that

$$G^{-}(2n, n, n; 0) = iG_{I}(2n, n, n; 0) \sim \frac{i}{\pi\sqrt{3}n} \left(1 + \frac{1}{6n^{2}} + \frac{47}{72n^{4}} + \frac{3047}{432n^{6}} + \frac{1630\,243}{10\,368n^{8}} + \frac{123\,577\,081}{20\,736n^{10}} + \frac{256\,585\,238\,971}{746\,496n^{12}} + \frac{41\,881\,050\,557\,657}{1492\,992n^{14}} + \frac{24\,505\,855\,348\,810\,649}{7962\,624n^{16}} + \frac{563\,629\,394\,387\,436\,037\,523}{1289\,945\,088n^{18}} + \cdots \right)$$
(8.25)

as $n \to \infty$. If we compare (8.25) with the general expansion (8.17) it is found that the coefficient of $1/n^{2m}$ in (8.25) is given by $\tilde{b}_{2m}^{(2)}(0)$, where $m = 0, 1, 2, \ldots$. It should be noted that, in the limit $w_1 \to 0+$, the asymptotic formula (8.17) represents the zero value for $G_{\rm R}(2n, n, n; 0)$ by negligible terms of $O(4^{-n})$, as $n \to \infty$.

8.3. Multiple turning points

Our main aim in this final subsection is to investigate the reasons for the breakdown of the asymptotic expansions (8.4) and (8.10) as $w \to \pm i\sqrt{3}$. We begin by making the transformation

$$y = v^{-(n+1)/2} (1-v)^{(n-1)/2} (1-9v)^{(3n-1)/2} Y$$
(8.26)

to the Heun equation (3.17), where *Y* is a new dependent variable. This procedure reduces (3.17) to the normal form

$$\frac{d^2Y}{dv^2} = \left[n^2 f(v) + g(v)\right]Y$$
(8.27)

where

$$f(v) = \left[\frac{(v - v_c)\left(27v + v_c^{-1}\right)}{2v(1 - v)(1 - 9v)}\right]^2$$
(8.28)

$$g(v) = -\frac{(1 - 12v + 102v^2 - 108v^3 + 81v^4)}{[2v(1 - v)(1 - 9v)]^2}$$
(8.29)

and

$$v_c = -\frac{\sqrt{3}}{9} \left(2 - \sqrt{3} \right). \tag{8.30}$$

We see that the differential equation (8.27) has turning points of multiplicity 2 (Olver 1977) at $v = v_c$ and $-1/(27v_c)$. If we make the substitution $w = \pm i\sqrt{3}$ in the transformation formula (3.29) it is found that $v(\pm i\sqrt{3}) = v_c$. It follows, therefore, that the expansions (8.4) and (8.10) break down as $w \to \pm i\sqrt{3}$ because the Heun equation (3.17) is associated with a *multiple turning point* at $v = v_c$. It should be noted that the turning point at $v = -1/(27v_c)$ does not affect the asymptotic behaviour of G(2n, n, n; w) because the point $v = -1/(27v_c)$ lies *outside* the region \mathcal{D}_1 shown in figure 1.

In a similar manner, we find that the second Heun equation (3.19) also has a normal form of the type (8.27) with turning points of multiplicity 2 at $v = -3v_c$ and $1/(9v_c)$. Fortunately, *both* these turning points are outside the region \mathcal{D}_1 of physical interest in the v plane.

Asymptotic representations for G(2n, n, n; w) which are uniformly valid in the immediate neighbourhood of $w = \pm i\sqrt{3}$ could be established by applying the sophisticated methods developed by Olver (1977, 1978) to the turning point $v = v_c$ of the differential equation (8.27). One would expect that the leading-order terms in these representations are expressible in terms of modified Bessel functions of order 1/4. For the special case $w = \pm i\sqrt{3}$ we can use (7.47) and (8.1) to derive the asymptotic expansion

$$G\left(2n, n, n; \pm i\sqrt{3}\right) \sim \mp i \frac{\Gamma\left(\frac{1}{4}\right)}{4\pi^{3/2} 2^{1/4} 3^{1/8}} \left(\frac{\sqrt{3}-1}{\sqrt{2}}\right)^{4n} \frac{1}{n^{3/4}} \left[1 - \frac{7\sqrt{3}}{128n} - \frac{77}{2(128n)^2} + \frac{5929\sqrt{3}}{2(128n)^3} + \frac{4384\,611}{8(128n)^4} - \frac{329\,524\,657\sqrt{3}}{8(128n)^5} + \frac{49\,140\,081\,463}{16(128n)^6} - \frac{4034\,376\,432\,471\sqrt{3}}{16(128n)^7} + \frac{22\,612\,364\,314\,605\,219}{128(128n)^8} - \frac{2471\,042\,735\,575\,208\,333\sqrt{3}}{128(128n)^9} + \cdots\right]$$
(8.31)

as $n \to \infty$. A striking feature of this expansion is that the amplitude factor $n^{-3/4}$ does not obey the expected n^{-1} decay law.

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

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

$$B_1^{(1)}(1, v) = -\frac{1}{16}(1 - v)(1 - 9v)(1 + 3v)^2$$

$$B_1^{(1)}(2, v) = \frac{1}{1120}(1 - v)^2(1 - 9v)(1 + 9v)(1 - 78v + 72v^2 - 162v^3 - 729v^4)$$

$$\begin{split} B_1^{(1)}(3,v) &= -\frac{1}{73\,920}(1-v)^3(1-9v)(1-90v+4428v^2+49\,572v^3\\ &\quad -65\,610v^4+669\,222v^5-708\,588v^6+4782\,969v^8) \\ B_1^{(1)}(4,v) &= \frac{1}{4804\,800}(1-v)^3(1-9v)(1-116v+6642v^2-285\,660v^3\\ &\quad -3342\,465v^4+7925\,688v^5-83\,377\,188v^6+299\,024\,136v^7\\ &\quad -884\,849\,265v^8+1052\,253\,180v^9+774\,840\,978v^{10}\\ &\quad -4649\,045\,868v^{11}+3486\,784\,401v^{12}) \\ B_1^{(2)}(0,v) &= 0\\ B_1^{(2)}(1,v) &= \frac{1}{16}(1+18v-27v^2)\\ B_1^{(2)}(2,v) &= -\frac{1}{1120}(1-2v+9v^2)(1+18v-27v^2)(1-90v+81v^2)\\ B_1^{(2)}(3,v) &= \frac{1}{73\,920}(1+18v-27v^2)(1-114v+7044v^2-32\,724v^3\\ &\quad +185\,166v^4-607\,986v^5+1\,338\,444v^6-1\,417\,176v^7+531\,441v^8)\\ B_1^{(2)}(4,v) &= -\frac{1}{4804\,800}(1-2v+9v^2)(1+18v-27v^2)(1-90v+81v^2)\\ &\quad \times(1-48v+5196v^2-14\,904v^3+121\,014v^4-559\,872v^5\\ &\quad +1338\,444v^6-1417\,176v^7+531\,441v^8) \end{split}$$

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

$$\begin{split} B_2^{(1)}(0,v) &= 1 \\ B_2^{(1)}(1,v) &= -\frac{1}{48}(1-v)^3(1-9v) \\ B_2^{(1)}(2,v) &= \frac{1}{3360}(1-v)^3(1-9v)(1-12v+30v^2-44v^3+9v^4) \\ B_2^{(1)}(3,v) &= -\frac{1}{221760}(1-v)^3(1-9v)(1-24v+204v^2-786v^3+1710v^4-2196v^5+2628v^6-594v^7+81v^8) \\ B_2^{(1)}(4,v) &= \frac{1}{14414400}(1-v)^3(1-9v)(1-36v+522v^2-3980v^3+17895v^4-51816v^5+102156v^6-144792v^7+146\,655v^8-163\,380v^9+37\,962v^{10}-7452v^{11}+729v^{12}) \\ B_2^{(2)}(0,v) &= 0 \\ B_2^{(2)}(1,v) &= \frac{1}{48}(1-6v-3v^2) \\ B_2^{(2)}(2,v) &= -\frac{1}{3360}(1-2v+9v^2)(1-6v-3v^2)(1-10v+v^2) \\ B_2^{(2)}(3,v) &= \frac{1}{221760}(1-6v-3v^2)(1-24v+204v^2-834v^3+2286v^4-3636v^5+7044v^6-1026v^7+81v^8) \\ B_2^{(2)}(4,v) &= -\frac{1}{14414400}(1-2v+9v^2)(1-6v-3v^2)(1-10v+v^2) \\ \times (1-24v+204v^2-768v^3+1494v^4-1656v^5+5196v^6-432v^7+81v^8) \end{split}$$

References

Berlin T H and Kac M 1952 Phys. Rev. 86 821-35

Borwein J M and Borwein P B 1987 Pi and the AGM (New York: Wiley)

Delves R T and Joyce G S 2001 Ann. Phys. 291 71-133

Duffin R J 1953 Duke Math. J. 20 233–51

Erdélyi A, Magnus W, Oberhettinger F and Tricomi F G 1953 *Higher Transcendental Functions* vol 1 (New York: McGraw-Hill)

Glasser M L and Boersma J 2000 J. Phys. A: Math. Gen. 33 5017-23

Ince E L 1927 Ordinary Differential Equations (London: Longmans)

Joyce G S 1972 *Phase Transitions and Critical Phenomena* vol 2 ed C Domb and M S Green (London: Academic) pp 375–442

Joyce G S 1973 Phil. Trans. R. Soc. A 273 583-610

Joyce G S 1994 Proc. R. Soc. A 445 463-77

Joyce G S 1998 J. Phys. A: Math. Gen. 31 5105-15

Joyce G S 2002 J. Phys. A: Math. Gen. 35 9811–28

Joyce G S and Delves R T 2004 J. Phys. A: Math. Gen. 37 3645-71

Katsura S and Inawashiro S 1973 Prog. Theor. Phys. 50 82–94

Katsura S, Inawashiro S and Abe Y 1971a J. Math. Phys. 12 895–9

Katsura S, Morita T, Inawashiro S, Horiguchi T and Abe Y 1971b J. Math. Phys. 12 892–5

Kobelev V, Kolomeisky A B and Fisher M E 2002 J. Chem. Phys. 116 7589-98

Koster G F and Slater J C 1954 Phys. Rev. 96 1208–23

Luke Y L 1969 The Special Functions and their Approximations vol 1 (New York: Academic)

Maradudin A A, Montroll E W, Weiss G H, Herman R and Milnes H W 1960 Green's Functions for Monatomic Simple Cubic Lattices (Bruxelles: Académie Royale de Belgique)

Milne-Thomson L M 1981 The Calculus of Finite Differences (New York: Chelsea)

Montroll E W and Weiss G H 1965 J. Math. Phys. 6 167-81

Morita T 1975 J. Phys. A: Math. Gen. 8 478-89

Olver F W J 1977 SIAM J. Math. Anal. 8 127-54

Olver F W J 1978 Phil. Trans. R. Soc. A 289 501-48

Orr W M 1900 Proc. Camb. Phil. Soc. 10 93-100

Ronveaux A 1995 Heun's Differential Equations (Oxford: Oxford University Press)

Snow C 1952 Hypergeometric and Legendre Functions with Applications to Integral Equations of Potential Theory (Applied Mathematics Series) vol 19 (Washington, DC: National Bureau of Standards)

Watson G N 1939 Q. J. Math. Oxford 10 266-76

Watson G N 1944 A Treatise on the Theory of Bessel Functions 2nd edn (Cambridge: Cambridge University Press)

Wolfram T and Callaway J 1963 Phys. Rev. 130 2207–17

Zeilberger D 1990 Discrete Math. 80 207–11