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Derivation of exact product forms for the simple cubic lattice Green function using Fourier generating functions and Lie group identities

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Abstract

The simple cubic lattice Green function

$$G(\ell_1, \ell_2, \ell_3; \alpha, w) = \frac{1}{(2\pi)^3} \times \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{\exp\left[-\mathrm{i}(\ell_1\theta_1 + \ell_2\theta_2 + \ell_3\theta_3)\right]}{w - \alpha\cos\theta_1 - \cos\theta_2 - \cos\theta_3}\, \mathrm{d}\theta_1\, \mathrm{d}\theta_2\, \mathrm{d}\theta_3$$

is investigated, where $\{\ell_1, \ell_2, \ell_3\}$ is a set of integers, $w = w_1 + \mathrm{i}w_2$ is a complex variable and α is a real parameter in the interval $(0, \infty)$. In particular, a new and direct method is used to prove that $G(2n, n, n; \alpha, w)$ and $G(n, n, n; 1, w)$ can be expressed in terms of a product of two ${}_2F_1$ hypergeometric functions, where $n = 0, 1, 2, \ldots$. In earlier work, Delves and Joyce obtained these ${}_2F_1$ product forms by solving complicated fourth-order linear differential equations of the Fuchsian type. In this paper Fourier generating functions and a known Lie group addition theorem play crucial roles in the derivation of the product forms. Many-term recurrence relations are also derived for $G(2n, n, n; \alpha, w)$ and $G(n, n, n; \alpha, w)$.

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1. Introduction

In this paper we shall consider the simple cubic lattice Green function

$$G(\ell_1, \ell_2, \ell_3; \alpha, w) = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{\exp\left[-\mathrm{i}(\ell_1\theta_1 + \ell_2\theta_2 + \ell_3\theta_3)\right]}{w - \alpha\cos\theta_1 - \cos\theta_2 - \cos\theta_3}\, \mathrm{d}\theta_1\, \mathrm{d}\theta_2\, \mathrm{d}\theta_3 \qquad (1.1)$$

where $\{\ell_1, \ell_2, \ell_3\}$ is a set of integers, $w = w_1 + \mathrm{i}w_2$ is a complex variable and α is a real nonzero parameter in the interval $(-\infty, \infty)$ (see Berlin and Kac (1952), Montroll and Potts (1955), Montroll (1956), Maradudin *et al* (1960), Katsura *et al* (1971), Joyce (1973), Delves and Joyce (2001), Kobelev and Kolomeisky (2002), Joyce *et al* (2003)). It is readily seen from (1.1) that

$$G(\ell_1, \ell_2, \ell_3; -\alpha, w) = (-1)^{\ell_1} G(\ell_1, \ell_2, \ell_3; \alpha, w). \tag{1.2}$$

We shall, therefore, restrict our attention to the case $\alpha \in (0, \infty)$. It should also be noted that $G(\ell_1, \ell_2, \ell_3; \alpha, w)$ is an *even* function of the integer variables $\{\ell_1, \ell_2, \ell_3\}$.

The triple integral (1.1) defines a single-valued analytic function $G(\ell_1, \ell_2, \ell_3; \alpha, w)$ in the complex (w_1, w_2) plane provided that a cut is made along the real axis from $w = -2 - \alpha$ to $w = 2 + \alpha$. We shall denote the set of points (w_1, w_2) in this cut plane by $\mathcal{C}^-$. For many applications in solid-state physics (Koster and Slater 1954, Wolfram and Callaway 1963, Katsura *et al* 1971) one requires the limiting behaviour of $G(\ell_1, \ell_2, \ell_3; \alpha, w)$ 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

$$G^{\pm}(\ell_1, \ell_2, \ell_3; \alpha, w_1) = \lim_{\nu \to 0+} G(\ell_1, \ell_2, \ell_3; \alpha, w_1 \pm \mathrm{i}\nu) \tag{1.3}$$

where $-2 - \alpha < w_1 < 2 + \alpha$.

Recently, Delves and Joyce (2006) have shown that the function $G(2n, n, n; \alpha, w)$ can be expressed in terms of a product of two hypergeometric functions of the type ${}_2F_1\left(\frac{1}{4}, \frac{3}{4}; n+1; \eta_\pm\right)$, where $n = 0, 1, 2, \ldots,$ and $\eta_\pm \equiv \eta_\pm(\alpha, w)$ are algebraic functions of (α, w). This product form was obtained by first proving that $wG(2n, n, n; \alpha, w)$ is a solution of a fourth-order linear differential equation of the Fuchsian type with seven regular singular points. It was then shown that any solution of this differential equation could be written in terms of a product of solutions of two second-order differential equations in normal form. Finally, Schwarzian transformation theory was used to solve the second-order differential equations in terms of ${}_2F_1$ hypergeometric functions. Similar methods have also been used by Joyce and Delves (2004) to demonstrate that $G(n, n, n; 1, w)$ can be evaluated in terms of a product of two hypergeometric functions of the type ${}_2F_1\left(\frac{1}{3}, \frac{2}{3}; n+1; \xi_\pm\right)$, where $\xi_\pm \equiv \xi_\pm(w)$ are algebraic functions of w.

Our main aim in this paper is to develop a new and direct method for deriving the ${}_2F_1$ product forms for $G(2n, n, n; \alpha, w)$ and $G(n, n, n; 1, w)$. In section 2 we shall first determine an exact formula for the Fourier generating function

$$\mathcal{F}_{2,1}(\psi, \alpha, w) = \sum_{n=-\infty}^{\infty} G(2n, n, n; \alpha, w)\Omega^n \tag{1.4}$$

where $\Omega = \exp(\mathrm{i}\psi)$. From this result we obtain the integral representation

$$G(2n, n, n; \alpha, w) = \frac{1}{\pi} \int_0^{\pi} \mathcal{F}_{2,1}(\psi, \alpha, w) \cos(n\psi)\, \mathrm{d}\psi. \tag{1.5}$$

Next a known Lie group addition theorem (Miller 1968) is used to establish a new integration formula which enables one to express (1.5) in the required ${}_2F_1$ product form. A similar procedure is used in section 3 to obtain the ${}_2F_1$ product form for $G(n, n, n; 1, w)$. Finally, in section 4 many-term recurrence relations are derived for $G(2n, n, n; \alpha, w)$ and $G(n, n, n; \alpha, w)$.

2. Results for $G(2n, n, n; \alpha, w)$

In this section we shall illustrate the new method by deriving the ${}_2F_1$ product form for $G(2n, n, n; \alpha, w)$.

2.1. Fourier generating function $\mathcal{F}_{2,1}(\psi, \alpha, w)$

We begin by defining the more general Fourier generating function

$$\mathcal{F}_{\lambda_1,\lambda_2}(\psi, \alpha, w) \equiv \sum_{n=-\infty}^{\infty} G(\lambda_1 n, \lambda_2 n, n; \alpha, w) \exp(\mathrm{i}n\psi) \tag{2.1}$$

where $\lambda_1, \lambda_2 = 0, 1, 2 \ldots,$ and λ_1, λ_2 have no common factors. Next, we introduce the Fourier series

$$f_{\lambda_1,\lambda_2}(\psi, \alpha, w; \theta_1, \theta_2) = \sum_{n=-\infty}^{\infty} \exp(\mathrm{i}n\psi) \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp(-\mathrm{i}n\theta) f_{\lambda_1,\lambda_2}(\theta, \alpha, w; \theta_1, \theta_2)\, \mathrm{d}\theta \tag{2.2}$$

where

$$f_{\lambda_1,\lambda_2}(\psi, \alpha, w; \theta_1, \theta_2) \equiv \left[w - \alpha\cos\theta_1 - \cos\theta_2 - \cos(\psi - \lambda_1\theta_1 - \lambda_2\theta_2)\right]^{-1}. \tag{2.3}$$

The integration variable in (2.2) is now changed from θ to θ_3 using the substitution $\theta = \theta_3 + \lambda_1\theta_1 + \lambda_2\theta_2$, and then both sides of (2.2) are integrated with respect to θ_1 and θ_2 from $-\pi$ to π. This procedure yields

$$\mathcal{F}_{\lambda_1,\lambda_2}(\psi, \alpha, w) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} f_{\lambda_1,\lambda_2}(\psi, \alpha, w; \theta_1, \theta_2)\, \mathrm{d}\theta_1\, \mathrm{d}\theta_2. \tag{2.4}$$

For the particular case $\lambda_1 = 2, \lambda_2 = 1$ it can be shown that $\mathcal{F}_{2,1}(\psi, \alpha, w)$ is an odd function of w which is single-valued and analytic in the w plane provided that $|w| > 2+\alpha$. In order to determine $\mathcal{F}_{2,1}(\psi, \alpha, w)$ we shall assume, at least initially, that w is real and positive with $w \in (2+\alpha, \infty)$. After performing the integration over θ_2 it is found that

$$\mathcal{F}_{2,1}(\psi, \alpha, w) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left[q_1(\psi, \alpha, w; \theta_1)\right]^{-\frac{1}{2}} \mathrm{d}\theta_1 \tag{2.5}$$

where

$$q_1(\psi, \alpha, w; \theta_1) = w^2 - 2\alpha w\cos\theta_1 + \left[\alpha^2 - 4\cos^2\left(\frac{\psi}{2}\right)\right]\cos^2\theta_1 - 8\sin\left(\frac{\psi}{2}\right)\cos\left(\frac{\psi}{2}\right)\sin\theta_1\cos\theta_1 - 4\sin^2\left(\frac{\psi}{2}\right)\sin^2\theta_1. \tag{2.6}$$

General methods for evaluating trignometric integrals of the type (2.5) have been developed by Jacobi (1969, p 195). From this work we find that

$$\mathcal{F}_{2,1}(\psi, \alpha, w) = \frac{1}{\sqrt{X_+}}\, {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{X_-}{X_+}\right) \tag{2.7}$$

where

$$X_\pm = \frac{1}{2}\left(w^2 + 4 - \alpha^2\right) \pm \frac{1}{2}\left[w^4 - 2\left(4+\alpha^2\right)w^2 + \left(16 + \alpha^4 - 8\alpha^2\cos\psi\right)\right]^{\frac{1}{2}} \tag{2.8}$$

are the solutions of the quadratic equation

$$Q(X; \psi, \alpha, w) \equiv X^2 - \left(w^2 + 4 - \alpha^2\right)X + 2\left(2w^2 - \alpha^2 + \alpha^2\cos\psi\right) = 0. \tag{2.9}$$

It should be noted that the Jacobi method usually involves solutions $\{X_j : j = 1, 2, 3\}$ of a *cubic* equation. However, for the particular integral (2.5) this cubic equation can be written in the simpler form $XQ(X; \psi, \alpha, w) = 0$.

It is possible to simplify (2.7) and extend its range of validity by applying the standard transformation formula (Erdélyi *et al* 1953, p 113, equation (34))

$${}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; z\right) = (1+z)^{-\frac{1}{2}}\, {}_2F_1\left[\frac{1}{4}, \frac{3}{4}; 1; \frac{4z}{(1+z)^2}\right]. \tag{2.10}$$

Hence, we obtain

$$w\mathcal{F}_{2,1}(\psi,\alpha,w) = \left(\frac{w^2}{w^2+4-\alpha^2}\right)^{\frac{1}{2}} {}_2F_1\left(\frac{1}{4},\frac{3}{4};1;x_4\right) \tag{2.11}$$

where

$$x_4 \equiv x_4(\psi,\alpha,w) = 8\frac{\left(2w^2-\alpha^2+\alpha^2\cos\psi\right)}{\left(w^2+4-\alpha^2\right)^2}. \tag{2.12}$$

Formula (2.11) is valid in a region $\mathcal{D}_1(\psi,\alpha)$ of the cut w plane which includes the neighbourhood $|w| > 2+\alpha$. The boundary of $\mathcal{D}_1(\psi,\alpha)$ lies inside the circle $|w| = 2+\alpha$ and consists of a point set $\mathcal{S}(\psi,\alpha)$ defined by $\{w : x_4(\psi,\alpha,w) \in (\Lambda_1,\infty)\}$, where

$$\Lambda_1 \equiv \Lambda_1(\psi,\alpha) = \mathrm{Max}\left[1, \frac{4}{4-\alpha^2\cos^2\left(\frac{\psi}{2}\right)}\right]. \tag{2.13}$$

The special points $w = \pm\sqrt{\alpha^2-4}$ are also on the boundary of $\mathcal{D}_1(\psi,\alpha)$, and are limit points of $\mathcal{S}(\psi,\alpha)$. When $w \notin \mathcal{D}_1(\psi,\alpha)$ it is necessary to replace the ${}_2F_1$ function in (2.11) by its analytic continuation on a second Riemann sheet (see Delves and Joyce (2006), p 4130).

Finally, it follows from (2.1) and (2.11) that

$$wG(2n,n,n;\alpha,w) = \left(\frac{w^2}{w^2+4-\alpha^2}\right)^{\frac{1}{2}} \times\frac{1}{\pi}\int_0^{\pi} {}_2F_1\left[\frac{1}{4},\frac{3}{4};1;8\frac{\left(2w^2-\alpha^2+\alpha^2\cos\psi\right)}{\left(w^2+4-\alpha^2\right)^2}\right]\cos(n\psi)\,\mathrm{d}\psi. \tag{2.14}$$

2.2. Lie Group addition formula given by Miller

Joyce and Delves (2004) have used raising and lowering operators to derive recursion formulae for the two Heun functions which occur in the product form for $G(n,n,n;1,w)$. It was noted that these operators can be related to the generators for the Lie algebra $\mathcal{G}(1,0)$. We shall now show that an addition formula for the Lie Group $G(1,0)$ enables one to establish an ${}_2F_1$ product form for the integral in (2.14).

In the work of Miller (1968) on the representations of the Lie group $G(1,0)$ it is proved that the ${}_2F_1$ hypergeometric function satisfies the addition formula (see Miller (1968), p 160, equation (5.15))

$$(1+b/a)^{-s}(1+ac)^{-t}(a+1)^k\phi\left[s,t;k;\frac{(c+b/a)(a+1)}{(1+b/a)(1+ac)}\right] = \sum_{j=-\infty}^{\infty} a^j\phi(s,t+j-k;j;b)\phi(s-j,t;-j+k;c) \tag{2.15}$$

where s,t are arbitrary complex numbers (not integers), k is an integer and

$$\phi(\alpha,\beta;\gamma;z) \equiv \frac{1}{\Gamma(\gamma+1)}\,{}_2F_1(\alpha,\beta;\gamma+1;z) \tag{2.16}$$

provided that $\gamma \neq -N$, where $N = 1,2,\ldots$. For the special case $\gamma = -N$ it is necessary to adopt the alternative definition (see Miller (1968), p 325, equation (A.5))

$$\phi(\alpha,\beta;-N;z) \equiv \frac{(\alpha)_N(\beta)_N}{N!}z^N{}_2F_1(N+\alpha,N+\beta;N+1;z). \tag{2.17}$$

For the purposes of this paper we substitute $s = t$ and $k = 0$ in (2.15) and make use of equations (2.16) and (2.17). Hence, we find that

$$\left(1+\frac{b}{a}\right)^{-t}(1+ac)^{-t}{}_2F_1\left[t,t;1;\frac{(c+b/a)(a+1)}{(1+b/a)(1+ac)}\right] = {}_2F_1(t,t;1;b)\,{}_2F_1(t,t;1;c) + \sum_{j=1}^{\infty}(-1)^j\left[(ac)^j+\left(\frac{b}{a}\right)^j\right] \times \frac{(t)_j(1-t)_j}{(j!)^2}\,{}_2F_1(t,j+t;j+1;b)\,{}_2F_1(t,j+t;j+1;c). \qquad (2.18)$$

Next the standard transformation (Erdélyi *et al* 1953, p 105, equation (3))

$$_2F_1(\alpha,\beta;\gamma;z) = (1-z)^{-\alpha}\,{}_2F_1[\alpha,\gamma-\beta;\gamma;z/(z-1)] \qquad (2.19)$$

is applied to all the $_2F_1$ functions in (2.18). This procedure yields the simplified result

$$_2F_1\left[t,1-t;1;-\frac{(c+b/a)(a+1)}{(1-b)(1-c)}\right] = {}_2F_1\left[t,1-t;1;\frac{b}{b-1}\right]{}_2F_1\left[t,1-t;1;\frac{c}{c-1}\right] + \sum_{j=1}^{\infty}(-1)^j\left[(ac)^j+\left(\frac{b}{a}\right)^j\right]\frac{(t)_j(1-t)_j}{(j!)^2}\,{}_2F_1\left[t,1-t;j+1;\frac{b}{b-1}\right] \times {}_2F_1\left[t,1-t;j+1;\frac{c}{c-1}\right]. \qquad (2.20)$$

We now make the substitution $a = -(b/c)^{1/2}\exp(\mathrm{i}\psi)$ in formula (2.20). Hence, we obtain

$$_2F_1\left[t,1-t;1;y(1-x)+x(1-y)+2\sqrt{xy(1-x)(1-y)}\cos\psi\right] = {}_2F_1(t,1-t;1;x)\,{}_2F_1(t,1-t;1;y) + 2\sum_{j=1}^{\infty}\frac{(t)_j(1-t)_j}{(j!)^2}\left[\frac{xy}{(1-x)(1-y)}\right]^{j/2} \times {}_2F_1(t,1-t;j+1;x)\,{}_2F_1(t,1-t;j+1;y)\cos(j\psi) \qquad (2.21)$$

where $x \equiv b/(b-1)$ and $y \equiv c/(c-1)$. Formula (2.21) is valid for arbitrary complex values of (x, y) provided that (x, y) lies in a sufficiently small neighbourhood of the origin $x = y = 0$.

It is convenient to introduce the functions

$$A \equiv A(x,y) = y(1-x)+x(1-y) \qquad (2.22)$$

$$B \equiv B(x,y) = 2\sqrt{xy(1-x)(1-y)}. \qquad (2.23)$$

By solving equations (2.22) and (2.23) we can determine the appropriate algebraic functions $x = x(A, B)$ and $y = y(A, B)$. These inverse functions enable one to express (2.21) in the useful alternative form

$$_2F_1(t,1-t;1;A+B\cos\psi) = {}_2F_1(t,1-t;1;\vartheta_+)\,{}_2F_1(t,1-t;1;\vartheta_-) + 2\sum_{j=1}^{\infty}\frac{(t)_j(1-t)_j}{(j!)^2}\left[\frac{1}{2B}\left(\sqrt{1-A-B}-\sqrt{1-A+B}\right)^2\right]^j \times {}_2F_1(t,1-t;j+1;\vartheta_+)\,{}_2F_1(t,1-t;j+1;\vartheta_-)\cos(j\psi) \qquad (2.24)$$

where

$$\vartheta_\pm \equiv \vartheta_\pm(A,B) = \frac{1}{2}\pm\frac{1}{2}\sqrt{A^2-B^2}-\frac{1}{2}\sqrt{(1-A)^2-B^2}. \qquad (2.25)$$

Finally, from the restricted Miller addition formula (2.24) we readily obtain the important result

$$
\begin{aligned}
I_n(t; A, B) &\equiv \frac{1}{\pi}\int_0^{\pi} {}_2F_1(t, 1-t; 1; A + B\cos\psi)\cos(n\psi)\,\mathrm{d}\psi \\
&= \frac{(t)_n(1-t)_n}{(n!)^2}\left[\frac{1}{2B}\left(\sqrt{1-A-B}-\sqrt{1-A+B}\right)^2\right]^n \\
&\quad\times {}_2F_1(t, 1-t; n+1; \vartheta_+)\,{}_2F_1(t, 1-t; n+1; \vartheta_-)
\end{aligned}
\tag{2.26}
$$

where $\vartheta_\pm \equiv \vartheta_\pm(A, B)$ are defined in (2.25). When $n = 0$ and $t = \frac{1}{2}$ this integral formula is in agreement with the earlier work of Iwata (1969), Rashid (1980), Montaldi (1981) and Joyce *et al* (2003). In the appendix it is shown that formula (2.26) can also be derived by *generalizing* the method first developed by Iwata (1969). The disadvantage of this alternative more routine procedure is that it does not give the deeper insight which is provided by the group-theoretic approach.

2.3. *Product form for* $G(2n, n, n; \alpha, w)$

The application of formula (2.26), with $t = \frac{1}{4}$, to the integral in (2.14) yields the required product form

$$
\begin{aligned}
wG(2n, n, n; \alpha, w) &= \left(\frac{w^2}{w^2+4-\alpha^2}\right)^{\frac{1}{2}}\frac{\left(\frac{1}{4}\right)_n\left(\frac{3}{4}\right)_n}{(n!)^2} \\
&\quad\times\left[\frac{w^2}{8\alpha}\left(\sqrt{1-\frac{(2-\alpha)^2}{w^2}}-\sqrt{1-\frac{(2+\alpha)^2}{w^2}}\right)^2\right]^{2n} \\
&\quad\times {}_2F_1\left(\frac{1}{4}, \frac{3}{4}; n+1; \eta_+\right){}_2F_1\left(\frac{1}{4}, \frac{3}{4}; n+1; \eta_-\right)
\end{aligned}
\tag{2.27}
$$

where

$$
\begin{aligned}
\eta_\pm \equiv \eta_\pm(\alpha, w) &= \frac{1}{2} + \frac{w^2}{2\left(w^2+4-\alpha^2\right)^2}\left[\pm 16\sqrt{1-\frac{\alpha^2}{w^2}}\right. \\
&\quad\left. - \left(w^2-4-\alpha^2\right)\sqrt{1-\frac{(2-\alpha)^2}{w^2}}\sqrt{1-\frac{(2+\alpha)^2}{w^2}}\right].
\end{aligned}
\tag{2.28}
$$

The region of validity $\mathcal{D}(\alpha)$ in the w plane for (2.27) has been determined by Delves and Joyce (2006, pp 4130–1) for all $\alpha \in (0, \infty)$. A detailed discussion of the analytic and asymptotic properties of (2.27) is also given in this paper.

3. Results for $G(n, n, n; \alpha, w)$

In this section we shall derive the ${}_2F_1$ product form for $G(n, n, n; 1, w)$.

3.1. *Fourier generating function* $\mathcal{F}_{1,1}(\psi, \alpha, w)$

Our main purpose in this subsection is to obtain an exact formula for the general Fourier generating function

$$
\mathcal{F}_{1,1}(\psi, \alpha, w) = \sum_{n=-\infty}^{\infty} G(n, n, n; \alpha, w)\exp(\mathrm{i}n\psi)
\tag{3.1}
$$

where $\alpha \in (0, \infty)$. From (2.4) we find that

$$\mathcal{F}_{1,1}(\psi, \alpha, w) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{1}{w - \alpha \cos\theta_1 - \cos\theta_2 - \cos(\psi - \theta_1 - \theta_2)} \, d\theta_1 \, d\theta_2. \tag{3.2}$$

In order to determine (3.2) we shall assume, at least initially, that w is real with $w \in (\Delta, \infty)$, where $\Delta > 0$ is sufficiently large. After performing the integration over θ_2 it is found that

$$\mathcal{F}_{1,1}\big(\psi, \alpha, w\big) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \big[q_2(\psi, \alpha, w; \theta_1)\big]^{-\frac{1}{2}} \, d\theta_1 \tag{3.3}$$

where

$$q_2(\psi, \alpha, w; \theta_1) = \big(w^2 - 2 + \alpha^2\big) - 2(\alpha w + \cos\psi)\cos\theta_1 - 2\sin\psi \sin\theta_1 - \alpha^2 \sin^2\theta_1. \tag{3.4}$$

Although it is possible to evaluate the integral (3.3) by applying the method of Jacobi (1969, p 195), we shall find that it is more useful to convert (3.3) into an elliptic integral by making the substitution $u = \tan(\theta_1/2)$. In this manner we obtain

$$\mathcal{F}_{1,1}(\psi, \alpha, w) = \frac{1}{\pi} \int_{-\infty}^{\infty} \big(c_0 + 4c_1 u + 6c_2 u^2 + 4c_3 u^3 + c_4 u^4\big)^{-\frac{1}{2}} \, du \tag{3.5}$$

where

$$c_0 \equiv c_0(\psi, \alpha, w) = (w - \alpha)^2 - 2(1 + \cos\psi) \tag{3.6}$$

$$c_1 \equiv c_1(\psi) = -\sin\psi \tag{3.7}$$

$$c_2 \equiv c_2(\alpha, w) = \frac{1}{3}\big(w^2 - \alpha^2 - 2\big) \tag{3.8}$$

$$c_3 \equiv c_3(\psi) = -\sin\psi \tag{3.9}$$

$$c_4 \equiv c_4(\psi, \alpha, w) = (w + \alpha)^2 - 2(1 - \cos\psi). \tag{3.10}$$

We are now able to use the work of Cayley (1889, 1895) to express (3.5) in the form

$$\mathcal{F}_{1,1}(\psi, \alpha, w) = \left[\frac{4}{3g_2}\big(1 + 14x_2 + x_2^2\big)\right]^{\frac{1}{4}} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; x_2\right). \tag{3.11}$$

In this formula $x_2 \equiv x_2(\psi, \alpha, w)$ is the appropriate solution of the sextic equation

$$\frac{108x(1 - x)^4}{\big(1 + 14x + x^2\big)^3} = \frac{1}{J} \tag{3.12}$$

where

$$J \equiv J(\psi, \alpha, w) = \frac{g_2^3}{g_2^3 - 27g_3^2} \tag{3.13}$$

and

$$g_2 \equiv g_2(\psi, \alpha, w) = c_0 c_4 - 4c_1 c_3 + 3c_2^2 \tag{3.14}$$

$$g_3 \equiv g_3(\psi, \alpha, w) = c_0 c_2 c_4 - c_0 c_3^2 - c_1^2 c_4 - c_2^3 + 2c_1 c_2 c_3. \tag{3.15}$$

The required solution x_2 of equation (3.12) has a Taylor series representation about $w = \infty$ which is given by

$$x_2 \equiv x_2(\psi, \alpha, w) = \frac{\alpha^2}{4w^6} \sum_{j=0}^{\infty} \frac{d_j(\psi, \alpha)}{(\alpha w)^j} \tag{3.16}$$

where $d_0(\psi, \alpha) = 1$,

$$d_1(\psi, \alpha) = (2\alpha^2 + 1)\cos\psi \tag{3.17}$$

$$d_2(\psi, \alpha) = \frac{1}{4}\Big[(18\alpha^4 + 32\alpha^2 + 1) + 2\alpha^2(\alpha^2 + 2)\cos(2\psi)\Big]. \tag{3.18}$$

Cayley (1889, 1895) has proved that the other solutions of equation (3.12) are $1/x_2$ and

$$\left\{\left(\frac{1 - \mathrm{i}^k x_2^{\frac{1}{4}}}{1 + \mathrm{i}^k x_2^{\frac{1}{4}}}\right)^4 : k = 0, 1, 2, 3\right\}. \tag{3.19}$$

We see, therefore, that $x_2 \equiv x_2(\psi, \alpha, w)$ is the *only* solution which tends to zero as $w \to \infty$.

The problem of deriving an explicit closed-form expression for x_2 can be avoided by applying the transformation formula (Goursat 1881, p S.142, equation (136))

$${}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; x\right) = (1 + 14x + x^2)^{-\frac{1}{4}}\, {}_2F_1\left[\frac{1}{12}, \frac{5}{12}; 1; \frac{108x(1-x)^4}{(1 + 14x + x^2)^3}\right] \tag{3.20}$$

to the ${}_2F_1$ function in (3.11). Hence, we obtain the much simplified result

$$w\mathcal{F}_{1,1}(\psi, \alpha, w) = \left(\frac{4w^4}{3g_2}\right)^{\frac{1}{4}} {}_2F_1\left(\frac{1}{12}, \frac{5}{12}; 1; \frac{1}{J}\right) \tag{3.21}$$

where

$$g_2 = \frac{4}{3}\left[w^4 - 2(\alpha^2 + 2)w^2 + (\alpha^2 - 1)^2 - 6\alpha w\cos\psi\right] \tag{3.22}$$

$$\begin{aligned} J = {} & \frac{8}{27}(w + \alpha\cos\psi)^{-2}\left[w^4 - 2(\alpha^2 + 2)w^2 + (\alpha^2 - 1)^2 - 6\alpha w\cos\psi\right]^3 \\ & \times \Big[8\alpha^2 w^4 + 8\alpha w^3\cos\psi - 2(8\alpha^4 + 20\alpha^2 - 1)w^2 - 36\alpha w(2\alpha^2 + 1)\cos\psi \\ & + (8\alpha^6 - 24\alpha^4 - 3\alpha^2 - 8) - 27\alpha^2\cos(2\psi)\Big]^{-1}. \end{aligned} \tag{3.23}$$

When the variable x is real the Goursat transformation (3.20) is valid provided that $-\frac{1}{4}(\sqrt{3} - 1)^4 < x \leqslant (\sqrt{2} - 1)^4$. It is clear from (3.16) that x_2 will always satisfy this restrictive condition when $w \in (\Delta, \infty)$, where $\Delta > 0$ is sufficiently large.

A more detailed analysis shows that the final result (3.21) is, in fact, valid in a region $\mathcal{D}_2(\psi, \alpha)$ of the cut w plane which includes a neighbourhood of the point $w = \infty$. The boundary of $\mathcal{D}_2(\psi, \alpha)$ consists of a point set defined by $\{w : [J(\psi, \alpha, w)]^{-1} \in [1, \infty)\}$. When $w \notin \mathcal{D}_2(\psi, \alpha)$ it is necessary to replace the ${}_2F_1$ function in (3.21) by its analytic continuation on a second Riemann sheet. We can construct this analytic continuation by first applying the transformation formula (Erdélyi *et al* 1953, p 111, equation (10))

$${}_2F_1\left(a, b; a + b + \frac{1}{2}; z\right) = {}_2F_1\left(2a, 2b; a + b + \frac{1}{2}; \frac{1}{2} - \frac{1}{2}\sqrt{1 - z}\right) \tag{3.24}$$

to (3.21). Hence, we find that

$$w\mathcal{F}_{1,1}(\psi, \alpha, w) = \left(\frac{4w^4}{3g_2}\right)^{\frac{1}{4}} {}_2F_1\left(\frac{1}{6}, \frac{5}{6}; 1; \frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{1}{J}}\right) \tag{3.25}$$

where $g_2 \equiv g_2(\psi, \alpha, w)$ and $J \equiv J(\psi, \alpha, w)$ are defined in (3.22) and (3.23), respectively. This formula is valid for all $w \in \mathcal{D}_2(\psi, \alpha)$. The analytic continuation of $w\mathcal{F}_{1,1}$ on the second Riemann sheet can now be obtained by simply changing the *sign* of the square root in (3.25).

3.2. Product form for $G(n, n, n; 1, w)$

In order to investigate the existence of an ${}_2F_1$ product form for $G(n, n, n; \alpha, w)$ we shall now consider the further transformation formula (Goursat 1881, p S.140, equation (126))

$$ {}_2F_1\left[\frac{1}{12}, \frac{5}{12}; 1; \frac{64x^3(1-x)}{(9-8x)^3}\right] = \left(1 - \frac{8x}{9}\right)^{\frac{1}{4}} {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; x\right). \tag{3.26} $$

This formula is valid when $|x| \leqslant \frac{3}{4}(3 - \sqrt{3})$. If we apply (3.26) to the ${}_2F_1$ function in (3.21) it is found that

$$ w\mathcal{F}_{1,1}(\psi, \alpha, w) = \left[\frac{4w^4}{3g_2}\left(1 - \frac{8x_3}{9}\right)\right]^{\frac{1}{4}} {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; x_3\right) \tag{3.27} $$

where $x_3 \equiv x_3(\psi, \alpha, w)$ is a solution of the quartic equation

$$ \frac{64x^3(1-x)}{(9-8x)^3} = \frac{1}{J} \tag{3.28} $$

which tends to zero as $w \to \infty$.

The four solutions of equation (3.28) are expressible in the closed-form

$$ x_\pm^{(1)} = \left\{1 + \frac{J^{\frac{1}{3}}}{9}\left[\pm\sqrt{1 - \frac{1}{J^{\frac{1}{3}}}} + \sqrt{2\sqrt{1 + \frac{1}{J^{\frac{1}{3}}} + \frac{1}{J^{\frac{2}{3}}}} - \left(1 + \frac{2}{J^{\frac{1}{3}}}\right)}\,\right]^2\right\}^{-1} \tag{3.29} $$

$$ x_\pm^{(2)} = \left\{1 - \frac{J^{\frac{1}{3}}}{9}\left[\pm\mathrm{i}\sqrt{1 - \frac{1}{J^{\frac{1}{3}}}} + \sqrt{2\sqrt{1 + \frac{1}{J^{\frac{1}{3}}} + \frac{1}{J^{\frac{2}{3}}}} + \left(1 + \frac{2}{J^{\frac{1}{3}}}\right)}\,\right]^2\right\}^{-1} \tag{3.30} $$

where $J \equiv J(\psi, \alpha, w)$ is defined in (3.23). It follows from (3.29) and (3.30) that $x_+^{(1)}$ and $x_\pm^{(2)}$ all tend to zero as $w \to \infty$. We can, therefore, take any one of these solutions as the required solution x_3. However, it is particularly instructive to associate x_3 with $x_+^{(1)}$. We find that the solution $x_+^{(1)}$ has a Taylor series representation about $w = \infty$ which is given by

$$ x_+^{(1)} \equiv x_3(\psi, \alpha, w) = \frac{27\alpha^{\frac{2}{3}}}{4w^2}\left[1 + \frac{1}{3\alpha w}(2\alpha^2 + 1)\cos\psi + \sum_{k=2}^{\infty} \frac{e_k(\psi, \alpha)}{w^k}\right] \tag{3.31} $$

where the coefficient $e_k(\psi, \alpha)$ is a function of ψ and α.

For general values of $\alpha \in (0, \infty)$ it is evident from (3.23) and (3.29) that x_3 is a complicated function of (ψ, α, w) which cannot be reduced to the restricted Miller form $A + B\cos\psi$. However, for the special case $\alpha = 1$ the quartic equation (3.28), with $J \equiv J(\psi, 1, w)$, is expressible in terms of a product of two polynomials of degrees 1 and 3 in the variable x. The linear factor yields the simple result

$$ x_3 \equiv x_3(\psi, 1, w) = \frac{27}{4w^3}(w + \cos\psi). \tag{3.32} $$

We see from (3.32) that the coefficients $\{e_k(\psi, \alpha) : k = 2, 3, \ldots\}$ in expansion (3.31) must all be zero when $\alpha = 1$. If equation (3.32) is substituted in (3.27) we obtain the important result

$$ w\mathcal{F}_{1,1}(\psi, 1, w) = {}_2F_1\left[\frac{1}{3}, \frac{2}{3}; 1; \frac{27}{4w^3}(w + \cos\psi)\right]. \tag{3.33} $$

Formula (3.33) is valid in a region $\mathcal{D}_3(\psi)$ of the cut w plane which includes the neighbourhood $|w| > 3$. The boundary of $\mathcal{D}_3(\psi)$ lies inside the circle $|w| = 3$ and consists of the point set $\{w : x_3(\psi, 1, w) \in (\Lambda_3, \infty)\}$, where

$$\Lambda_3 \equiv \Lambda_3(\psi) = \mathrm{Max}\left[1, \frac{1}{\cos^2\psi}\right]. \tag{3.34}$$

For the special case $\psi = \frac{\pi}{2}$ formula (3.33) is valid throughout the w plane provided that a cut is made along the real axis from $w = -\frac{3\sqrt{3}}{2}$ to $w = \frac{3\sqrt{3}}{2}$.

It follows from (3.1) and (3.33) that

$$wG(n, n, n; 1, w) = \frac{1}{\pi}\int_0^\pi {}_2F_1\left[\frac{1}{3}, \frac{2}{3}; 1; \frac{27}{4w^3}(w + \cos\psi)\right]\cos(n\psi)\,\mathrm{d}\psi. \tag{3.35}$$

We now apply (2.26) with $t = \frac{1}{3}$ to the integral in (3.35). This procedure leads to the required product form

$$wG(n, n, n; 1, w) = \frac{\left(\frac{1}{3}\right)_n\left(\frac{2}{3}\right)_n}{(n!)^2}\left[\frac{w}{3}\left(1 - \sqrt{1 - \frac{9}{w^2}}\right)\right]^{3n} {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; n+1; \xi_+\right)$$
$$\times\, {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; n+1; \xi_-\right) \tag{3.36}$$

where

$$\xi_\pm \equiv \xi_\pm(w) = \frac{1}{8w^2}\left[4w^2 + \left(9 - 4w^2\right)\sqrt{1 - \frac{9}{w^2}} \pm 27\sqrt{1 - \frac{1}{w^2}}\right]. \tag{3.37}$$

The region of validity $\mathcal{D}_4$ in the w plane for (3.36) has been determined by Joyce and Delves (2004, p 3664). A detailed discussion of the analytic and asymptotic properties of (3.36) is also given in this paper.

Finally, we note that formula (2.11) for $w\mathcal{F}_{2,1}(\psi, \alpha, w)$ can also be established by applying the method of Cayley (1889, 1895) to the integral (2.5). This alternative procedure involves the transformation (Goursat 1881, p S.138, equation (118))

$${}_2F_1\left[\frac{1}{12}, \frac{5}{12}; 1; \frac{27x^2(1-x)}{(4-3x)^3}\right] = \left(1 - \frac{3x}{4}\right)^{\frac{1}{4}} {}_2F_1\left(\frac{1}{4}, \frac{3}{4}; 1; x\right). \tag{3.38}$$

4. Recurrence relations

In this last section we shall use the Fourier generating functions to derive recurrence relations for $G(2n, n, n; \alpha, w)$ and $G(n, n, n; \alpha, w)$.

4.1. Recurrence relation for $G(2n, n, n; \alpha, w)$

In the first stage of the analysis we write the Fourier generating function (2.11) in the form

$$w\mathcal{F}_{2,1} = \left(\frac{w^2}{w^2 + 4 - \alpha^2}\right)^{\frac{1}{2}} {}_2F_1\left(\frac{1}{4}, \frac{3}{4}; 1; z\right) \tag{4.1}$$

where

$$z = \frac{4\left[2\left(2w^2 - \alpha^2\right) + \alpha^2\left(\Omega + \Omega^{-1}\right)\right]}{\left(w^2 + 4 - \alpha^2\right)^2} \tag{4.2}$$

and $\Omega = \exp(\mathrm{i}\psi)$. We can now use this formula and the standard hypergeometric differential equation (Erdélyi *et al* 1953, p 56, equation (1)) to show that

$$P_0(\alpha, w; \Omega)\frac{\partial^2 \mathcal{F}_{2,1}}{\partial\Omega^2} + P_1(\alpha, w; \Omega)\frac{\partial \mathcal{F}_{2,1}}{\partial\Omega} + P_2(\alpha, w; \Omega)\mathcal{F}_{2,1} = 0 \tag{4.3}$$

where

$$\begin{aligned} P_0(\alpha, w; \Omega) &= 4\Omega^2(\Omega^2 - 1)\left[\alpha^2\Omega^2 + 2(2w^2 - \alpha^2)\Omega + \alpha^2\right] \\ &\quad \times \left\{4\alpha^2\Omega^2 - \left[w^4 - 2w^2(\alpha^2 + 4) + (\alpha^4 + 16)\right]\Omega + 4\alpha^2\right\} \end{aligned} \tag{4.4}$$

$$\begin{aligned} P_1(\alpha, w; \Omega) &= 4\Omega^2\Big\{8\alpha^4\Omega^5 - \alpha^2(w^2 + 4w - \alpha^2 - 4)(w^2 - 4w - \alpha^2 - 4) \\ &\quad \times (\Omega^4 - 4\Omega^2 - 1) - 16\alpha^4\Omega^3 + 4\Big[2w^6 - (5\alpha^2 + 16)w^4 \\ &\quad + 4(\alpha^4 + 2\alpha^2 + 8)w^2 - \alpha^2(\alpha^4 + 6\alpha^2 + 16)\Big]\Omega\Big\} \end{aligned} \tag{4.5}$$

$$P_2(\alpha, w; \Omega) = 3\alpha^4(\Omega^2 - 1)^3. \tag{4.6}$$

Next we substitute the generating function series (1.4) in the differential equation (4.3). In this manner we obtain the following seven-term recurrence relation:

$$\begin{aligned} &\alpha^4(4n + 9)(4n + 11)G^{(1)}_{n+3} - \alpha^4(4n - 9)(4n - 11)G^{(1)}_{n-3} \\ &\quad - 4\alpha^2(w^2 + 4w - \alpha^2 - 4)(w^2 - 4w - \alpha^2 - 4) \\ &\quad \times \left[(n + 2)^2G^{(1)}_{n+2} + 4nG^{(1)}_n - (n - 2)^2G^{(1)}_{n-2}\right] \\ &\quad - 8w^2\left[2w^4 - (5\alpha^2 + 16)w^2 + 4(\alpha^4 + 2\alpha^2 + 8)\right] \\ &\quad \times \left[(n + 1)(n + 2)G^{(1)}_{n+1} - (n - 1)(n - 2)G^{(1)}_{n-1}\right] \\ &\quad + \alpha^2\left[8(\alpha^4 + 2\alpha^2 + 16)n^2 + (16\alpha^4 + 87\alpha^2 + 256)\right]\left(G^{(1)}_{n+1} - G^{(1)}_{n-1}\right) \\ &\quad + 8\alpha^2n(3\alpha^4 + 14\alpha^2 + 48)\left(G^{(1)}_{n+1} + G^{(1)}_{n-1}\right) = 0 \end{aligned} \tag{4.7}$$

where $G^{(1)}_n \equiv G(2n, n, n; \alpha, w)$ and $n = 0, \pm1, \pm2, \ldots$. Delves and Joyce (2006, p 4143) have also given a five-term relation for $G^{(1)}_n$ which was derived by extending the methods developed by Iwata (1979). This shorter relation is of degree 3 in the variable n.

4.2. Recurrence relation for $G(n, n, n; \alpha, w)$

We can derive a recurrence relation for the diagonal Green function $G(n, n, n; \alpha, w)$ by applying the method described in the previous subsection to the Fourier generating function (3.21). A complicated calculation eventually leads to the following eleven-term relation:

$$\begin{aligned} &9\alpha^4w\left[81n\left(G^{(2)}_{n+5} + G^{(2)}_{n-5}\right) + (9n^2 + 182)\left(G^{(2)}_{n+5} - G^{(2)}_{n-5}\right)\right] \\ &\quad - 12\alpha^3n\left[16w^4 - 9(22\alpha^2 + 23)w^2 + 54(\alpha^2 - 1)^2\right]\left(G^{(2)}_{n+4} + G^{(2)}_{n-4}\right) \\ &\quad - 12\alpha^3\Big\{n^2\left[2w^4 - 27(\alpha^2 + 1)w^2 + 9(\alpha^2 - 1)^2\right] \end{aligned}$$

$$
\begin{aligned}
&+\Big[32w^4-2\big(182\alpha^2+199\big)w^2+77\big(\alpha^2-1\big)^2\Big]\Big\}\big(G_{n+4}^{(2)}-G_{n-4}^{(2)}\big)\\
&-\alpha^2wn\Big[16\big(31\alpha^2+26\big)w^4-8\big(284\alpha^4+863\alpha^2+311\big)w^2\\
&+3\big(592\alpha^6-696\alpha^4-951\alpha^2+488\big)\Big]\big(G_{n+3}^{(2)}+G_{n-3}^{(2)}\big)\\
&-\alpha^2w\Big\{n^2\Big[16\big(5\alpha^2+4\big)w^4-8\big(52\alpha^4+139\alpha^2+52\big)w^2\\
&+3\big(112\alpha^6-120\alpha^4-177\alpha^2+104\big)\Big]+6\Big[16\big(8\alpha^2+7\big)w^4\\
&-8\big(65\alpha^4+223\alpha^2+78\big)w^2+\big(392\alpha^6-508\alpha^4-643\alpha^2+276\big)\Big]\Big\}\\
&\times\big(G_{n+3}^{(2)}-G_{n-3}^{(2)}\big)-16\alpha n\Big[4\big(4\alpha^4+15\alpha^2+2\big)w^6\\
&-\big(48\alpha^6+296\alpha^4+326\alpha^2+41\big)w^4+3\big(16\alpha^8+52\alpha^6-225\alpha^4-13\alpha^2+8\big)w^2\\
&-\big(\alpha^2-1\big)^2\big(16\alpha^6-48\alpha^4-33\alpha^2-16\big)\Big]\big(G_{n+2}^{(2)}+G_{n-2}^{(2)}\big)\\
&-8\alpha\Big\{n^2\Big[4\big(2\alpha^4+6\alpha^2+1\big)w^6-2\big(12\alpha^6+68\alpha^4+68\alpha^2+11\big)w^4\\
&+3\big(8\alpha^8+24\alpha^6-93\alpha^4+\alpha^2+6\big)w^2-\big(\alpha^2-1\big)^2\big(8\alpha^6-24\alpha^4-3\alpha^2-8\big)\Big]\\
&+\Big[16\big(2\alpha^4+9\alpha^2+1\big)w^6-4\big(24\alpha^6+160\alpha^4+190\alpha^2+19\big)w^4\\
&+6\big(16\alpha^8+56\alpha^6-262\alpha^4-27\alpha^2+4\big)w^2\\
&-\big(\alpha^2-1\big)^2\big(32\alpha^6-96\alpha^4-105\alpha^2-32\big)\Big]\Big\}\big(G_{n+2}^{(2)}-G_{n-2}^{(2)}\big)\\
&-2wn\Big[96\alpha^2\big(2\alpha^2+1\big)w^6-8\big(72\alpha^6+67\alpha^4+56\alpha^2-3\big)w^4\\
&+4\big(144\alpha^8-412\alpha^6-1129\alpha^4-25\alpha^2-36\big)w^2\\
&-3\big(64\alpha^{10}-696\alpha^8+1012\alpha^6-13\alpha^4-60\alpha^2-64\big)\Big]\big(G_{n+1}^{(2)}+G_{n-1}^{(2)}\big)\\
&-2w\Big\{n^2\Big[32\alpha^2\big(2\alpha^2+1\big)w^6-8\big(24\alpha^6+27\alpha^4+22\alpha^2-1\big)w^4\\
&+4\big(48\alpha^8-76\alpha^6-247\alpha^4+44\alpha^2-12\big)w^2\\
&-\big(64\alpha^{10}-488\alpha^8+820\alpha^6-415\alpha^4+164\alpha^2-64\big)\Big]\\
&+2\Big[32\alpha^2\big(2\alpha^2+1\big)w^6-8\big(24\alpha^6+20\alpha^4+17\alpha^2-1\big)w^4\\
&+12\big(16\alpha^8-53\alpha^6-147\alpha^4-10\alpha^2-4\big)w^2\\
&-\big(64\alpha^{10}-764\alpha^8+1090\alpha^6+107\alpha^4-118\alpha^2-64\big)\Big]\Big\}\big(G_{n+1}^{(2)}-G_{n-1}^{(2)}\big)\\
&-8\alpha n\Big[16\big(\alpha^2+1\big)\big(2\alpha^2+1\big)w^6-4\big(24\alpha^6+112\alpha^4+76\alpha^2+25\big)w^4\\
&+3\big(32\alpha^8+80\alpha^6-342\alpha^4-53\alpha^2+40\big)w^2\\
&-2\big(\alpha^2-1\big)^2\big(16\alpha^6-48\alpha^4-33\alpha^2-16\big)\Big]G_n^{(2)}=0
\end{aligned}
\tag{4.8}
$$

where $G_n^{(2)} \equiv G(n,n,n;\alpha,w)$ and $n = 0, \pm 1, \pm 2, \ldots$.

The recurrence relation (4.8) has been used to investigate the detailed asymptotic behaviour of $G(n,n,n;\alpha,w)$ as $n \to \infty$. We hope to discuss this application in a future publication.

Appendix. Alternative evaluation of the integral $I_n(t; A, B)$

In this appendix we shall evaluate the integral

$$I_n(t;\, A,\, B) \equiv \frac{1}{\pi}\int_0^{\pi} {}_2F_1(t,\, 1-t;\, 1;\, A + B\cos\psi)\cos(n\psi)\,\mathrm{d}\psi \tag{A.1}$$

by generalizing the method of Iwata (1969). In the first stage of the analysis we apply the Gaussian hypergeometric series to the ${}_2F_1$ function in (A.1) and then integrate term by term. This procedure gives

$$I_n(t;\, A,\, B) = \sum_{m=0}^{\infty} \frac{(t)_m(1-t)_m}{(m!)^2}\,\Xi_{n,m}(A,\, B) \tag{A.2}$$

where

$$\Xi_{n,m}(A,\, B) \equiv \frac{1}{\pi}\int_0^{\pi} (A + B\cos\psi)^m \cos(n\psi)\,\mathrm{d}\psi. \tag{A.3}$$

We shall assume that $|A|$ and $|B|$ are sufficiently small to ensure the convergence of the series (A.2).

Next the integral (A.3) is expressed in the alternative form

$$\Xi_{n,m}(A,\, B) \equiv \frac{y_+^m}{2\pi}\int_0^{2\pi} [1 + \rho\exp(\mathrm{i}\psi)]^m[1 + \rho\exp(-\mathrm{i}\psi)]^m \cos(n\psi)\,\mathrm{d}\psi \tag{A.4}$$

where $\rho = (y_-/y_+)^{1/2}$ and

$$y_\pm \equiv y_\pm(A,\, B) = \frac{1}{2}\left(A \pm \sqrt{A^2 - B^2}\right). \tag{A.5}$$

The integral (A.4) can be readily evaluated using the method of residues. Hence, we find that

$$\Xi_{n,m}(A,\, B) = \rho^n y_+^m \sum_{j=0}^{m-n} \binom{m}{j}\binom{m}{n+j}\rho^{2j}. \tag{A.6}$$

We now substitute (A.6) in (A.2) and interchange the order of the two summations. After some algebraic simplifications we eventually obtain

$$I_n(t;\, A,\, B) = \frac{(t)_n(1-t)_n}{(n!)^2}(y_+y_-)^{n/2}F_4(n+t,\, n+1-t;\, n+1,\, n+1;\, y_+,\, y_-) \tag{A.7}$$

where $F_4(\alpha,\, \beta;\, \gamma,\, \gamma';\, x,\, y)$ is an Appell hypergeometric series of two variables (see Erdélyi *et al* (1953), p 224). From the work of Bailey (1933, 1934) it is known that

$$F_4[\alpha,\, \beta;\, \gamma,\, \alpha+\beta-\gamma+1;\, x(1-y),\, y(1-x)] = {}_2F_1(\alpha,\, \beta;\, \gamma;\, x)\, {}_2F_1(\alpha,\, \beta;\, \alpha+\beta-\gamma+1;\, y). \tag{A.8}$$

This result is valid inside simply-connected regions surrounding $x = 0$, $y = 0$, for which

$$|x(1-y)|^{\frac{1}{2}} + |y(1-x)|^{\frac{1}{2}} < 1. \tag{A.9}$$

The application of (A.8) to the F_4 series in (A.7) leads to the product form

$$I_n(t;\, A,\, B) = \frac{(t)_n(1-t)_n}{(n!)^2}(y_+y_-)^{n/2}\, {}_2F_1(n+t,\, n+1-t;\, n+1;\, \vartheta_+) \times {}_2F_1(n+t,\, n+1-t;\, n+1;\, \vartheta_-) \tag{A.10}$$

where $\vartheta_\pm \equiv \vartheta_\pm(A,\, B)$ are defined in (2.25).

Finally, we use the standard formula (Erdélyi *et al* 1953, p 105, equation (2))

$${}_2F_1(n+t,\, n+1-t;\, n+1;\, \vartheta) = (1-\vartheta)^{-n}\, {}_2F_1(t,\, 1-t;\, n+1;\, \vartheta) \tag{A.11}$$

to write (A.10) in the required form

$$I_n(t;A,B) = \frac{(t)_n(1-t)_n}{(n!)^2}\left[\frac{1}{2B}\left(\sqrt{1-A-B}-\sqrt{1-A+B}\right)^2\right]^n \times {}_2F_1(t,1-t;n+1;\vartheta_+)\,{}_2F_1(t,1-t;n+1;\vartheta_-). \tag{A.12}$$

This result is in agreement with (2.26) which was derived from the Lie group addition formula (2.15).

The evaluation of $I_n(t;A,B)$ can be simplified when $B=A$. For this special case, we find that

$$\Xi_{n,m}(A,A) = \frac{(2m)!}{(n+m)!(m-n)!}\left(\frac{A}{2}\right)^m \tag{A.13}$$

and (A.7) reduces to

$$I_n(t;A,A) = \frac{(t)_n(1-t)_n}{(n!)^2}\left(\frac{A}{2}\right)^n {}_3F_2\left(n+t,n+1-t,n+\frac{1}{2};n+1,2n+1;2A\right). \tag{A.14}$$

We can now use the theorem of Clausen (1828)

$${}_3F_2\left(2\alpha,2\beta,\alpha+\beta;\alpha+\beta+\frac{1}{2},2\alpha+2\beta;z\right) = \left[{}_2F_1\left(\alpha,\beta;\alpha+\beta+\frac{1}{2};z\right)\right]^2 \tag{A.15}$$

to write (A.14) in the form

$$I_n(t;A,A) = \frac{(t)_n(1-t)_n}{(n!)^2}\left(\frac{A}{2}\right)^n \left\{{}_2F_1\left[\frac{1}{2}(n+t),\frac{1}{2}(n+1-t);n+1;2A\right]\right\}^2. \tag{A.16}$$

The application of the transformation formula (3.24) to the ${}_2F_1$ in (A.16) gives

$$I_n(t;A,A) = \frac{(t)_n(1-t)_n}{(n!)^2}\left(\frac{A}{2}\right)^n \left[{}_2F_1\left(n+t,n+1-t;n+1;\frac{1}{2}-\frac{1}{2}\sqrt{1-2A}\right)\right]^2. \tag{A.17}$$

This result is in agreement with (A.10) when $B=A$.

Finally, we note that this alternative method can also be used for the case $B=-A$ because

$$\Xi_{n,m}(A,-A) = (-1)^n\,\Xi_{n,m}(A,A). \tag{A.18}$$

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