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Exact evaluation of the Green functions for the anisotropic face-centred and simple cubic lattices

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Abstract

The analytic properties of the lattice Green functions

$$G_1(\alpha_1, w_1) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{\mathrm{d}\theta_1\,\mathrm{d}\theta_2\,\mathrm{d}\theta_3}{w_1 - \cos\theta_1\cos\theta_2 - \cos\theta_2\cos\theta_3 - \alpha_1\cos\theta_3\cos\theta_1}$$

and

$$G_2(\alpha_2, w_2) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{\mathrm{d}\theta_1\,\mathrm{d}\theta_2\,\mathrm{d}\theta_3}{w_2 - \cos\theta_1 - \cos\theta_2 - \alpha_2\cos\theta_3}$$

are investigated, where w_1, w_2 are complex variables and α_1, α_2 are real parameters in the interval $(0, \infty)$. In particular, simple and direct methods are developed which enable one to evaluate $G_1(\alpha_1, w_1)$ and $G_2(\alpha_2, w_2)$ in terms of products of two complete elliptic integrals of the first kind. Kampé de Fériet series are also used to derive new transformation formulae which give connections between $G_1(\alpha_1, w_1)$ and $G_2(\alpha_2, w_2)$.

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1. Introduction

In this paper we shall investigate the analytic properties of the lattice Green functions

$$G_j(\alpha_j, w_j) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{\mathrm{d}\theta_1\,\mathrm{d}\theta_2\,\mathrm{d}\theta_3}{w_j - \Theta_j(\alpha_j : \theta_1, \theta_2, \theta_3)} \qquad (j = 1, 2) \tag{1.1}$$

where w_1, w_2 are complex variables,

$$\Theta_1(\alpha_1 : \theta_1, \theta_2, \theta_3) = \cos\theta_1\cos\theta_2 + \cos\theta_2\cos\theta_3 + \alpha_1\cos\theta_3\cos\theta_1 \tag{1.2}$$

$$\Theta_2(\alpha_2 : \theta_1, \theta_2, \theta_3) = \cos\theta_1 + \cos\theta_2 + \alpha_2\cos\theta_3 \tag{1.3}$$

and α_1, α_2 are real parameters in the interval $(0, \infty)$. The Green function $G_1(\alpha_1, w_1)$ is frequently encountered in lattice statistical problems which involve the face-centred cubic (fcc) lattice with partially anisotropic interactions, while $G_2(\alpha_2, w_2)$ is important in similar problems involving the simple cubic (sc) lattice (Berlin and Kac 1952, Maradudin *et al* 1960, Montroll and Weiss 1965, Joyce 1972a, Kobelev and Kolomeisky 2002).

The integral (1.1) with $j = 1$ defines a single-valued analytic function $G_1(\alpha_1, w_1)$ in the w_1 complex plane provided that a cut is made along the real axis from $w_1 = \min(-\alpha_1, -2+\alpha_1)$ to $w_1 = 2+\alpha_1$. A similar property holds for the integral (1.1) with $j = 2$ provided that the cut is made along the real axis of the w_2 plane from $w_2 = -2-\alpha_2$ to $w_2 = 2+\alpha_2$. We shall denote the set of points in the w_1 and w_2 cut planes by $\mathcal{C}_1^-$ and $\mathcal{C}_2^-$, respectively. Taylor series representations for $\{G_j(\alpha_j, w_j) : j = 1, 2\}$ can be obtained by expanding the integrand in (1.1) in inverse powers of w_j and then integrating term-by-term. Hence, we find that

$$w_j G_j(\alpha_j, w_j) = 1 + \sum_{n=2}^{\infty} \frac{\mu_n^{(j)}(\alpha_j)}{w_j^n} \tag{1.4}$$

where $|w_j| \geqslant 2+\alpha_j$,

$$\mu_n^{(j)}(\alpha_j) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi [\Theta_j(\alpha_j : \theta_1, \theta_2, \theta_3)]^n \,\mathrm{d}\theta_1\,\mathrm{d}\theta_2\,\mathrm{d}\theta_3 \tag{1.5}$$

and $j = 1, 2$. In the appendix we list formulae for $\left\{\mu_n^{(1)}(\alpha_1) : n = 2, 3, \ldots, 10\right\}$. It has also been shown (Delves and Joyce 2001) that

$$\mu_{2n}^{(2)}(\alpha_2) = \frac{\left(\frac{1}{2}\right)_n}{n!}\alpha_2^{2n}\,{}_3F_2\left[\begin{matrix}-n, & -n, & \frac{1}{2}; & \\ & & & 4\big/\alpha_2^2\\ 1, & 1; & & \end{matrix}\right] \tag{1.6}$$

where $(b)_n$ is the Pochhammer symbol and ${}_3F_2$ is a generalized hypergeometric series. We note that $\mu_n^{(2)}(\alpha_2)$ is equal to zero when n is an odd positive integer.

The Green function $G_1(\alpha_1, w_1)$ was first evaluated by Joyce (1971) in terms of a product of two complete elliptic integrals of the first kind. In section 2 of the present paper we shall derive the Joyce product form by following an *alternative* procedure in which the triple integral for $G_1(\alpha_1, w_1)$ is first reduced to a single integral of the type

$$I(A, B) \equiv \frac{2}{\pi^2}\int_0^\pi K\left(\sqrt{A + B\cos\psi}\right)\mathrm{d}\psi \tag{1.7}$$

where A, B are complex variables and $K(k)$ is a complete elliptic integral of the first kind with a modulus k. The required product form for $G_1(\alpha_1, w_1)$ is then obtained by applying the method of Iwata (1969) to (1.7). In section 3 we shall show that $I(A, B)$ can be represented as a Kampé de Fériet series of the type $F_{1:0;1}^{2:0;1}$ (see Srivastava and Karlsson 1985). Two further Kampé de Fériet representations for $I(A, B)$ of the type $F_{1:0;1}^{1:1;2}$ and $F_{1:1;1}^{3:0;0}$ are also obtained by applying transformation formulae to the $F_{1:0;1}^{2:0;1}$ series. We shall find in section 4 that these series representations for $I(A, B)$ play a crucial role in the evaluation of $G_2(\alpha_2, w_2)$.

Recently, Delves and Joyce (2001) have carried out a detailed investigation of the analytic properties of the Green function $G_2(\alpha_2, w_2)$. In particular, it was shown that the function $y \equiv w_2 G_2(\alpha_2, w_2)$ is a solution of a fourth-order linear differential equation of the type

$$\sum_{j=0}^{4} f_j(\alpha_2, z)\mathrm{D}^{4-j} y = 0 \tag{1.8}$$

where $\{f_j(\alpha_2, z) : j = 0, 1, \ldots, 4\}$ is a set of polynomials in the variables α_2 and z, $\mathrm{D} \equiv \mathrm{d}/\mathrm{d}z$ and $z = 1\big/w_2^2$. It was then proved that all the solutions of this differential equation can be expressed in terms of a product of two functions $H_1(\alpha_2, z)$ and $H_2(\alpha_2, z)$ which satisfy second-order linear differential equations of the normal type

$$[\mathrm{D}^2 + U_+(\alpha_2, z)]y = 0 \tag{1.9}$$

$$[\mathrm{D}^2 + U_-(\alpha_2, z)]y = 0 \tag{1.10}$$

respectively, where $U_\pm(\alpha_2, z)$ are complicated *algebraic* functions of α_2 and z. Next these second-order differential equations were both reduced to the Gauss hypergeometric differential equation by using Schwarzian transformation theory. Finally, it was deduced from this result that $w_2 G_2(\alpha_2, w_2)$ could be expressed in terms of a product form of the type $K(k_+)K(k_-)$, where the moduli $k_\pm$ are algebraic functions of α_2 and z.

Our main aim in section 4 of this paper is to derive the Delves–Joyce product form by a *new* and *direct* method which *avoids* the use of complicated differential equations and *non-linear* Schwarzian transformation theory. In the first stage of the analysis the triple integral for $G_2(\alpha_2, w_2)$ is reduced to a single integral of the type

$$J(C, D) \equiv \frac{2}{\pi^2}\int_0^\pi K(C + D\cos\psi)\,\mathrm{d}\psi \tag{1.11}$$

where C, D are complex variables. Next it is shown that $J(C, D)$ has a Kampé de Fériet series representation which is directly related to the $F^{3:0;0}_{1:1;1}$ series given in section 3 for the integral $I(A, B)$. Finally, this important relationship and known results for $I(A, B)$ are used to derive the Delves–Joyce product form for $w_2 G(\alpha_2, w_2)$. In section 5 we shall establish new transformation formulae which enable one to make *connections* between $G_1(\alpha_1, w_1)$ and $G_2(\alpha_2, w_2)$.

2. Evaluation of the fcc lattice Green function $G_1(\alpha_1, w_1)$

In this section we shall derive an exact product form for $G_1(\alpha_1, w_1)$ by generalizing the methods developed by Mannari and Kawabata (1964) and Iwata (1969) for the case $\alpha_1 = 1$.

2.1. Reduction of $G_1(\alpha_1, w_1)$ to a single integral

In the first stage of the analysis we perform the integration over the variable θ_3 in (1.1), with $j = 1$ and then make the changes of variable $\theta_1 = 2\vartheta_1$ and $\theta_2 = 2\vartheta_2$. This procedure gives

$$G_1(\alpha_1, w_1) = \frac{4}{(w_1 + \alpha_1)\pi^2}\int_0^{\pi/2}\mathrm{d}\vartheta_2\int_0^{\pi/2}\frac{\mathrm{d}\vartheta_1}{[(1 - a\cos^2\vartheta_1)(1 - b\sin^2\vartheta_1)]^{1/2}} \tag{2.1}$$

where

$$a = [4\cos^2\vartheta_2 - 2(1 - \alpha_1)]/(w_1 + \alpha_1) \tag{2.2}$$

$$b = [4\sin^2\vartheta_2 - 2(1 - \alpha_1)]/(w_1 + \alpha_1). \tag{2.3}$$

We can now use the standard result (see Mannari and Kawabata 1964)

$$\int_0^{\pi/2}\frac{\mathrm{d}\vartheta_1}{[(1 - a\cos^2\vartheta_1)(1 - b\sin^2\vartheta_1)]^{1/2}} = K\left(\sqrt{a + b - ab}\right) \tag{2.4}$$

where $K(k)$ is the complete elliptic integral of the first kind with a modulus k, to write (2.1) in the form

$$G_1(\alpha_1, w_1) = \frac{1}{w_1 + \alpha_1} I(A_1, B_1) \tag{2.5}$$

where

$$A_1 \equiv A_1(\alpha_1, w_1) = 2(2\alpha_1 w_1 + 1)/(w_1 + \alpha_1)^2 \tag{2.6}$$

$$B_1 \equiv B_1(\alpha_1, w_1) = 2/(w_1 + \alpha_1)^2 \tag{2.7}$$

and

$$I(A, B) \equiv \frac{2}{\pi^2} \int_0^\pi K\left(\sqrt{A + B\cos\psi}\right) \mathrm{d}\psi. \tag{2.8}$$

In general, the variables (A, B) in the definition (2.8) can be taken to be *independent* complex variables. However, it should be noted that for a given value of α_1 the particular set of points $\{A_1(\alpha_1, w_1), B_1(\alpha_1, w_1) : w_1 \in \mathcal{C}_1^-\}$ is *restricted* to lie on the complex *rational* curve

$$\left[A_1 + \left(2\alpha_1^2 - 1\right) B_1\right]^2 - 8\alpha_1^2 B_1 = 0. \tag{2.9}$$

2.2. Exact product forms for $I(A, B)$ and $G_1(\alpha_1, w_1)$

Next we apply the Gaussian hypergeometric series

$$\frac{2}{\pi} K(k) = \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{(1)_n^2} k^{2n} \tag{2.10}$$

to the integrand in (2.8). In this manner, we obtain

$$I(A, B) = \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{(1)_n^2} \Omega_n(A, B) \tag{2.11}$$

where

$$\Omega_n(A, B) = \frac{1}{\pi} \int_0^\pi (A + B\cos\psi)^n \,\mathrm{d}\psi \tag{2.12}$$

and $(a)_n$ denotes the Pochhammer symbol. The integral (2.12) can be readily evaluated using the method of residues. Hence, we obtain

$$\Omega_n(A, B) = (x_+)^n \sum_{m=0}^{n} \binom{n}{m}^2 \left(\frac{x_-}{x_+}\right)^m \tag{2.13}$$

where

$$x_\pm = \tfrac{1}{2}\left(A \pm \sqrt{A^2 - B^2}\right). \tag{2.14}$$

If (2.13) is substituted in (2.11) and the order of the resulting two summations is interchanged we find that it is possible to express $I(A, B)$ in the form

$$I(A, B) = F_4\left(\tfrac{1}{2}, \tfrac{1}{2}; 1, 1; x_+, x_-\right) \tag{2.15}$$

where $F_4(\alpha, \beta; \gamma, \gamma'; x, y)$ is the fourth Appell hypergeometric function in two variables x and y.

In the final stage of the analysis we simplify (2.15) by using the Bailey (1933) identity

$$F_4[\alpha, \beta; \gamma, \alpha + \beta - \gamma + 1; x(1 - y), y(1 - x)]$$
$$= {}_2F_1(\alpha, \beta; \gamma; x)\, {}_2F_1(\alpha, \beta; \alpha + \beta - \gamma + 1; y). \tag{2.16}$$

This procedure yields the important *general* formula

$$I(A, B) = \left(\frac{2}{\pi}\right)^2 K(k_+) K(k_-) \tag{2.17}$$

where

$$k_\pm^2 \equiv k_\pm^2(A, B) = \tfrac{1}{2} \pm \tfrac{1}{2}\sqrt{A^2 - B^2} - \tfrac{1}{2}\sqrt{(1 - A)^2 - B^2}. \tag{2.18}$$

If we now substitute (2.17) in (2.5) and apply the relations (2.6) and (2.7) we obtain the required result

$$w_1 G_1(\alpha_1, w_1) = \frac{1}{1 + \alpha_1 z_1}\left(\frac{2}{\pi}\right)^2 K(k_+)K(k_-) \tag{2.19}$$

where

$$\begin{aligned} k_\pm^2 \equiv k_\pm^2(\alpha_1, w_1) = \frac{1}{2} \pm \frac{2\alpha_1 z_1}{(1 + \alpha_1 z_1)^2}\left(1 + \frac{z_1}{\alpha_1}\right)^{1/2} \\ - \frac{(1 - \alpha_1 z_1)}{2(1 + \alpha_1 z_1)^2}[1 + (2 - \alpha_1)z_1]^{1/2}[1 - (2 + \alpha_1)z_1]^{1/2} \end{aligned} \tag{2.20}$$

and $z_1 = 1/w_1$. The product form (2.19) is in agreement with the work of Joyce (1971).

It can be shown that the formula (2.19) is valid provided that z_1 lies in a certain finite region $\mathcal{R}_1(\alpha_1)$ of the cut z_1 plane which surrounds the point $z_1 = 0$. The points z_1 on the boundary of $\mathcal{R}_1(\alpha_1)$ are associated with values of k_+^2 which lie in the interval $\frac{1}{2} + \frac{1}{2}\left[1 + \left(1/\alpha_1^2\right)\right]^{1/2} \leqslant k_+^2 < \infty$. We can extend the range of validity of (2.19) across the boundary curve by constructing the analytic continuation of $K(k_+)$ onto the appropriate adjacent Riemann sheet (see Morita and Horiguchi 1971).

When $\alpha_1 = 1$ the product form (2.19) reduces to the Iwata (1969) formula for $w_1 G_1(1, w_1)$, while for the special case $\alpha_1 = 1$ and $w_1 = 3$ we find that k_+ becomes the complementary modulus k'_- and $k_- = k_3$, where k_N denotes the Nth singular value for the modulus (see Borwein and Borwein 1987). From these results and (2.19) we obtain the well-known result (Watson 1939)

$$G_1(1, 3) = \frac{\sqrt{3}}{4}\left[\frac{2}{\pi}K(k_3)\right]^2 \tag{2.21}$$

where

$$k_3 = \frac{\sqrt{3} - 1}{2\sqrt{2}}. \tag{2.22}$$

3. Kampé de Fériet series for $I(A, B)$

From the analysis in the previous section and the work of Iwata (1969), Rashid (1980) and Montaldi (1981) it is clear that the integral $I(A, B)$ and the product formula (2.17) are of particular importance in the evaluation of three-dimensional lattice Green functions. In this section we shall derive various representations for $I(A, B)$ in terms of the Kampé de Fériet series (see Srivastava and Karlsson 1985)

$$\begin{aligned} F^{p:r;u}_{q:s;v}\left[\begin{matrix} \alpha_1, \ldots, \alpha_p : & \gamma_1, \ldots, \gamma_r; & \rho_1, \ldots, \rho_u; & \\ & & & x, y \\ \beta_1, \ldots, \beta_q : & \delta_1, \ldots, \delta_s; & \sigma_1, \ldots, \sigma_v; & \end{matrix}\right] \\ = \sum_{\ell,m=0}^{\infty} \frac{\prod_{j=1}^{p}(\alpha_j)_{\ell+m}\prod_{j=1}^{r}(\gamma_j)_\ell\prod_{j=1}^{u}(\rho_j)_m}{\prod_{j=1}^{q}(\beta_j)_{\ell+m}\prod_{j=1}^{s}(\delta_j)_\ell\prod_{j=1}^{v}(\sigma_j)_m}\frac{x^\ell}{\ell!}\frac{y^m}{m!}. \end{aligned} \tag{3.1}$$

We shall see in section 4 that these new representations play a *crucial* role in the evaluation of the sc lattice Green function $G_2(\alpha_2, w_2)$.

3.1. Basic results

We first consider the expansion (2.11) and use the change of variable $\psi = 2\vartheta$ to write the integral $\Omega_n(A, B)$ in the alternative form

$$\Omega_n(A, B) = \frac{2}{\pi}\int_0^{\pi/2} [(A - B) + 2B\cos^2\vartheta]^n \, \mathrm{d}\vartheta. \tag{3.2}$$

After applying the binomial theorem to the integrand in (3.2) we obtain the formula

$$\Omega_n(A, B) = \sum_{m=0}^{n} \binom{n}{m} \frac{\left(\frac{1}{2}\right)_m}{(1)_m} (A - B)^{n-m} (2B)^m. \tag{3.3}$$

We now substitute (3.3) in (2.11) and reverse the order of the resulting two summations. This procedure gives

$$I(A, B) = \sum_{\ell,m=0}^{\infty} \frac{\left(\frac{1}{2}\right)^2_{\ell+m} \left(\frac{1}{2}\right)_m}{(1)_{\ell+m}(1)_m} \frac{(A - B)^\ell}{\ell!} \frac{(2B)^m}{m!}. \tag{3.4}$$

If we compare the double series (3.4) with the general definition (3.1) we obtain the Kampé de Fériet series representation

$$I(A, B) = F^{2:0;1}_{1:0;1}\left[\begin{matrix} \frac{1}{2}, \frac{1}{2} : & -; & \frac{1}{2}; & \\ & & & A - B, 2B \\ 1 : & -; & 1; & \end{matrix}\right]. \tag{3.5}$$

When $B = A$ it is readily seen that (3.5) reduces to

$$I(A, A) = {}_3F_2\left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 1, 1; 2A\right) \tag{3.6}$$

where ${}_3F_2$ is a generalized hypergeometric series.

3.2. Generalized Euler transformation formula

Next we shall prove the generalized Euler transformation formula

$$F^{2:0;1}_{1:0;1}\left[\begin{matrix} \frac{1}{2}, \frac{1}{2} : & -; & \frac{1}{2}; & \\ & & & x, y \\ 1 : & -; & 1; & \end{matrix}\right] = \frac{1}{(1 - x)^{1/2}} F^{1:1;2}_{1:0;1}\left[\begin{matrix} \frac{1}{2} : & \frac{1}{2}; & \frac{1}{2}, \frac{1}{2}; & \\ & & & \frac{x}{x-1}, \frac{y}{1-x} \\ 1 : & -; & 1; & \end{matrix}\right]. \tag{3.7}$$

We begin by using (3.1) to express the right-hand side of equation (3.7) in the form

$$\Lambda(x, y) = \sum_{\ell,m=0}^{\infty} \frac{\left(\frac{1}{2}\right)_{\ell+m} \left(\frac{1}{2}\right)_\ell \left(\frac{1}{2}\right)^2_m}{(1)_{\ell+m}(1)_m \ell! m!} \frac{(-1)^\ell x^\ell y^m}{(1 - x)^{\ell+m+\frac{1}{2}}}. \tag{3.8}$$

Next the binomial expansion

$$(1 - x)^{-(\ell+m+\frac{1}{2})} = \sum_{t=0}^{\infty} \frac{\left(\ell + m + \frac{1}{2}\right)_t}{t!} x^t \tag{3.9}$$

and the identity

$$\left(\ell + m + \frac{1}{2}\right)_t = \frac{\left(\frac{1}{2}\right)_{\ell+m+t}}{\left(\frac{1}{2}\right)_{\ell+m}} \tag{3.10}$$

are applied to (3.8) and the resulting double series in powers of x is rearranged by introducing the summation variable $n = \ell + t$. In this manner, we find that

$$\Lambda(x, y) = \sum_{n,m=0}^{\infty} \frac{\left(\frac{1}{2}\right)_{n+m} \left(\frac{1}{2}\right)^2_m}{(1)_m} f(n, m) \frac{x^n}{n!} \frac{y^m}{m!} \tag{3.11}$$

where

$$f(n,m) = \frac{1}{m!}\,{}_2F_1\left(-n, \frac{1}{2}; m+1; 1\right). \tag{3.12}$$

The application of the Gauss summation formula to (3.12) gives

$$f(n,m) = \frac{\left(\frac{1}{2}\right)_{n+m}}{\left(\frac{1}{2}\right)_m (1)_{n+m}}. \tag{3.13}$$

If the result (3.13) is substituted in (3.11) we see that $\Lambda(x, y)$ has been reduced to the left-hand side of equation (3.7), and the proof of the identity (3.7) is complete.

We now apply the transformation formula (3.7) to (3.5). Hence, we obtain the second Kampé de Fériet series representation

$$I(A,B) = \frac{1}{(1-A+B)^{1/2}} F^{1:1;2}_{1:0;1}\left[\begin{matrix} \frac{1}{2}: & \frac{1}{2}; & \frac{1}{2}, \frac{1}{2}; & \\ & & & -\frac{A-B}{1-A+B}, \frac{2B}{1-A+B} \\ 1: & -; & 1; & \end{matrix}\right]. \tag{3.14}$$

3.3. Generalized Bailey transformation formula

Recently, Karlsson *et al* (2000) have established the transformation formula

$$F^{1:2;2}_{1:1;1}\left[\begin{matrix} \gamma+\gamma'-1: & \alpha,\beta; & \alpha,\beta; & \\ & & & x, y \\ \alpha+\beta: & \gamma; & \gamma'; & \end{matrix}\right]$$

$$= F^{3:0;0}_{1:1;1}\left[\begin{matrix} \gamma+\gamma'-1, \alpha, \beta: & -; & -; & \\ & & & x(1-y), y(1-x) \\ \alpha+\beta: & \gamma; & \gamma'; & \end{matrix}\right]. \tag{3.15}$$

When $\gamma + \gamma' = \alpha + \beta + 1$ this result reduces to the well-known Bailey identity (2.16).

If we consider (3.15) with $\alpha = \beta = \gamma = \frac{1}{2}$ and $\gamma' = 1$ it is seen that the $F^{1:2;2}_{1:1;1}$ series in (3.15) reduces to the same type of Kampé de Fériet series which occurs in (3.14). It follows, therefore, that we can also write

$$I(A,B) = \frac{1}{(1-A+B)^{1/2}}$$

$$\times F^{3:0;0}_{1:1;1}\left[\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}: & -; & -; & \\ & & & -\frac{(A-B)(1-A-B)}{(1-A+B)^2}, \frac{2B}{(1-A+B)^2} \\ 1: & \frac{1}{2}; & 1; & \end{matrix}\right]. \tag{3.16}$$

4. Evaluation of the sc lattice Green function $G_2(\alpha_2, w_2)$

Our main aim in this section is to give a *new, simple* and *direct* derivation of the Delves–Joyce (2001) product form for $G_2(\alpha_2, w_2)$.

4.1. Reduction of $G_2(\alpha_2, w_2)$ to a single integral

We begin by performing the integration over the variable θ_1 in (1.1), with $j = 2$. In this manner, it is found that

$$G_2(\alpha_2, w_2) = \frac{1}{\pi^2}\int_0^\pi d\theta_3 \int_0^\pi \frac{d\theta_2}{[(c-\cos\theta_2)(d-\cos\theta_2)]^{1/2}} \tag{4.1}$$

where

$$c = w_2 + 1 - \alpha_2 \cos\theta_3 \tag{4.2}$$

$$d = w_2 - 1 - \alpha_2 \cos\theta_3. \tag{4.3}$$

If we now apply the standard result

$$\int_0^\pi \frac{\mathrm{d}\theta_2}{[(c-\cos\theta_2)(d-\cos\theta_2)]^{1/2}} = \frac{2}{[(c-1)(d+1)]^{1/2}} K(k) \tag{4.4}$$

where

$$k^2 = \frac{2(c-d)}{(c-1)(d+1)} \tag{4.5}$$

to (4.1) we obtain the formula

$$G_2(\alpha_2, w_2) = \frac{2}{\pi^2}\int_0^\pi \frac{1}{w_2 - \alpha_2\cos\theta_3} K\left(\frac{2}{w_2 - \alpha_2\cos\theta_3}\right) \mathrm{d}\theta_3. \tag{4.6}$$

Next the integration variable in (4.6) is changed from θ_3 to ψ using the transformation

$$\cos\theta_3 = \frac{w_2\cos\psi + \alpha_2}{w_2 + \alpha_2\cos\psi}. \tag{4.7}$$

Hence, we find that

$$G_2(\alpha_2, w_2) = \frac{1}{\left(w_2^2 - \alpha_2^2\right)^{1/2}} J(C_2, D_2) \tag{4.8}$$

where

$$C_2 \equiv C_2(\alpha_2, w_2) = 2w_2\big/\left(w_2^2 - \alpha_2^2\right) \tag{4.9}$$

$$D_2 \equiv D_2(\alpha_2, w_2) = 2\alpha_2\big/\left(w_2^2 - \alpha_2^2\right) \tag{4.10}$$

and

$$J(C, D) \equiv \frac{2}{\pi^2}\int_0^\pi K(C + D\cos\psi)\,\mathrm{d}\psi. \tag{4.11}$$

In general, the variables (C, D) in the definition (4.11) can be taken to be *independent* complex variables. However, it should be noted that the particular set of points $\{C_2(\alpha_2, w_2), D_2(\alpha_2, w_2) : w_2 \in \mathcal{C}_2^-\}$ is *restricted* to lie on the complex curve

$$\alpha_2\left(C_2^2 - D_2^2\right) - 2D_2 = 0. \tag{4.12}$$

4.2. *Connection between* $J(C, D)$ *and* $I(A, B)$

We now establish a link between $J(C, D)$ and $I(A, B)$. In the first stage of the analysis the hypergeometric series (2.10) is substituted in (4.11). This procedure gives

$$J(C, D) = \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{(1)_n^2} \Omega_{2n}(C, D) \tag{4.13}$$

where

$$\Omega_{2n}(C, D) = \frac{1}{\pi}\int_0^\pi (C + D\cos\psi)^{2n}\,\mathrm{d}\psi. \tag{4.14}$$

If the binomial theorem is applied to the integrand in (4.14) it is found that

$$\Omega_{2n}(C, D) = \sum_{m=0}^{n} \binom{2n}{2m} \frac{\left(\frac{1}{2}\right)_m}{(1)_m} C^{2n-2m} D^{2m}. \tag{4.15}$$

Next we substitute (4.15) in (4.13) and reverse the order of the resulting two summations. In this manner, we obtain

$$J(C, D) = \sum_{\ell,m=0}^{\infty} \frac{\left(\frac{1}{2}\right)^3_{\ell+m}}{(1)_{\ell+m}\left(\frac{1}{2}\right)_\ell (1)_m} \frac{C^{2\ell}}{\ell!} \frac{D^{2m}}{m!}. \tag{4.16}$$

From the double series (4.16) and the definition (3.1) we see that

$$J(C, D) = F^{3:0;0}_{1:1;1} \left[\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} : & -; & -; & \\ & & & C^2, D^2 \\ 1 : & \frac{1}{2}; & 1; & \end{matrix} \right]. \tag{4.17}$$

Finally, a comparison of (4.17) with (3.16) yields the required connection formula

$$J(C, D) = (1 - A + B)^{1/2} I(A, B) \tag{4.18}$$

where A and B are *appropriate* solutions of the simultaneous equations

$$C^2 = -\frac{(A - B)(1 - A - B)}{(1 - A + B)^2} \tag{4.19}$$

$$D^2 = \frac{2B}{(1 - A + B)^2} \tag{4.20}$$

and the integral $I(A, B)$ is defined in (2.8).

4.3. Exact product forms for $J(C, D)$ and $G_2(\alpha_2, w_2)$

We shall now use the relation (4.18) to derive an exact formula for the general integral $J(C, D)$. From the algebraic equations (4.19) and (4.20) we find that the relevant solutions for A and B are given by

$$A = \frac{1}{4D^2}[(C^2 - D^2)^2 + 2D^2 - 1 + (C^2 - D^2 + 1)S(C, D)] \tag{4.21}$$

$$B = \frac{1}{4D^2}[(C^2 - D^2)^2 - 2C^2 + 1 + (C^2 - D^2 - 1)S(C, D)] \tag{4.22}$$

where

$$S(C, D) = [(C^2 - D^2)^2 - 2(C^2 + D^2) + 1]^{1/2}. \tag{4.23}$$

Next we substitute (2.17) in (4.18) and apply equations (4.21) and (4.22). After a considerable amount of algebraic simplification it is found that

$$J(C, D) = \frac{2}{\sqrt{(1 - D)^2 - C^2} + \sqrt{(1 + D)^2 - C^2}} \left(\frac{2}{\pi}\right)^2 K(k_+)K(k_-) \tag{4.24}$$

where

$$\begin{aligned} k_\pm^2 \equiv k_\pm^2(C, D) = {} & \frac{1}{2} - \frac{1}{2C} \left[\sqrt{(1 - D)^2 - C^2} + \sqrt{(1 + D)^2 - C^2}\right]^{-3} \\ & \times \left[(C + D)\sqrt{1 - (C - D)^2} + (C - D)\sqrt{1 - (C + D)^2}\right] \\ & \times \left\{\pm 4C\sqrt{C^2 - D^2} + \left[\sqrt{(1 + C)^2 - D^2} + \sqrt{(1 - C)^2 - D^2}\right]^2\right\}. \end{aligned} \tag{4.25}$$

This formula is valid provided that (C, D) lies in a sufficiently small neighbourhood of the origin point $(C, D) = (0, 0)$.

Finally, we can use (4.24) and (4.8)–(4.10) to derive an exact product form for $G_2(\alpha_2, w_2)$. In particular, we deduce that

$$w_2 G_2(\alpha_2, w_2) = \frac{2}{\sqrt{1-(2-\alpha_2)^2 z_2^2} + \sqrt{1-(2+\alpha_2)^2 z_2^2}} \left[\frac{2}{\pi} K(k_+)\right] \left[\frac{2}{\pi} K(k_-)\right] \tag{4.26}$$

where

$$\begin{aligned} k_\pm^2 \equiv k_\pm^2(\alpha_2, z_2) = \frac{1}{2} - \frac{1}{2} &\left[\sqrt{1-(2-\alpha_2)^2 z_2^2} + \sqrt{1-(2+\alpha_2)^2 z_2^2}\right]^{-3} \\ &\times \left[\sqrt{1+(2-\alpha_2)z_2}\,\sqrt{1-(2+\alpha_2)z_2} + \sqrt{1-(2-\alpha_2)z_2}\,\sqrt{1+(2+\alpha_2)z_2}\right] \\ &\times \left\{\pm 16 z_2^2 + \sqrt{1-\alpha_2^2 z_2^2}\left[\sqrt{1+(2-\alpha_2)z_2}\,\sqrt{1+(2+\alpha_2)z_2}\right.\right. \\ &\left.\left. + \sqrt{1-(2-\alpha_2)z_2}\,\sqrt{1-(2+\alpha_2)z_2}\right]^2\right\} \end{aligned} \tag{4.27}$$

and $z_2 = 1/w_2$. It can be shown that this basic formula is valid for *all* values of $w_2 \in \mathcal{C}_2^-$. A detailed investigation of the analytic properties of (4.26) has already been given by Delves and Joyce (2001).

When $\alpha_2 = 1$ the product form (4.26) yields results which are in agreement with the work of Joyce (1972b, 1973). For the special case $\alpha_2 = 1$ and $w_2 = 3$ we find that (4.26) gives

$$G_2(1, 3) = \frac{2\sqrt{2}}{\pi^2} K(k_+) K(k_-) \tag{4.28}$$

where

$$k_\pm^2 = -\tfrac{1}{2}\left(2\sqrt{3} - 1 \pm \sqrt{6}\right). \tag{4.29}$$

It can be shown (see Joyce 1973, p 602) that (4.28) can be expressed in the alternative form

$$G_2(1, 3) = \left(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}\right)\left[\frac{2}{\pi} K(k_6)\right]^2 \tag{4.30}$$

where

$$k_6 = \left(2 - \sqrt{3}\right)\left(\sqrt{3} - \sqrt{2}\right). \tag{4.31}$$

The formula (4.30) was first derived by Watson (1939) using a completely different method.

5. Connections between $G_1(\alpha_1, w_1)$ and $G_2(\alpha_2, w_2)$

In this concluding section we shall derive transformation formulae which provide one with direct connections between the Green functions $G_1(\alpha_1, w_1)$ and $G_2(\alpha_2, w_2)$. We begin by applying the general result (4.18) to equation (2.5). This procedure gives

$$G_1(\alpha_1, w_1) = \frac{1}{(w_1 - \alpha_1)} J(C_1, D_1) \tag{5.1}$$

where

$$C_1^2 = -\frac{4\alpha_1 w_1(w_1+2-\alpha_1)(w_1-2-\alpha_1)}{(w_1-\alpha_1)^4} \tag{5.2}$$

$$D_1^2 = \frac{4(w_1+\alpha_1)^2}{(w_1-\alpha_1)^4}. \tag{5.3}$$

We now compare (5.1) with (4.8) and impose the conditions

$$C_1^2(\alpha_1, w_1) \equiv C_2^2(\alpha_2, w_2) \qquad \text{and} \qquad D_1^2(\alpha_1, w_1) \equiv D_2^2(\alpha_2, w_2). \tag{5.4}$$

In this manner, we obtain the connection formula

$$w_1 G_1(\alpha_1, w_1) = \left[\frac{w_1(\alpha_1 w_1 + 1)}{\alpha_1(w_1+2-\alpha_1)(w_1-2-\alpha_1)}\right]^{1/2} w_2 G_2(\alpha_2, w_2) \tag{5.5}$$

where

$$w_2^2 \equiv w_2^2(\alpha_1, w_1) = -\frac{\alpha_1 w_1(w_1+2-\alpha_1)(w_1-2-\alpha_1)}{(\alpha_1 w_1+1)^2} \tag{5.6}$$

$$\alpha_2 \equiv \alpha_2(\alpha_1, w_1) = \frac{w_1+\alpha_1}{\alpha_1 w_1 + 1}. \tag{5.7}$$

In order to check equations (5.5)–(5.7) we have used the series (1.4) with $j = 2$ and the transformations (5.6) and (5.7) to expand the right-hand side of (5.5) in inverse powers of w_1. The resulting series coefficients $\{\mu_n^{(1)}(\alpha_1) : n = 2, 3, \ldots\}$ were found to be in agreement with those listed in the appendix. If (5.5)–(5.7) are evaluated for the special case $\alpha_1 = 1$ and $w_1 = -3$ we obtain the interesting relation

$$G_2(1, 3) = -\sqrt{2} G_1(1, -3). \tag{5.8}$$

Finally, we note that equations (5.6) and (5.7) can also be used to derive the *inverse* connection formula

$$G_2(\alpha_2, w_2) = -\frac{1}{2\alpha_2}\left[\sqrt{w_2^2 - (2+\alpha_2)^2} + \sqrt{w_2^2 - (2-\alpha_2)^2}\right] G_1(\alpha_1, w_1) \tag{5.9}$$

where

$$\begin{aligned} w_1 \equiv w_1(\alpha_2, w_2) = -\frac{1}{4\alpha_2}\Bigg\{&\left(w_2^2 - 4 - \alpha_2^2\right) + \sqrt{w_2^2-\alpha_2^2}\left[\sqrt{w_2^2-(2+\alpha_2)^2}\right. \\ &\left.+\sqrt{w_2^2-(2-\alpha_2)^2}\right] + \sqrt{w_2^2-(2+\alpha_2)^2}\sqrt{w_2^2-(2-\alpha_2)^2}\Bigg\} \end{aligned} \tag{5.10}$$

$$\begin{aligned} \alpha_1 \equiv \alpha_1(\alpha_2, w_2) = -\frac{1}{4\alpha_2}\Bigg\{&\left(w_2^2 - 4 - \alpha_2^2\right) - \sqrt{w_2^2-\alpha_2^2}\left[\sqrt{w_2^2-(2+\alpha_2)^2}\right. \\ &\left.+\sqrt{w_2^2-(2-\alpha_2)^2}\right] + \sqrt{w_2^2-(2+\alpha_2)^2}\sqrt{w_2^2-(2-\alpha_2)^2}\Bigg\}. \end{aligned} \tag{5.11}$$

We have used the series (1.4) with $j = 1$ and the transformations (5.10) and (5.11) to expand the right-hand side of (5.9) in inverse powers of w_2. It was found that the resulting series coefficients $\{\mu_{2n}^{(2)}(\alpha_2) : n = 1, 2, \ldots\}$ were in agreement with the formula (1.6).

Appendix. Formulae for the coefficients $\{\mu_n^{(1)}(\alpha_1) : n = 2, 3, \ldots, 10\}$

$$\mu_2^{(1)}(\alpha_1) = \tfrac{1}{4}\left(2+\alpha_1^2\right)$$
$$\mu_3^{(1)}(\alpha_1) = \tfrac{3}{4}\alpha_1$$
$$\mu_4^{(1)}(\alpha_1) = \tfrac{9}{64}\left(6+8\alpha_1^2+\alpha_1^4\right)$$
$$\mu_5^{(1)}(\alpha_1) = \tfrac{45}{32}\alpha_1\left(2+\alpha_1^2\right)$$
$$\mu_6^{(1)}(\alpha_1) = \tfrac{5}{256}\left(100+333\alpha_1^2+90\alpha_1^4+5\alpha_1^6\right)$$
$$\mu_7^{(1)}(\alpha_1) = \tfrac{525}{256}\alpha_1\left(1+\alpha_1^2\right)\left(5+\alpha_1^2\right)$$
$$\mu_8^{(1)}(\alpha_1) = \tfrac{175}{16\,384}\left(490+3\,104\alpha_1^2+1\,944\alpha_1^4+224\alpha_1^6+7\alpha_1^8\right)$$
$$\mu_9^{(1)}(\alpha_1) = \tfrac{525}{4\,096}\alpha_1\left(294+652\alpha_1^2+252\alpha_1^4+21\alpha_1^6\right)$$
$$\mu_{10}^{(1)}(\alpha_1) = \tfrac{441}{65\,536}\left(2\,268+23\,450\alpha_1^2+26\,800\alpha_1^4+7\,050\alpha_1^6+450\alpha_1^8+9\alpha_1^{10}\right).$$

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