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Exact evaluation of the simple cubic lattice Green function for a general lattice point

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Abstract

The simple cubic lattice Green function

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

is investigated, where $\{l, m, n\}$ denotes a set of integers and $w = u + iv$ is a complex variable in the (u, v) plane. In particular, it is shown that the modified Green function

$$\overline{G}(l,m,n;w) \equiv (3/w)^{l+m+n} wG(l,m,n;w)$$

can be expressed in the ξ-parametric form

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

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

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

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

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

and $\{R_j(l,m,n;\xi) : j = 0,1,2,3\}$ is a set of rational functions of ξ. It is found that the complete elliptic integral formulae for the Green functions $\{\overline{G}(n,n,n;w) : n = 1,2,3,4\}$ and $\{\overline{G}(2n,n,n;w) : n = 1,2,3,4\}$ can be factorized as a product of two linear forms in $K(k)$ and $E(k)$ whose coefficients are *rational* functions of the parameter ξ. On the basis of these explicit results it is *conjectured* that this factorization propery is valid for *all* integer values of n.

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1. Introduction

The lattice Green function

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

where $\{l,m,n\}$ denotes a set of integers and $w = u + \mathrm{i}v$ is a complex variable in the (u, v) plane, plays an important role 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, Katsura *et al* 1971). We shall assume, without loss of generality, that $l \geqslant m \geqslant n \geqslant 0$. The triple integral (1.1) defines a single-valued analytic function $G(l,m,n;w)$ in the complex (u, v) plane provided that a cut is made along the real axis from $w = -3$ to $w = +3$. The set of points (u, v) in this cut plane will be denoted by $\mathcal{C}^-$. We readily find from (1.1) that $G(l,m,n;w)$ satisfies the symmetry relation

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

It follows, therefore, that the analytic function $G(l,m,n;w)$ is an even or odd function of w according as $l+m+n$ is an odd or even number respectively. In most applications one usually requires the limiting behaviour of $G(l,m,n;w)$ as w approaches the real u axis. It is convenient, therefore, to introduce the further definitions

$$G^{\pm}(l,m,n;u) \equiv \lim_{\epsilon\to 0+} G(l,m,n;u\pm\mathrm{i}\epsilon) \tag{1.3}$$

where $-\infty < u < \infty$ and ϵ is a real positive number. When $|u| \geqslant 3$ it can be shown that the imaginary part of $G^{\pm}(l,m,n;u)$ is always equal to zero. In this paper we shall also make use of the more compact notation

$$G_l(w) \equiv G(l,0,0;w) \tag{1.4}$$

where $l = 0, 1, 2, \ldots$.

An exact evaluation of the lattice Green function $G_0(w)$ was first carried out by Watson (1939) for the special case $w = 3$. In particular, he established the formula

$$G_0(3) = \left(18+12\sqrt{2}-10\sqrt{3}-7\sqrt{6}\right)\left[\frac{2}{\pi}K\left(\left(2-\sqrt{3}\right)\left(\sqrt{3}-\sqrt{2}\right)\right)\right]^2 \tag{1.5}$$

where $K(k)$ denotes the complete elliptic integral of the first kind with modulus k. It is also possible to express $G_0(3)$ in terms of the gamma function using the work of Borwein and Zucker (1992). We find that

$$G_0(3) = \frac{1}{96\pi^3}\left(\sqrt{3}-1\right)\left[\Gamma\left(\frac{1}{24}\right)\Gamma\left(\frac{11}{24}\right)\right]^2. \tag{1.6}$$

From these results we obtain the numerical value

$$G_0(3) = 0.505\,462\,019\,717\,326\,006\,052\,004\,053\,227\ldots. \tag{1.7}$$

More generally, it was shown by Joyce (1972, 1973) that the function $G_0(w)$ could be expressed in the following form:

$$wG_0(w) = \left(1-\frac{3}{4}x_1\right)^{\frac{1}{2}}(1-x_1)^{-1}\left[\frac{2}{\pi}K(k_+)\right]\left[\frac{2}{\pi}K(k_-)\right] \tag{1.8}$$

where

$$k_\pm^2 \equiv k_\pm^2(x_2) = \tfrac{1}{2} \pm \tfrac{1}{4}x_2(4-x_2)^{\frac{1}{2}} - \tfrac{1}{4}(2-x_2)(1-x_2)^{\frac{1}{2}} \tag{1.9}$$

$$x_1 = \tfrac{1}{2} + \tfrac{1}{2}(3/w^2) - \tfrac{1}{2}\left[1 - (9/w^2)\right]^{\frac{1}{2}}\left[1 - (1/w^2)\right]^{\frac{1}{2}} \tag{1.10}$$

$$x_2 = x_1/(x_1 - 1). \tag{1.11}$$

From a detailed study of the algebraic relations (1.9)–(1.11) it is found that we can use the formula (1.8) to calculate $G_0(w)$ at *any* point in the cut plane $\mathcal{C}^-$. It has been shown (Joyce 1973, p 602) that for $w = 3$ the formula (1.8) reduces to the Watson result (1.5).

It was later established by Morita (1975) that it is always possible, *at least in principle*, to express the Green function (1.1) for an *arbitrary* lattice site (l, m, n) in terms of the three basic functions $G_0(w)$, $G_2(w)$ and $G_3(w)$ by making successive applications of certain recurrence relations. Horiguchi and Morita (1975) were also able to derive the following formulae for $G_2(w)$ and $G_3(w)$:

$$\begin{aligned} G_2(w) = &-\tfrac{2}{3}w - \tfrac{1}{3}(1 - 2w^2)G_0(w) - \tfrac{4}{3}w(5 - w^2)G_0'(w) \\ &+ \tfrac{2}{3}(9 - 10w^2 + w^4)G_0''(w) \end{aligned} \tag{1.12}$$

$$\begin{aligned} G_3(w) = &-\tfrac{1}{3}(3 + 4w^2) - \tfrac{1}{3}w(3 - 5w^2)G_0(w) + \tfrac{1}{3}(9 - 80w^2 + 15w^4)G_0'(w) \\ &+ \tfrac{7}{3}w(9 - 10w^2 + w^4)G_0''(w) \end{aligned} \tag{1.13}$$

where $G_0'(w)$ and $G_0''(w)$ denote the first and second derivatives of $G_0(w)$ with respect to w respectively. (It should be noted that the differential relation given by Horiguchi and Morita 1975 for $G_3(w)$ contains two minor errors. Equation (1.13) gives the corrected version for their relation.) If the formula (1.8) is now applied to the relations (1.12) and (1.13) we readily see that $G_2(w)$ and $G_3(w)$ can be evaluated exactly in terms of products of complete elliptic integrals of the first and second kind (see Horiguchi and Morita 1975 for further details). It is then possible to use the work of Morita (1975) to derive similar closed-form expressions for $G(l, m, n; w)$ at other lattice points. Unfortunately, the complicated algebraic structure of the formula (1.8) makes this procedure for evaluating $G(l, m, n; w)$ difficult to apply in practice, and no simple explicit closed forms for $G(l, m, n; w)$ appear to have been obtained using these methods.

Recently, Joyce (1994, 1998) has shown that the application of the transformation

$$w^2 = \frac{(1 - 9\xi^4)^2}{4\xi^2(1 - \xi^2)(1 - 9\xi^2)} \tag{1.14}$$

to (1.8) leads to the *simplified* parametric representation

$$wG_0(w) = \frac{(1 - 9\xi^4)}{(1 - \xi)^3(1 + 3\xi)}\left[\frac{2}{\pi}K(k)\right]^2 \tag{1.15}$$

where

$$k^2 \equiv k^2(\xi) = \frac{16\xi^3}{(1 - \xi)^3(1 + 3\xi)} \tag{1.16}$$

and the parameter ξ lies in a certain finite region $\mathcal{R}_4$ of the complex plane. If the inverse relation (Joyce 1994)

$$\xi \equiv \xi(w) = (1/w)\left[1 + \sqrt{1 - (9/w^2)}\right]^{-\frac{1}{2}}\left[1 + \sqrt{1 - (1/w^2)}\right]^{-\frac{1}{2}} \tag{1.17}$$

is substituted in (1.15) then we obtain, at least in principle, an explicit formula for $G_0(w)$.

In this paper we shall combine the result (1.15) with the earlier work of Horiguchi and Morita (1975) and Morita (1975) in order to prove that $G(l, m, n; w)$ can be written in the form

$$\overline{G}(l,m,n;w) = R_0(l,m,n;\xi) + R_1(l,m,n;\xi)\left[\frac{2}{\pi}K(k)\right]^2 + R_2(l,m,n;\xi)\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] + R_3(l,m,n;\xi)\left[\frac{2}{\pi}E(k)\right]^2 \tag{1.18}$$

where $\{R_j(l,m,n;\xi) : j = 0,1,2,3\}$ denotes a set of rational functions of ξ,

$$\overline{G}(l,m,n;w) \equiv (3/w)^{l+m+n} w G(l,m,n;w) \tag{1.19}$$

$E(k)$ is the complete elliptic integral of the second kind and $\xi = \xi(w)$ is defined in (1.17). Explicit expressions for $\overline{G}(l,m,n;w)$ of the type (1.18) are given for $l+m+n \leqslant 4$. A simplified formula for $G(l,m,n;3)$ is also derived which is in agreement with the recent independent work of Glasser and Boersma (2000). Finally, it is noted that for the special cases $G(n,n,n;w)$ and $G(2n,n,n;w)$ the formula (1.18) can be expressed as a *product* of two linear forms in $K(k)$ and $E(k)$ whose coefficients are rational functions of the parameter ξ.

2. Analysis of $G_2(w)$ and $G_3(w)$

In this section we obtain parametric representations for the derivatives $G_0'(w)$ and $G_0''(w)$. These results are then used in combination with (1.12) and (1.13) to determine closed-form expressions for the Green functions $G_2(w)$ and $G_3(w)$ of the type (1.18). The special case $w = 3$ is also investigated.

2.1. Formulae for $G_2(w)$ and $G_3(w)$

The derivative $G_0'(w)$ can be determined from (1.15) by applying the standard formula (Whittaker and Watson 1927, p 521)

$$\frac{\mathrm{d}K(k)}{\mathrm{d}k} = \frac{1}{k(1-k^2)}[E(k) - (1-k^2)K(k)]. \tag{2.1}$$

In this manner, we find that

$$G_0'(w) = \frac{4\xi^2(1+\xi)(1-3\xi)}{(1-\xi)^2(1-18\xi^2+9\xi^4)(1-2\xi^2+9\xi^4)} \times \left\{2(1-5\xi^2)\left[\frac{2}{\pi}K(k)\right]^2 - 3(1-\xi)^3(1+3\xi)\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right]\right\} \tag{2.2}$$

where $k \equiv k(\xi)$ and $\xi \equiv \xi(w)$ are defined in (1.16) and (1.17) respectively.

We can now obtain the second derivative $G_0''(w)$ by using (2.2) and the further relation (Whittaker and Watson 1927, p 521)

$$\frac{\mathrm{d}E(k)}{\mathrm{d}k} = \frac{1}{k}[E(k) - K(k)]. \tag{2.3}$$

The final result is

$$wG_0''(w) = \frac{2\xi^2(1+\xi)(1-3\xi)(1-9\xi^4)}{(1-\xi)^2(1-18\xi^2+9\xi^4)^3(1-2\xi^2+9\xi^4)^3} \times \left\{-(5 - 108\xi^2 + 1344\xi^4 - 3964\xi^6 - 18990\xi^8 + 79164\xi^{10} - 56376\xi^{12} + 8748\xi^{14} + 6561\xi^{16})\left[\frac{2}{\pi}K(k)\right]^2 + 12\xi^2(1-\xi)^3(1+3\xi)(5+19\xi^2\right.$$

$$+450\xi^4 - 2538\xi^6 + 2025\xi^8 - 729\xi^{10})\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right]$$

$$+9(1-\xi)^6(1+3\xi)^2(1-18\xi^2+9\xi^4)(1-2\xi^2+9\xi^4)\left[\frac{2}{\pi}E(k)\right]^2\Bigg\}. \qquad (2.4)$$

Next we substitute (1.14), (1.15), (2.2) and (2.4) in the differential relation (1.12). After a considerable amount of algebraic manipulation we obtain the required result

$$\overline{G}(2,0,0;w) = -6 + \frac{3(5-21\xi^2-21\xi^4-27\xi^6)}{(1-\xi)^3(1+3\xi)(1+3\xi^2)}\left[\frac{2}{\pi}K(k)\right]^2 - \frac{36(1-5\xi^2)}{(1-9\xi^4)}\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] + \frac{27(1-\xi)^3(1+3\xi)}{(1-9\xi^4)}\left[\frac{2}{\pi}E(k)\right]^2 \qquad (2.5)$$

where the modified Green function $\overline{G}(2,0,0;w)$ is defined in (1.19). If we make the same substitutions in relation (1.13) it is found that

$$\overline{G}(3,0,0;w) = -\frac{36(1+3\xi^2-48\xi^4+27\xi^6+81\xi^8)}{(1-9\xi^4)^2} + \frac{9(5-9\xi^2)(1-6\xi^2-3\xi^4)(7-15\xi^2-39\xi^4-81\xi^6)}{2(1-\xi)^3(1+3\xi)(1-9\xi^4)^2}\left[\frac{2}{\pi}K(k)\right]^2 - \frac{81(5-30\xi^2-24\xi^4+150\xi^6+27\xi^8)}{(1-9\xi^4)^2}\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] + \frac{567(1-\xi)^3(1+3\xi)}{2(1-9\xi^4)}\left[\frac{2}{\pi}E(k)\right]^2 \qquad (2.6)$$

where $\overline{G}(3,0,0;w)$ is defined in (1.19). The formulae (2.5) and (2.6) can be used to calculate $G_2(w)$ and $G_3(w)$ for all values of $w \in \mathcal{C}^-$.

2.2. *Special case $w = 3$*

We shall now demonstrate that a considerable simplification of the basic results (2.5) and (2.6) can be achieved when $w = 3$. For this special case we find that the formula (2.5) becomes

$$G_2(3) = -2 + \frac{1}{2}\left(78 - 48\sqrt{2} - 42\sqrt{3} + 29\sqrt{6}\right)\left[\frac{2}{\pi}K(k_0)\right]^2 - 2\left(3+\sqrt{2}\right)\left[\frac{2}{\pi}K(k_0)\right]\left[\frac{2}{\pi}E(k_0)\right] + \sqrt{3}\left(2+2\sqrt{3}-\sqrt{2}\right)\left[\frac{2}{\pi}E(k_0)\right]^2 \qquad (2.7)$$

where

$$k_0^2 = \left(\sqrt{2}-1\right)^2\left(\sqrt{3}-1\right)^2\left(\sqrt{3}+\sqrt{2}\right). \qquad (2.8)$$

Next we use the transformation formulae for the ${}_2F_1$ hypergeometric function (Erdélyi *et al* 1953) to obtain the following relations:

$$K(k_0) = \sqrt{2}\left(\sqrt{3}-\sqrt{2}\right)\left(\sqrt{2}+1\right)K(k_6) \qquad (2.9)$$

$$E(k_0) = \left(2-\sqrt{2}\right)\left(\sqrt{3}+\sqrt{2}\right)E(k_6) - \left(2+\sqrt{2}\right)\left(2-\sqrt{3}\right)K(k_6) \qquad (2.10)$$

where

$$k_6 = \left(2-\sqrt{3}\right)\left(\sqrt{3}-\sqrt{2}\right). \qquad (2.11)$$

The substitution of (2.9) and (2.10) in (2.7) yields

$$G_2(3) = -2 + \left(78 + 52\sqrt{2} - 38\sqrt{3} - 27\sqrt{6}\right)\left[\frac{2}{\pi}K(k_6)\right]^2 - 4\left(3 + \sqrt{2} + 2\sqrt{3} + \sqrt{6}\right)\left[\frac{2}{\pi}K(k_6)\right]\left[\frac{2}{\pi}E(k_6)\right] + 2\left(6 + 2\sqrt{3} + \sqrt{6}\right)\left[\frac{2}{\pi}E(k_6)\right]^2. \quad (2.12)$$

The modulus k_6 is called the *singular value* of order 6 and has the property that

$$\frac{K'(k_6)}{K(k_6)} = \sqrt{6} \quad (2.13)$$

where $K'(k)$ denotes the complementary complete elliptic integral of the first kind. It can also be shown (Borwein and Borwein 1987) that $E(k_6)$ and $K(k_6)$ are connected by the further relation

$$E(k_6) = \frac{\pi}{4\sqrt{6}K(k_6)} + \frac{1}{\sqrt{6}}\left(1 + \sqrt{2}\right)^2\left(1 + 2\sqrt{2} - 2\sqrt{3}\right)K(k_6). \quad (2.14)$$

We now substitute (2.14) in (2.12) in order to obtain the formula

$$G_2(3) = -2 + \frac{10}{3}\left(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}\right)\left[\frac{2}{\pi}K(k_6)\right]^2 + \frac{1}{12}\left(6 + 2\sqrt{3} + \sqrt{6}\right)[K(k_6)]^{-2}. \quad (2.15)$$

Finally, we use (1.5) to write (2.15) in the alternative simplified form

$$G_2(3) = -2 + \tfrac{10}{3}G_0(3) + 2[\pi^2 G_0(3)]^{-1}. \quad (2.16)$$

From (1.7) and (2.16) we obtain the numerical value

$$G_2(3) = 0.085\,778\,629\,084\,731\,494\,127\,660\,697\,895\ldots. \quad (2.17)$$

The formula (2.6) can also be analysed in a similar manner when $w = 3$. In particular, we find that

$$G_3(3) = -13 + 7\left(36 - 21\sqrt{2} - 19\sqrt{3} + 13\sqrt{6}\right)\left[\frac{2}{\pi}K(k_0)\right]^2 - 21\left(3 + \sqrt{2}\right)\left[\frac{2}{\pi}K(k_0)\right]\left[\frac{2}{\pi}E(k_0)\right] + \frac{21}{2}\sqrt{3}\left(2 + 2\sqrt{3} - \sqrt{2}\right)\left[\frac{2}{\pi}E(k_0)\right]^2 \quad (2.18)$$

where the modulus k_0 is defined in (2.8). If we apply (2.9), (2.10), (2.14) and (1.5) to this result we obtain the simplified formula

$$G_3(3) = -13 + \tfrac{35}{2}G_0(3) + 21[\pi^2 G_0(3)]^{-1}. \quad (2.19)$$

From (2.19) we can calculate the numerical value

$$G_3(3) = 0.055\,090\,260\,336\,475\,582\,430\,366\,396\,424\ldots. \quad (2.20)$$

The formulae (2.16) and (2.19) have also been derived by Glasser and Boersma (2000) using different methods.

3. Recurrence relations for $G(l, m, n; w)$

In this section we shall use the recurrence relations developed by Horiguchi (1971) and Morita (1975) to express the general Green function $G(l, m, n; w)$ in terms of the known functions $G_0(w)$, $G_2(w)$ and $G_3(w)$. It will be assumed, without loss of generality, that $l \geqslant m \geqslant n \geqslant 0$.

3.1. Relations for $G(l, m, 0; w)$ with $l + m \leqslant 4$

We begin by considering the basic recurrence formula (Montroll and Weiss 1965, Horiguchi 1971)

$$G(l+1, m, n; w) + G(l-1, m, n; w) + G(l, m+1, n; w) + G(l, m-1, n; w) + G(l, m, n+1; w) + G(l, m, n-1; w) = -2\delta_{l,0}\delta_{m,0}\delta_{n,0} + 2wG(l, m, n; w) \tag{3.1}$$

where δ denotes the Kronecker symbol. If we make the substitutions $l = m = n = 0$; $l = 1, m = n = 0$ and $l = 2, m = n = 0$ in (3.1) we obtain the relations

$$3G(1, 0, 0; w) = -1 + wG_0(w) \tag{3.2}$$

$$4G(1, 1, 0; w) = -G_0(w) + 2wG(1, 0, 0; w) - G_2(w) \tag{3.3}$$

$$4G(2, 1, 0; w) = -G(1, 0, 0; w) + 2wG_2(w) - G_3(w) \tag{3.4}$$

respectively. From these results it is readily seen that

$$12G(1, 1, 0; w) = -2w - (3 - 2w^2)G_0(w) - 3G_2(w) \tag{3.5}$$

$$12G(2, 1, 0; w) = 1 - wG_0(w) + 6wG_2(w) - 3G_3(w). \tag{3.6}$$

Next we use equations [4.9*a*], [4.9*b*], [4.10*a*], [4.10*b*], [4.12*a*] and [4.12*b*] derived by Morita (1975) to obtain the following set of recurrence relations:

$$\begin{aligned}(2p+1)[G(p+2, p, 0; w) + G(p+1, p+1, 0; w)] &= 2(4p+1)wG(p+1, p, 0; w) - 4p[G(p+1, p-1, 0; w) + w^2G(p, p, 0; w)] \\ &\quad - (2p-1)[G(p, p-2, 0; w) + G(p-1, p-1, 0; w)] \\ &\quad + 2(4p-1)wG(p, p-1, 0; w)\end{aligned} \tag{3.7}$$

$$\begin{aligned}3G(p+3, p-1, 0; w) + 4G(p+2, p, 0; w) + G(p+1, p+1, 0; w) &= 2w[5G(p+2, p-1, 0; w) + 3G(p+1, p, 0; w)] - 6G(p+2, p-2, 0; w) \\ &\quad - 8w^2G(p+1, p-1, 0; w) - 2G(p, p, 0; w) - 3G(p+1, p-3, 0; w) \\ &\quad + 2w[5G(p+1, p-2, 0; w) + 3G(p, p-1, 0; w)] - 4G(p, p-2, 0; w) \\ &\quad - G(p-1, p-1, 0; w)\end{aligned} \tag{3.8}$$

$$\begin{aligned}3G(p+3, p-1, 0; w) + 4(p+1)G(p+2, p, 0; w) - (4p+3)G(p+1, p+1, 0; w) &= 2(p+4)wG(p+2, p-1, 0; w) - 2(p-2)wG(p+1, p, 0; w) \\ &\quad - 3G(p+2, p-2, 0; w) - 4[1 + (p+1)w^2]G(p+1, p-1, 0; w) \\ &\quad - (1 - 4pw^2)G(p, p, 0; w) + 2(p+1)wG(p+1, p-2, 0; w) \\ &\quad - 2(p-1)wG(p, p-1, 0; w)\end{aligned} \tag{3.9}$$

where $p \geqslant 1$. It should be noted that the equations [4.12*a*] and [4.12*b*] as given by Morita (1975) contain several errors. For the isotropic case ($\gamma = 1$) the corrected equations (in the notation of Morita) are given by

$$3G'(2p+2, 4, 0) + 4(1+p)G'(2p+2, 2, 0) - (3+4p)G'(2p+2, 0, 0) = N'_4 \qquad [4.12a]$$

and

$$N_4' = 2(p+4)tG'(2p+1,3,0) - 2(p-2)tG'(2p+1,1,0) - 3G'(2p,4,0) \\ - 4[1+(p+1)t^2]G'(2p,2,0) - (1-4pt^2)G'(2p,0,0) \\ + 2(p+1)tG'(2p-1,3,0) - 2(p-1)tG'(2p-1,1,0). \qquad [4.12b]$$

It is now possible to determine relations for $G(4,0,0;w)$, $G(3,1,0;w)$ and $G(2,2,0;w)$ by solving equations (3.7)–(3.9) with $p = 1$. This procedure yields

$$9G(4,0,0;w) = 5G_0(w) - 30wG(1,0,0;w) - 16(1-2w^2)G(1,1,0;w) \\ + 4(11-6w^2)G_2(w) - 32wG(2,1,0;w) + 30wG_3(w) \qquad (3.10)$$

$$9G(3,1,0;w) = -2G_0(w) + 12wG(1,0,0;w) + (1-8w^2)G(1,1,0;w) \\ - 14G_2(w) + 20wG(2,1,0;w) \qquad (3.11)$$

$$9G(2,2,0;w) = -G_0(w) + 6wG(1,0,0;w) - 4(1+w^2)G(1,1,0;w) \\ + 2G_2(w) + 10wG(2,1,0;w). \qquad (3.12)$$

The application of (3.2), (3.5) and (3.6) to these results gives

$$27G(4,0,0;w) = 2w(15-8w^2) + (27-54w^2+16w^4)G_0(w) \\ + 144(1-w^2)G_2(w) + 114wG_3(w) \qquad (3.13)$$

$$108G(3,1,0;w) = -2w(15-8w^2) - (27-54w^2+16w^4)G_0(w) \\ - 9(19-16w^2)G_2(w) - 60wG_3(w) \qquad (3.14)$$

$$54G(2,2,0;w) = -w(3-4w^2) + w^2(9-4w^2)G_0(w) \\ + 18(1+2w^2)G_2(w) - 15wG_3(w). \qquad (3.15)$$

We have now established the required relations for all the Green functions $G(l,m,0;w)$ which have $l+m \leqslant 4$.

3.2. Relations for $G(l,m,0;w)$ with $l+m \geqslant 5$

We begin the analysis of the case $l+m \geqslant 5$ by using equations [4.7] and [4.8] given by Morita (1975) to obtain the following recurrence formulae:

$$G(p+2,p-1,0;w) + G(p+1,p,0;w) \\ = 3wG(p+1,p-1,0;w) + wG(p,p,0;w) - 2G(p+1,p-2,0;w) \\ - 2w^2G(p,p-1,0;w) + 3wG(p,p-2,0;w) + wG(p-1,p-1,0;w) \\ - G(p,p-3,0;w) - G(p-1,p-2,0;w) \qquad (3.16)$$

$$p[G(p+2,p-1,0;w) + 3G(p+1,p,0;w)] \\ = (4p-1)w[G(p+1,p-1,0;w) + G(p,p,0;w)] \\ - (2p-1)[G(p+1,p-2,0;w) + (1+2w^2)G(p,p-1,0;w)] \\ + (4p-3)w[G(p,p-2,0;w) + G(p-1,p-1,0;w)] \\ - (p-1)[G(p,p-3,0;w) + 3G(p-1,p-2,0;w)] \qquad (3.17)$$

where $p \geqslant 2$. From these results it is evident that we can derive recurrence relations for $G(p+2,p-1,0;w)$ and $G(p+1,p,0;w)$ in terms of $G(l,m,0;w)$ with $2p-3 \leqslant l+m \leqslant 2p$. When $p = 2$ this procedure enables one to evaluate $G(4,1,0;w)$ and $G(3,2,0;w)$ in terms of *known* $G(l,m,0;w)$ which have $1 \leqslant l+m \leqslant 4$.

Next we make the substitutions $l' = 2p - 1$ and $m' = 2q - 1$ in equation [4.4] given by Morita (1975). In this manner we find that

$$\begin{aligned}
&2qG(p+q+1, p-q, 0; w)\\
&\quad = -2q[2G(p+q, p-q-1, 0; w) + G(p+q-1, p-q-2, 0; w)]\\
&\quad\quad + 2(4q-1)w[G(p+q, p-q, 0; w) + G(p+q-1, p-q-1, 0; w)]\\
&\quad\quad - 2(2q-1)[G(p+q, p-q+1, 0; w) + 2w^2 G(p+q-1, p-q, 0; w)\\
&\quad\quad + G(p+q-2, p-q-1, 0; w)] + 2(4q-3)w[G(p+q-1, p-q+1, 0; w)\\
&\quad\quad + G(p+q-2, p-q, 0; w)] - 2(q-1)[G(p+q-1, p-q+2, 0; w)\\
&\quad\quad + 2G(p+q-2, p-q+1, 0; w) + G(p+q-3, p-q, 0; w)] \qquad (3.18)
\end{aligned}$$

where $p \geqslant 2$ and $2 \leqslant q \leqslant p$. From (3.18) and the relations for $G(p+2, p-1, 0; w)$ and $G(p+1, p, 0; w)$ it is possible to express $\{G(p+q+1, p-q, 0; w) : q = 2, \ldots, p\}$ in terms of $G(l, m, 0; w)$ with $2p-3 \leqslant l+m \leqslant 2p$. Recurrence relations have now been established for all Green functions $G(l, m, 0; w)$ which have $l+m = 2p+1$, with $p \geqslant 2$.

For the case $l+m = 2p+2$ we can use (3.7)–(3.9) to evaluate $G(p+3, p-1, 0; w)$, $G(p+2, p, 0; w)$ and $G(p+1, p+1, 0; w)$ in terms of the Green functions $G(l, m, 0; w)$ with $2p-2 \leqslant l+m \leqslant 2p+1$. We also make the substitutions $l' = 2p$ and $m' = 2q$ in equation [4.4] given by Morita (1975). This procedure yields the further relation

$$\begin{aligned}
&(2q+1)G(p+q+2, p-q, 0; w)\\
&\quad = -(2q+1)[2G(p+q+1, p-q-1, 0; w) + G(p+q, p-q-2, 0; w)]\\
&\quad\quad + 2(4q+1)w[G(p+q+1, p-q, 0; w) + G(p+q, p-q-1, 0; w)]\\
&\quad\quad - 4q[G(p+q+1, p-q+1, 0; w) + 2w^2 G(p+q, p-q, 0; w)\\
&\quad\quad + G(p+q-1, p-q-1, 0; w)] + 2(4q-1)w[G(p+q, p-q+1, 0; w)\\
&\quad\quad + G(p+q-1, p-q, 0; w)] - (2q-1)[G(p+q, p-q+2, 0; w)\\
&\quad\quad + 2G(p+q-1, p-q+1, 0; w) + G(p+q-2, p-q, 0; w)] \qquad (3.19)
\end{aligned}$$

where $p \geqslant 2$ and $2 \leqslant q \leqslant p$. This formula and the relations for $G(p+3, p-1, 0; w)$ and $G(p+2, p, 0; w)$ enable one to express $\{G(p+q+2, p-q, 0; w) : q = 2, \ldots, p\}$ in terms of $G(l, m, 0; w)$ with $2p-2 \leqslant l+m \leqslant 2p+1$. It has now been shown that we can derive recurrence relations for all Green functions $G(l, m, 0; w)$ which have $l+m = 2p+2$, with $p \geqslant 2$.

If the whole procedure described in section 3.2 is carried out for increasing values of p in the range $2 \leqslant p \leqslant p_{\max}$ then it is possible, at least in principle, to evaluate all the Green functions $G(l, m, 0; w)$ with $l+m \leqslant 2p_{\max}+2$ in terms of the basic functions $G_0(w)$, $G_2(w)$ and $G_3(w)$. The complicated algebra involved in these calculations has been performed using *Mathematica* (Wolfram 1991) for $p_{\max} = 3$ and the final formulae for $G(l, m, 0)$ are listed in the appendix for $l+m \leqslant 8$.

3.3. Relations for $G(l, m, n; w)$ with $n \geqslant 1$

If we assume that $G(l, m, 0)$ has been evaluated for $l+m \leqslant 2p_{\max}+2$, where $p_{\max} \geqslant 2$, then we can determine $G(l, m, n; w)$ with $n \geqslant 1$ by using the basic recurrence relation (3.1). For example, if we make the substitution $n = 0$ in (3.1) it is found that

$$\begin{aligned}
2G(l, m, 1; w) &= 2wG(l, m, 0; w) - G(l+1, m, 0; w) - G(l-1, m, 0; w)\\
&\quad - G(l, m+1, 0; w) - G(l, m-1, 0; w). \qquad (3.20)
\end{aligned}$$

From this result it is possible to calculate all the Green functions $G(l, m, 1; w)$ with $l + m \leqslant 2p_{\max} + 1$. By repeating this procedure for increasing values of n we are able to express all the Green functions $G(l, m, n; w)$ with $l+m+n \leqslant 2p_{\max}+2$ in terms of $G_0(w)$, $G_2(w)$ and $G_3(w)$. The final formulae are listed in the appendix for $l + m + n \leqslant 8$.

From the results in the appendix it is evident that, in general, we can express the Green function $G(l, m, n; w)$ in the form

$$G(l, m, n; w) = Q_0(l, m, n; w) + Q_1(l, m, n; w)G_0(w) + Q_2(l, m, n; w)G_2(w) + Q_3(l, m, n; w)G_3(w) \tag{3.21}$$

where $\{Q_j(l, m, n; w) : j = 0, 1, 2, 3\}$ is a set of polynomials in the variable w with rational coefficients which depend on l, m and n. It follows from the symmetry relation (1.2) that the polynomials Q_0 and Q_3 are odd functions of w for even values of $l+m+n$ and even functions of w for odd values of $l + m + n$, while the polynomials Q_1 and Q_2 are even functions of w for even values of $l + m + n$ and odd functions of w for odd values of $l + m + n$. A detailed inspection of the appendix also suggests that the degrees of the polynomials $\{Q_j : j = 0, 1, 2, 3\}$ are $p - 1, p, p - 2$ and $p - 3$ respectively, provided that $p = l + m + n \geqslant 4$. When $l + m + n \leqslant 3$ the relation (3.21) does not always involve all the polynomials $\{Q_j : j = 0, 1, 2, 3\}$.

4. Exact formulae for $G(l, m, n; w)$

We shall now use the results obtained in previous sections to derive exact formulae for the Green function $G(l, m, n; w)$ in terms of the complete elliptic integrals $K(k)$ and $E(k)$.

4.1. General results for arbitrary values of $w \in \mathcal{C}^-$

If equations (1.14), (1.15), (1.19), (2.5) and (2.6) are applied to equation (3.21) it is found that it is possible, at least in principle, to express the modified Green function

$$\overline{G}(l, m, n; w) \equiv (3/w)^{l+m+n} wG(l, m, n; w) \tag{4.1}$$

in the form

$$\overline{G}(l, m, n; w) = R_0(l, m, n; \xi) + R_1(l, m, n; \xi)\left[\frac{2}{\pi}K(k)\right]^2 + R_2(l, m, n; \xi)\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] + R_3(l, m, n; \xi)\left[\frac{2}{\pi}E(k)\right]^2 \tag{4.2}$$

where $\{R_j(l, m, n : \xi);\ j = 0, 1, 2, 3\}$ denotes a set of *rational* functions of ξ, the modulus $k = k(\xi)$ is defined in (1.16) and $\xi = \xi(w)$ is given by (1.17). The determination of the set of rational functions $\{R_j(l, m, n : \xi);\ j = 0, 1, 2, 3\}$ for particular values of l, m and n involves a large amount of tedious algebra which was carried out using *Mathematica* (Wolfram 1991). Some typical results are listed below:

$$\overline{G}(1, 1, 0; w) = -\frac{9}{4}(1+\xi)^2(1-3\xi)(1-\xi)^{-1}(1-3\xi^2)^{-1}\left[\frac{2}{\pi}K(k)\right]^2 + 9(1-5\xi^2)(1-9\xi^4)^{-1}\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] - \frac{27}{4}(1-\xi)^3(1+3\xi)(1-9\xi^4)^{-1}\left[\frac{2}{\pi}E(k)\right]^2 \tag{4.3}$$

$$\begin{aligned}\overline{G}(2,1,0;w) &= 36\xi^2(1-\xi^2)(1-9\xi^2)(1-9\xi^4)^{-2} \\ &\quad -\frac{9}{8}(1+\xi)(1-3\xi)(1-\xi)^{-2}(1-9\xi^4)^{-2} \\ &\quad \times(15-46\xi^2-306\xi^6+81\xi^8)\left[\frac{2}{\pi}K(k)\right]^2 \\ &\quad +\frac{27}{4}(7-50\xi^2+90\xi^6+81\xi^8)(1-9\xi^4)^{-2}\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] \\ &\quad -\frac{243}{8}(1-\xi)^3(1+3\xi)(1-9\xi^4)^{-1}\left[\frac{2}{\pi}E(k)\right]^2 \end{aligned} \tag{4.4}$$

$$\begin{aligned}\overline{G}(1,1,1;w) &= \frac{81}{8}(1+\xi)^3(1-3\xi)(1+\xi^2)(1-9\xi^2)(1-9\xi^4)^{-2}\left[\frac{2}{\pi}K(k)\right]^2 \\ &\quad -\frac{81}{4}(1-\xi^2)(1-9\xi^2)(1+3\xi^4)(1-9\xi^4)^{-2}\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] \\ &\quad +\frac{81}{8}(1-\xi)^3(1+3\xi)(1-9\xi^4)^{-1}\left[\frac{2}{\pi}E(k)\right]^2 \end{aligned} \tag{4.5}$$

$$\begin{aligned}\overline{G}(4,0,0;w) &= -216(1-9\xi^4)^{-2}(1+10\xi^2-118\xi^4+90\xi^6+81\xi^8) \\ &\quad +27(1-\xi)^{-3}(1+3\xi)^{-1}(1-9\xi^4)^{-3}(49-460\xi^2-620\xi^4 \\ &\quad +13276\xi^6-21450\xi^8-8148\xi^{10}-30636\xi^{12}+62532\xi^{14} \\ &\quad +18225\xi^{16})\left[\frac{2}{\pi}K(k)\right]^2-54(63-282\xi^2-2655\xi^4+12652\xi^6 \\ &\quad -3735\xi^8-12690\xi^{10}-4617\xi^{12})(1-9\xi^4)^{-3}\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] \\ &\quad +27(1-\xi)^3(1+3\xi)(1-9\xi^4)^{-3}(85+192\xi^2-3450\xi^4 \\ &\quad +1728\xi^6+6885\xi^8)\left[\frac{2}{\pi}E(k)\right]^2 \end{aligned} \tag{4.6}$$

$$\begin{aligned}\overline{G}(3,1,0;w) &= 432\xi^2(1-\xi^2)(1-9\xi^2)(1-9\xi^4)^{-2} \\ &\quad -\frac{27}{2}(1+\xi)(1-3\xi)(1-\xi)^{-2}(1-9\xi^4)^{-3}(7+24\xi^2-479\xi^4 \\ &\quad +600\xi^6+537\xi^8+1440\xi^{10}-81\xi^{12})\left[\frac{2}{\pi}K(k)\right]^2+27(1-9\xi^4)^{-3} \\ &\quad \times(9+6\xi^2-1197\xi^4+5144\xi^6-3501\xi^8-270\xi^{10}-1215\xi^{12}) \\ &\quad \times\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right]-\frac{27}{2}(1-\xi)^3(1+3\xi)(1-9\xi^4)^{-3} \\ &\quad \times(11+114\xi^2-1338\xi^4+1026\xi^6+891\xi^8)\left[\frac{2}{\pi}E(k)\right]^2 \end{aligned} \tag{4.7}$$

$$\begin{aligned}\overline{G}(2,2,0;w) &= -\frac{27}{4}(1+\xi)^3(1-3\xi)(1-9\xi^4)^{-2}(1+3\xi^2)^{-1} \\ &\quad \times(7-27\xi^2-39\xi^4+27\xi^6)\left[\frac{2}{\pi}K(k)\right]^2+\frac{27}{2}(1-9\xi^4)^{-3} \\ &\quad \times(9-102\xi^2+423\xi^4-1228\xi^6+1359\xi^8-270\xi^{10}-1215\xi^{12}) \end{aligned}$$

$$\times \left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] - \frac{27}{4}(1-\xi)^3(1+3\xi)(1-9\xi^4)^{-3}$$
$$\times (11 - 48\xi^2 + 282\xi^4 - 432\xi^6 + 891\xi^8)\left[\frac{2}{\pi}E(k)\right]^2 \tag{4.8}$$

$$\overline{G}(2,1,1;w) = \frac{81}{4}(1+\xi)^3(1-3\xi)(1-\xi^2)(1-9\xi^2)(1-3\xi^2)^{-2}(1-9\xi^4)^{-1}$$
$$\times \left[\frac{2}{\pi}K(k)\right]^2 - \frac{81}{2}(1-9\xi^2)(1-\xi^2)(1-9\xi^4)^{-3}(1+8\xi^2$$
$$- 46\xi^4 - 27\xi^8)\left[\frac{2}{\pi}K(k)\right]\left[\frac{2}{\pi}E(k)\right] + \frac{81}{4}(1-\xi)^3(1+3\xi)$$
$$\times (1-9\xi^4)^{-3}(1+18\xi^2-27\xi^4)(1-6\xi^2-3\xi^4)\left[\frac{2}{\pi}E(k)\right]^2 \tag{4.9}$$

where the modulus $k = k(\xi)$ is defined in (1.16) and the function $\xi = \xi(w)$ is given by (1.17). The results (4.3)–(4.9) are new representations for $\overline{G}(l, m, n; w)$ which can be used to calculate accurate numerical values of the Green function $G(l, m, n; w)$ at *any* point w in the complex cut plane $\mathcal{C}^-$. The relations listed in the appendix also enable one to derive further exact formulae of the type (4.2) for all $\overline{G}(l, m, n; w)$ which have $5 \leqslant l + m + n \leqslant 8$.

It is always possible, at least in principle, to separate $G(l, m, n; w)$ into its real and imaginary parts, and write

$$G(l, m, n; w) \equiv G_R(l, m, n; u, v) + iG_I(l, m, n; u, v) \tag{4.10}$$

where $w = u + iv$. We can achieve considerable insight into the global properties of $G(l, m, n; w)$ by constructing surface representations for G_R and G_I above the (u, v) cut plane $\mathcal{C}^-$. In order to illustrate this procedure we give in figure 1 the surface for $G_I(1, 1, 1; u, v)$ which was plotted by making a *direct* application of *Mathematica* (Wolfram 1991) to the formula (4.5). Figure 1 clearly shows the discontinuous behaviour of G_I along the edge of the cut and the branch-point singularities at $w = \pm 1$.

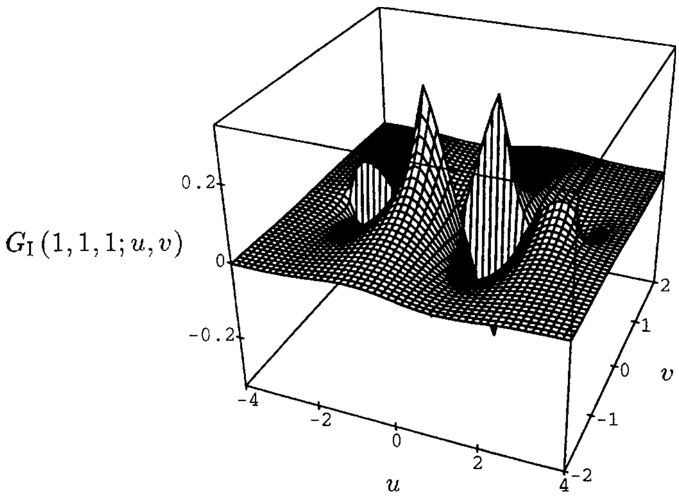

Figure 1. Surface for the imaginary part $G_I(1, 1, 1; u, v)$ of the simple cubic lattice Green function $G(1, 1, 1; w)$ plotted above the (u, v) plane.

4.2. Formulae for the special case $w = 3$

If we make the substitution $w = 3$ in (3.21) and then apply the formulae (2.16) and (2.19) it is found that

$$G(l, m, n; 3) = r_0(l, m, n) + r_1(l, m, n)G_0(3) + r_2(l, m, n)[\pi^2 G_0(3)]^{-1} \tag{4.11}$$

where $\{r_j(l, m, n) : j = 0, 1, 2\}$ denotes a set of rational numbers. Glasser and Boersma (2000) have also derived the result (4.11) using a different recursion scheme developed by Duffin and Shelly (1958). Explicit formulae for $G(l, m, n; 3)$ of the type (4.11) have been obtained for all lattice sites (l, m, n) which have $0 \leqslant n \leqslant m \leqslant l \leqslant 10$, and the numerical values of $G(l, m, n; 3)$ have been calculated to 45 figures for $0 \leqslant n \leqslant m \leqslant l \leqslant 20$. This material is available on request from the author in the form of unpublished tables.

Finally, the asymptotic behaviour of $G(l, m, n; 3)$ as $R \equiv (l^2 + m^2 + n^2)^{1/2} \to \infty$ has been determined using the work of Duffin (1953). In particular, we find that

$$\begin{aligned}G(l, m, n; 3) \sim{} & \frac{1}{2\pi R} + \frac{1}{8\pi R^7}[(l^4 + m^4 + n^4) - 3(l^2m^2 + l^2n^2 + m^2n^2)] \\ & + \frac{1}{64\pi R^{13}}[23(l^8 + m^8 + n^8) - 244(l^6m^2 + l^2m^6 + m^6n^2 \\ & + m^2n^6 + l^2n^6 + l^6n^2) + 621(l^4m^4 + m^4n^4 + l^4n^4) \\ & - 228(l^4m^2n^2 + l^2m^4n^2 + l^2m^2n^4)] + \cdots\end{aligned} \tag{4.12}$$

as $R \to \infty$. This result enables one to carry out useful checks on the exact results for $G(l, m, n; 3)$. For example, we find that

$$G(10, 10, 10; 3) = \frac{9103\,337\,588\,547\,750\,625\,\alpha - 22\,955\,005\,286\,093\,930\,166\,\beta}{61\,677\,742\,126\,000} \tag{4.13}$$

where

$$\alpha = G_0(3) \qquad \text{and} \qquad \beta = [\pi^2 G_0(3)]^{-1}. \tag{4.14}$$

From this result we obtain the numerical value

$$G(10, 10, 10; 3) = 0.009\,183\,702\,020\,546\,191\,790\,374\,219\,924\ldots \tag{4.15}$$

while (4.12) gives the approximation

$$G(10, 10, 10; 3) \sim 0.009\,183\,7015\ldots. \tag{4.16}$$

5. Concluding remarks on $G(n, n, n; w)$ and $G(2n, n, n; w)$

If computer algebra factorization methods are applied to the results (4.3)–(4.9) we make the surprising discovery that the formulae (4.5) and (4.9) can both 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! In particular, it is found that

$$\begin{aligned}\overline{G}(1, 1, 1; w) = {} & \frac{81(1 + 3\xi)}{8(1 - 9\xi^4)^2}\left(\frac{2}{\pi}\right)^2 [(1 + \xi)^2(1 - 3\xi)K(k) - (1 - \xi)(1 + 3\xi^2)E(k)] \\ & \times [(1 + \xi)(1 - 3\xi)(1 + \xi^2)K(k) - (1 - \xi)^2(1 - 3\xi^2)E(k)]\end{aligned} \tag{5.1}$$

$$\begin{aligned}\overline{G}(2, 1, 1; w) = {} & \frac{81(1 - \xi)(1 + 3\xi)}{4(1 - 9\xi^4)^3}\left(\frac{2}{\pi}\right)^2 [(1 + \xi)^3(1 - 3\xi)K(k) - (1 - 6\xi^2 - 3\xi^4)E(k)] \\ & \times[(1 + \xi)(1 - 3\xi)(1 + 3\xi^2)^2K(k) - (1 - \xi)^2 \\ & \times (1 + 18\xi^2 - 27\xi^4)E(k)].\end{aligned} \tag{5.2}$$

Further investigations show that this factorization property also holds for other lattice Green functions of the type $G(n, n, n; w)$ and $G(2n, n, n; w)$. Some examples of the higher-order product forms for the diagonal Green function are given below:

$$\overline{G}(2,2,2;w) = \frac{729(1-\xi)^2(1+3\xi)}{20(1-9\xi^4)^5}\left(\frac{2}{\pi}\right)^2 [(1+\xi)^3(1-3\xi)(1-36\xi^2+27\xi^4)K(k) - (1-9\xi^4)(1+6\xi-3\xi^2)(1-6\xi-3\xi^2)E(k)] \times [(1+\xi)^2(1-3\xi)(1-7\xi^2-27\xi^4-27\xi^6)K(k) - (1-\xi)(1-9\xi^4)(1-12\xi^2+9\xi^4)E(k)] \quad (5.3)$$

$$\overline{G}(3,3,3;w) = \frac{6561(1-\xi)^3(1+3\xi)}{35(1-9\xi^4)^8}\left(\frac{2}{\pi}\right)^2 [(1+\xi)^3(1-3\xi)(1-15\xi^2+24\xi^4 + 216\xi^6+729\xi^8+729\xi^{10})K(k) - (1-3\xi^2)(1-18\xi^2+57\xi^4 + 240\xi^6+513\xi^8-1458\xi^{10}+729\xi^{12})E(k)][(1+\xi)^3(1-3\xi) \times (1-51\xi^2+1212\xi^4-3132\xi^6+2187\xi^8-729\xi^{10})K(k) - (1+3\xi^2)(1-60\xi^2+1695\xi^4-8664\xi^6+15255\xi^8 - 4860\xi^{10}+729\xi^{12})E(k)] \quad (5.4)$$

$$\overline{G}(4,4,4;w) = \frac{2125764(1-\xi)^3(1+3\xi)}{1925(1-9\xi^4)^{11}}\left(\frac{2}{\pi}\right)^2 [(1+\xi)^3(1-3\xi)(1-24\xi^2 + 160\xi^4-16\xi^6-1260\xi^8-4968\xi^{10}-13608\xi^{12}+19683\xi^{16})K(k) - (1-9\xi^4)(1-12\xi^2+9\xi^4)(1-18\xi^2+85\xi^4-40\xi^6+765\xi^8 - 1458\xi^{10}+729\xi^{12})E(k)][(1+\xi)^3(1-3\xi)(1-68\xi^2+2074\xi^4 - 40364\xi^6+169020\xi^8-281772\xi^{10}+194886\xi^{12}-96228\xi^{14} + 19683\xi^{16})K(k) - (1-9\xi^4)(1+6\xi-3\xi^2)(1-6\xi-3\xi^2) \times (1-32\xi^2+1135\xi^4-5360\xi^6+10215\xi^8 - 2592\xi^{10}+729\xi^{12})E(k)]. \quad (5.5)$$

For the lattice Green function $G(2n, n, n; w)$ we obtain the following higher-order product forms:

$$\overline{G}(4,2,2;w) = \frac{6561(1-\xi)^2(1+3\xi)}{35(1-9\xi^4)^7}\left(\frac{2}{\pi}\right)^2 [(1+\xi)^3(1-3\xi)(1-12\xi^2+30\xi^4 - 44\xi^6+9\xi^8)K(k) - (1-10\xi^2+\xi^4)(1-6\xi^2-3\xi^4) \times (1-2\xi^2+9\xi^4)E(k)][(1+\xi)^2(1-3\xi)(1+9\xi^2) \times (1-78\xi^2+72\xi^4-162\xi^6-729\xi^8)K(k) - (1-\xi) \times (1-2\xi^2+9\xi^4)(1+18\xi^2-27\xi^4) \times (1-90\xi^2+81\xi^4)E(k)] \quad (5.6)$$

$$\overline{G}(6,3,3;w) = \frac{944784(1-\xi)^3(1+3\xi)}{385(1-9\xi^4)^{11}}\left(\frac{2}{\pi}\right)^2 [(1+\xi)^3(1-3\xi)(1-90\xi^2 + 4428\xi^4+49572\xi^6-65610\xi^8+669222\xi^{10}-708588\xi^{12} + 4782969\xi^{16})K(k) - (1+18\xi^2-27\xi^4)(1-114\xi^2+7044\xi^4$$

$$
\begin{aligned}
&- 32724\xi^{6} + 185166\xi^{8} - 607986\xi^{10} + 1338444\xi^{12} - 1417176\xi^{14} \\
&+ 531441\xi^{16})E(k)][(1+\xi)^{3}(1-3\xi)(1-24\xi^{2}+204\xi^{4}-786\xi^{6} \\
&+ 1710\xi^{8} - 2196\xi^{10} + 2628\xi^{12} - 594\xi^{14} + 81\xi^{16})K(k) \\
&- (1-6\xi^{2}-3\xi^{4})(1-24\xi^{2}+204\xi^{4}-834\xi^{6}+2286\xi^{8} \\
&- 3636\xi^{10} + 7044\xi^{12} - 1026\xi^{14} + 81\xi^{16})E(k)] \qquad (5.7)
\end{aligned}
$$

$$
\begin{aligned}
\overline{G}(8,4,4;w) = {}& \frac{918330048(1-\xi)^{3}(1+3\xi)}{25025(1-9\xi^{4})^{15}}\left(\frac{2}{\pi}\right)^{2}[(1+\xi)^{3}(1-3\xi)(1-116\xi^{2} \\
&+ 6642\xi^{4} - 285660\xi^{6} - 3342465\xi^{8} + 7925688\xi^{10} - 83377188\xi^{12} \\
&+ 299024136\xi^{14} - 884849265\xi^{16} + 1052253180\xi^{18} + 774840978\xi^{20} \\
&- 4649045868\xi^{22} + 3486784401\xi^{24})K(k) - (1-2\xi^{2}+9\xi^{4}) \\
&\times (1+18\xi^{2}-27\xi^{4})(1-90\xi^{2}+81\xi^{4})(1-48\xi^{2}+5196\xi^{4} \\
&- 14904\xi^{6} + 121014\xi^{8} - 559872\xi^{10} + 1338444\xi^{12} - 1417176\xi^{14} \\
&+ 531441\xi^{16})E(k)][(1+\xi)^{3}(1-3\xi)(1-36\xi^{2}+522\xi^{4}-3980\xi^{6} \\
&+ 17895\xi^{8} - 51816\xi^{10} + 102156\xi^{12} - 144792\xi^{14} + 146655\xi^{16} \\
&- 163380\xi^{18} + 37962\xi^{20} - 7452\xi^{22} + 729\xi^{24})K(k) \\
&- (1-10\xi^{2}+\xi^{4})(1-6\xi^{2}-3\xi^{4})(1-2\xi^{2}+9\xi^{4}) \\
&\times (1-24\xi^{2}+204\xi^{4}-768\xi^{6}+1494\xi^{8}-1656\xi^{10} \\
&+ 5196\xi^{12} - 432\xi^{14} + 81\xi^{16})E(k)]. \qquad (5.8)
\end{aligned}
$$

From the explicit results given in this section we *conjecture* that the elliptic integral formulae for Green functions of the type $G(n,n,n;w)$ and $G(2n,n,n;w)$ can be factorized as a product of two linear forms in $K(k)$ and $E(k)$ for *all* values of $n = 1, 2, \ldots$. The possibility of establishing a *general proof* of this conjecture is currently being investigated by the author in collaboration with R T Delves.

Appendix

In this section we list expressions for $G(l,m,n;w)$ in terms of $G_0(w)$, $G_2(w)$ and $G_3(w)$, where $l+m+n \leqslant 8$.

$$G(0,0,0;w) = G_0(w)$$

$$3G(1,0,0;w) = -1 + wG_0(w)$$

$$G(2,0,0;w) = G_2(w)$$

$$12G(1,1,0;w) = -2w - (3-2w^{2})G_0(w) - 3G_2(w)$$

$$G(3,0,0;w) = G_3(w)$$

$$12G(2,1,0;w) = 1 - wG_0(w) + 6wG_2(w) - 3G_3(w)$$

$$12G(1,1,1;w) = (3-2w^{2}) - 2w(3-w^{2})G_0(w) - 9wG_2(w) + 3G_3(w)$$

$$
\begin{aligned}
27G(4,0,0;w) = {}& 2w(15-8w^{2}) + (27-54w^{2}+16w^{4})G_0(w) \\
&+ 144(1-w^{2})G_2(w) + 114wG_3(w)
\end{aligned}
$$

$$
\begin{aligned}
108G(3,1,0;w) = {}& -2w(15-8w^{2}) - (27-54w^{2}+16w^{4})G_0(w) \\
&- 9(19-16w^{2})G_2(w) - 60wG_3(w)
\end{aligned}
$$

$$54G(2,2,0;w) = -w(3-4w^2) + w^2(9-4w^2)G_0(w) + 18(1+2w^2)G_2(w) - 15wG_3(w)$$

$$36G(2,1,1;w) = 4w(3-w^2) + (9-18w^2+4w^4)G_0(w) + 9(1-2w^2)G_2(w) + 6wG_3(w)$$

$$54G(5,0,0;w) = -(45-318w^2+148w^4) + w(315-540w^2+148w^4)G_0(w) + 90w(10-13w^2)G_2(w) + 15(27+46w^2)G_3(w)$$

$$72G(4,1,0;w) = (15-66w^2+28w^4) - w(69-108w^2+28w^4)G_0(w) - 18w(6-11w^2)G_2(w) - 3(51+26w^2)G_3(w)$$

$$216G(3,2,0;w) = (9-66w^2+28w^4) - w(63-108w^2+28w^4)G_0(w) - 18w(8-11w^2)G_2(w) + 3(27-26w^2)G_3(w)$$

$$36G(3,1,1;w) = -2(3-6w^2+2w^4) + w(15-18w^2+4w^4)G_0(w) - 9w(3+2w^2)G_2(w) + 6(3+w^2)G_3(w)$$

$$72G(2,2,1;w) = -(9-18w^2+4w^4) + w(9-2w^2)(3-2w^2)G_0(w) + 18w(2-w^2)G_2(w) - 3(3-2w^2)G_3(w)$$

$$675G(6,0,0;w) = w(3303+10278w^2-5956w^4) + (5616+2943w^2-19212w^4+5956w^6)G_0(w) + 9(3675-620w^2-4858w^4)G_2(w) + 3w(14001+7598w^2)G_3(w)$$

$$2700G(5,1,0;w) = -2w(2589+964w^2-1128w^4) - (6291-6282w^2-5312w^4+2256w^6)G_0(w) - 9(4075-3520w^2-1608w^4)G_2(w) - 24w(1447+231w^2)G_3(w)$$

$$2700G(4,2,0;w) = w(1893-2182w^2+564w^4) + (1296-4167w^2+3028w^4-564w^6)G_0(w) + 18(350-410w^2+201w^4)G_2(w) + 3w(1031-462w^2)G_3(w)$$

$$2700G(3,3,0;w) = 4w(153-297w^2+94w^4) + (189-1728w^2+1752w^4-376w^6)G_0(w) - 9(75+280w^2-268w^4)G_2(w) + 6w(177-154w^2)G_3(w)$$

$$60G(4,1,1;w) = 4w(2-w^2)(3+2w^2) + (33-36w^2-16w^4+8w^6)G_0(w) + 3(15+2w^2)(5-6w^2)G_2(w) + 6w(19+2w^2)G_3(w)$$

$$540G(3,2,1;w) = -2w(69-56w^2+12w^4) - (81-252w^2+148w^4-24w^6)G_0(w) - 9(25-10w^2+12w^4)G_2(w) + 12w(1+3w^2)G_3(w)$$

$$180G(2,2,2;w) = -w(63-42w^2+4w^4) - (36-117w^2+48w^4-4w^6)G_0(w) + 18w^2(10-w^2)G_2(w) - 3w(21-2w^2)G_3(w)$$

$$1350G(7,0,0;w) = -(10125-98022w^2-19772w^4+32944w^6) + w(112959-121968w^2-69188w^4+32944w^6)G_0(w) + 126w(3650-3145w^2-1828w^4)G_2(w) + 21(4725+20282w^2+5336w^4)G_3(w)$$

$$540G(6,1,0;w) = (1125-9276w^2+2504w^4+912w^6) - w(9837-14724w^2+1136w^4+912w^6)G_0(w) - 18w(1945-2240w^2-308w^4)G_2(w) - 3(3645+9172w^2+696w^4)G_3(w)$$

$$1800G(5,2,0;w) = -(825 - 4746w^2 + 3404w^4 - 608w^6) + w(4287 - 8724w^2 + 4316w^4 - 608w^6)G_0(w) + 6w(1200 - 2185w^2 + 616w^4)G_2(w) + 3(2325 + 1682w^2 - 464w^4)G_3(w)$$

$$5400G(4,3,0;w) = -(225 - 2994w^2 + 3356w^4 - 912w^6) + w(2043 - 6336w^2 + 4724w^4 - 912w^6)G_0(w) + 18w(250 - 405w^2 + 308w^4)G_2(w) - 3(675 - 898w^2 + 696w^4)G_3(w)$$

$$180G(5,1,1;w) = -2(45 - 258w^2 + 82w^4 + 16w^6) + w(567 - 834w^2 + 116w^4 + 32w^6)G_0(w) + 9w(185 - 250w^2 - 16w^4)G_2(w) + 6(165 + 161w^2 + 8w^4)G_3(w)$$

$$360G(4,2,1;w) = (3 - 4w^2)(15 - 14w^2 + 4w^4) - w(3 - 2w^2)^2(11 - 4w^2)G_0(w) + 18w(20 - 5w^2 - 4w^4)G_2(w) - 3(105 - 26w^2 - 8w^4)G_3(w)$$

$$540G(3,3,1;w) = -4w^2(1 - w^2)(3 - 4w^2) - w(9 - 18w^2 + 52w^4 - 16w^6)G_0(w) - 9w(5 + 2w^2)(5 + 4w^2)G_2(w) + 6w^2(23 + 4w^2)G_3(w)$$

$$1080G(3,2,2;w) = (135 - 522w^2 + 228w^4 - 16w^6) - w(549 - 828w^2 + 252w^4 - 16w^6)G_0(w) - 18w(30 - 55w^2 + 4w^4)G_2(w) + 3(45 - 114w^2 + 8w^4)G_3(w)$$

$$33075G(8,0,0;w) = 2w(419973 + 6483172w^2 - 1268472w^4 - 1027448w^6) + (2847987 + 10302282w^2 - 20238596w^4 - 545400w^6 + 2054896w^8)G_0(w) + 36(462400 + 903590w^2 - 1551619w^4 - 385382w^6)G_2(w) + 6w(5037691 + 6970776w^2 + 1075684w^4)G_3(w)$$

$$132300G(7,1,0;w) = -2w(748959 + 4333444w^2 - 1898808w^4 - 220320w^6) - (3123171 + 4911498w^2 - 15203552w^4 + 3136656w^6 + 440640w^8)G_0(w) - 9(2029675 + 1080080w^2 - 4287048w^4 - 287520w^6)G_2(w) - 12w(2285189 + 1839282w^2 + 80280w^4)G_3(w)$$

$$66150G(6,2,0;w) = w(220011 + 292876w^2 - 276432w^4 + 36720w^6) + (315792 - 146529w^2 - 637504w^4 + 331512w^6 - 36720w^8)G_0(w) + 18(103825 - 82570w^2 - 62698w^4 + 11980w^6)G_2(w) + 3w(657637 + 139056w^2 - 26760w^4)G_3(w)$$

$$132300G(5,3,0;w) = -4w(28704 - 45649w^2 + 30414w^4 - 7344w^6) - (81027 - 272268w^2 + 309064w^4 - 165720w^6 + 29376w^8)G_0(w) - 9(47275 - 56440w^2 + 29404w^4 - 19168w^6)G_2(w) - 6w(30661 - 14874w^2 + 10704w^4)G_3(w)$$

$$66150G(4,4,0;w) = -w(7923 - 36844w^2 + 38712w^4 - 11016w^6) - (2106 - 31761w^2 + 73906w^4 - 55236w^6 + 11016w^8)G_0(w) + 18(400 + 3110w^2 - 3051w^4 + 3594w^6)G_2(w) - 3w(4241 - 5496w^2 + 8028w^4)G_3(w)$$

$$3780G(6,1,1;w) = 4w(4341 + 5771w^2 - 3432w^4 - 240w^6) + (24273 - 7146w^2 - 45836w^4 + 12288w^6 + 960w^8)G_0(w)$$

$$
\begin{aligned}
&\quad + 9(15625 - 7810w^2 - 13824w^4 - 480w^6)G_2(w) \\
&\quad + 6w(27589 + 8472w^2 + 240w^4)G_3(w) \\
6300G(5, 2, 1; w) &= -2w(3399 - 1556w^2 - 428w^4 + 160w^6) \\
&\quad - (7281 - 13032w^2 + 2548w^4 + 1336w^6 - 320w^8)G_0(w) \\
&\quad - 9(4825 - 6170w^2 + 772w^4 + 160w^6)G_2(w) \\
&\quad - 12w(2354 - 313w^2 - 40w^4)G_3(w) \\
18900G(4, 3, 1; w) &= -2w(111 - 1984w^2 + 408w^4 + 240w^6) \\
&\quad + (891 + 3798w^2 - 6272w^4 + 96w^6 + 480w^8)G_0(w) \\
&\quad + 9(1075 + 680w^2 - 2208w^4 - 240w^6)G_2(w) \\
&\quad - 48w(139 - 183w^2 - 15w^4)G_3(w) \\
315G(4, 2, 2; w) &= 4w(1 - w^2)(39 - 19w^2 + w^4) \\
&\quad + (72 - 360w^2 + 343w^4 - 86w^6 + 4w^8)G_0(w) \\
&\quad + 9(25 - 20w^2 + 39w^4 - 2w^6)G_2(w) + 6w(1 - 20w^2 + w^4)G_3(w) \\
3780G(3, 3, 2; w) &= 4w(1 - w^2)(291 - 124w^2 + 8w^4) \\
&\quad + (513 - 2754w^2 + 2380w^4 - 576w^6 + 32w^8)G_0(w) \\
&\quad + 9(25 - 370w^2 + 256w^4 - 16w^6)G_2(w) + 6w(169 - 132w^2 + 8w^4)G_3(w)
\end{aligned}
$$

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