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On the cubic modular transformation and the cubic lattice Green functions

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Abstract. The elliptic modular transformation of order 3 is used to prove that the lattice Green functions at the origin for the face-centred cubic and simple cubic lattices can both be expressed in terms of the *square* of a complete elliptic integral of the first kind.

1. Introduction

We begin by defining the lattice Green functions at the origin for the body-centred cubic (bcc), face-centred cubic (fcc) and simple cubic (sc) lattices as

$$P(z)_{\mathrm{bcc}} = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{\mathrm{d}\theta_1\mathrm{d}\theta_2\mathrm{d}\theta_3}{1 - z\cos\theta_1\cos\theta_2\cos\theta_3}, \tag{1.1}$$

$$P(z)_{\mathrm{fcc}} = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{\mathrm{d}\theta_1\mathrm{d}\theta_2\mathrm{d}\theta_3}{1 - \frac{z}{3}\left(\cos\theta_1\cos\theta_2 + \cos\theta_2\cos\theta_3 + \cos\theta_3\cos\theta_1\right)}, \tag{1.2}$$

$$P(z)_{\mathrm{sc}} = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{\mathrm{d}\theta_1\mathrm{d}\theta_2\mathrm{d}\theta_3}{1 - \frac{z}{3}\left(\cos\theta_1 + \cos\theta_2 + \cos\theta_3\right)}, \tag{1.3}$$

respectively, where z is a complex variable in a suitably cut z plane. In the theory of random walks on cubic lattices these functions are of fundamental importance as probability generating functions (Montroll and Weiss 1965). The Green functions (1.1)–(1.3) also appear in the theory of lattice vibrations (Montroll 1956) and in many lattice statistical models of phase transitions such as the spherical model (Berlin and Kac 1952, Joyce 1972a).

An exact evaluation of the three triple integrals (1.1)–(1.3) was carried out by Watson (1939) for the special case $z = 1$. In particular, he found that

$$P(1)_{\mathrm{bcc}} = \left[\frac{2}{\pi}K\left(\frac{1}{\sqrt{2}}\right)\right]^2, \tag{1.4}$$

$$P(1)_{\mathrm{fcc}} = \frac{3\sqrt{3}}{4}\left[\frac{2}{\pi}K\left(\frac{\sqrt{3}-1}{2\sqrt{2}}\right)\right]^2, \tag{1.5}$$

$$P(1)_{\mathrm{sc}} = 3\left(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}\right)\left[\frac{2}{\pi}K\left(\left(2-\sqrt{3}\right)\left(\sqrt{3}-\sqrt{2}\right)\right)\right]^2, \tag{1.6}$$

where $K(k)$ denotes the complete elliptic integral of the first kind with modulus k. After Watson's work the problem of investigating the mathematical properties of the Green functions (1.1)–(1.3) for arbitrary values of $z \neq 1$ has been the subject of many papers (see Katsura *et al* 1971).

The main aim in this paper is to show that the elliptic modular transformation of order 3 (Cayley 1874, 1895; Borwein and Borwein 1987) can be used to express the lattice Green functions $P(z)_{\rm fcc}$ and $P(z)_{\rm sc}$ in terms of the *square* of the complete elliptic integral $K(k)$. These results which are valid for arbitrary values of z in a suitably cut z plane are natural generalizations of the Watson formulae (1.5) and (1.6). An important advantage of the modular transformation approach is that it provides one with considerable *insight* into the mathematical structure of the Green functions. In section 2 the various closed-form expressions that are known for the Green functions (1.1)–(1.3) are discussed and simplified parametric representations for $P(z)_{\rm fcc}$ and $P(z)_{\rm sc}$ are derived. In section 3 a concise background to the theory of elliptic modular functions is given. Finally, in section 4 the cubic modular transformation is applied to the parametric representations for $P(z)_{\rm fcc}$ and $P(z)_{\rm sc}$.

2. Formulae for the cubic lattice Green functions

A general formula for $P(z)_{\rm bcc}$ was first obtained by Maradudin (unpublished work) and the result was quoted by Maradudin *et al* (1960) as

$$P(z)_{\rm bcc} = \left[\frac{2}{\pi} K\left(\sqrt{\frac{1}{2} - \frac{1}{2}\sqrt{1-z^2}}\right)\right]^2. \tag{2.1}$$

Various authors (Katsura and Horiguchi 1971, Morita and Horiguchi 1971, Joyce 1971) have used (2.1) and the method of analytic continuation to determine the detailed analytic properties of $P(z)_{\rm bcc}$ in a z plane which is cut along the real axis from $z = -\infty$ to $z = -1$, and from $z = 1$ to $z = +\infty$.

From the work of Iwata (1969) it follows that the Green function $P(z)_{\rm fcc}$ can be expressed in the general product form

$$P(z)_{\rm fcc} = \frac{12}{\pi^2}(3+z)^{-1} K(k_+)\ K(k_-), \tag{2.2}$$

where

$$k_\pm^2 = k_\pm^2(\eta) = \frac{1}{2} \pm \frac{1}{4}\eta(4-\eta)^{\frac{1}{2}} - \frac{1}{4}(2-\eta)(1-\eta)^{\frac{1}{2}}, \tag{2.3}$$

$$\eta = \eta(z) = 4z/(3+z) \tag{2.4}$$

and the variable z lies in a certain finite region $\mathcal{R}_1$ of a complex z plane which is cut along the real axis from $z = -\infty$ to $z = -3$, and from $z = 1$ to $z = +\infty$. The region $\mathcal{R}_1$ which includes the unit disk $|z| \leqslant 1$ has been described by Joyce (1994). If the formula (2.2) is to be used outside the region $\mathcal{R}_1$ it is necessary to replace $K(k_+)$ by its analytic continuation onto the appropriate adjacent Riemann sheet (see Morita and Horiguchi 1971).

A simplification of the algebraic structure of (2.3) can be achieved by introducing the rational transformation

$$z = \frac{12\xi(1+\xi)(1-3\xi)}{(1+3\xi^2)^2}. \tag{2.5}$$

In this manner we obtain the alternative formula

$$P(z)_{\rm fcc} = \frac{4}{\pi^2}\,\frac{(1+3\xi^2)^2}{(1-\xi)^2(1+3\xi)^2}\, K(k_+)\ K(k_-), \tag{2.6}$$

where

$$k_+^2 = k_+^2(\xi) = \frac{16\xi}{(1-\xi)(1+3\xi)^3}, \tag{2.7}$$

$$k_-^2 = k_-^2(\xi) = \frac{16\xi^3}{(1-\xi)^3(1+3\xi)}, \tag{2.8}$$

$$\xi = \xi(z) = \left(1+\sqrt{1-z}\right)^{-1}\left(-1+\sqrt{1+\frac{z}{3}}\right). \tag{2.9}$$

We can use the sequence of equations (2.9)–(2.6) to calculate $P(z)_{\rm fcc}$ for any given value of $z \in \mathcal{R}_1$. It is also seen that equations (2.5)–(2.8) provide one with a parametric representation for $P(z)_{\rm fcc}$ which is valid in a sufficiently small neighbourhood of the origin $\xi = 0$.

A product formula was obtained for the Green function $P(z)_{\rm sc}$ by Joyce (1972b, 1973). In particular, it was found that

$$P(z)_{\rm sc} = \frac{4}{\pi^2}\left(1-\frac{3}{4}\beta\right)^{\frac{1}{2}}(1-\beta)^{-1}\,K(k_+)\,K(k_-), \tag{2.10}$$

where

$$k_\pm^2 = k_\pm^2(\eta) = \frac{1}{2} \pm \frac{1}{4}\eta(4-\eta)^{\frac{1}{2}} - \frac{1}{4}(2-\eta)(1-\eta)^{\frac{1}{2}}, \tag{2.11}$$

$$\eta = \eta(\beta) = \beta/(\beta-1), \tag{2.12}$$

$$\beta = \beta(z) = \frac{1}{2} + \frac{1}{6}z^2 - \frac{1}{2}\left(1-z^2\right)^{\frac{1}{2}}\left(1-\frac{z^2}{9}\right)^{\frac{1}{2}}. \tag{2.13}$$

This result can be used to determine $P(z)_{\rm sc}$ at *any* point in the z plane provided that cuts are made along the real axis from $z = -\infty$ to $z = -1$, and from $z = 1$ to $z = +\infty$.

The rather complicated structure of the formula (2.10) can be simplified by first applying the transformation (Joyce 1994)

$$z^2 = 36\xi^2(1-\xi^2)\,(1-9\xi^2)\,(1-9\xi^4)^{-2} \tag{2.14}$$

to equations (2.10)–(2.13). Hence we find

$$P(z)_{\rm sc} = \frac{4}{\pi^2}\,\frac{(1-9\xi^4)}{(1-\xi^2)\,(1-9\xi^2)}\,K(k_+)\,K(k_-), \tag{2.15}$$

where

$$k_+^2 = k_+^2(\xi) = \frac{1}{2} - \frac{\left(1+18\xi^2-27\xi^4\right)}{2\left(1-\xi^2\right)^{\frac{1}{2}}\left(1-9\xi^2\right)^{\frac{3}{2}}}, \tag{2.16}$$

$$k_-^2 = k_-^2(\xi) = \frac{1}{2} - \frac{\left(1-6\xi^2-3\xi^4\right)}{2\left(1-\xi^2\right)^{\frac{3}{2}}\left(1-9\xi^2\right)^{\frac{1}{2}}}. \tag{2.17}$$

Next we apply the following quadratic transformation formula (Erdélyi *et al* 1953, p 113, equation 30) to the complete elliptic integrals in (2.15):

$$K(\omega_\pm) = \left(1-\widetilde{k}_\pm^2\right)^{\frac{1}{4}}\,K(\widetilde{k}_\pm), \tag{2.18}$$

where

$$\omega_{\pm}^2 = \frac{1}{2} - \frac{1}{4}\left(2 - \widetilde{k}_{\pm}^2\right)\left(1 - \widetilde{k}_{\pm}^2\right)^{-\frac{1}{2}}, \tag{2.19}$$

$$\widetilde{k}_{+}^2 = \widetilde{k}_{+}^2(\xi) = \frac{16\xi}{(1-\xi)(1+3\xi)^3}, \tag{2.20}$$

$$\widetilde{k}_{-}^2 = \widetilde{k}_{-}^2(\xi) = \frac{16\xi^3}{(1-\xi)^3(1+3\xi)}. \tag{2.21}$$

This procedure yields the required result

$$P(z)_{\mathrm{sc}} = \frac{4}{\pi^2}\,\frac{(1-9\xi^4)}{(1-\xi)^2\,(1+3\xi)^2}\,K(\widetilde{k}_{+})\,K(\widetilde{k}_{-}), \tag{2.22}$$

where $\widetilde{k}_{\pm} = \widetilde{k}_{\pm}(\xi)$ are defined in (2.20) and (2.21). It can also be shown using equation (2.14) that the inverse transformation $\xi = \xi(z)$ is given by

$$\xi = \xi(z) = \left(1 + \sqrt{1-z^2}\,\right)^{-\frac{1}{2}}\left(1 - \sqrt{1 - \frac{z^2}{9}}\,\right)^{\frac{1}{2}}. \tag{2.23}$$

Equations (2.20)–(2.23) can be used to calculate $P(z)_{\mathrm{sc}}$ for any given value of z provided that z lies in a certain finite region $\mathcal{D}_1$ of the cut z plane. This region of validity is shown in figure 1. The points on the boundary of the region $\mathcal{D}_1$ are associated with values of $\widetilde{k}_{+}^2$ which lie in the interval $b < \widetilde{k}_{+}^2 \leqslant 2$, where

$$b = \frac{1}{32}\left(1+\sqrt{5}\right)^{\frac{9}{2}}\left[\left(1+\sqrt{5}\right)^{\frac{3}{2}} - 4\sqrt{2}\,\right], \tag{2.24}$$

$$= 1.014\,334\,296\,627\,\ldots\,. \tag{2.25}$$

It is possible to apply (2.22) outside the region $\mathcal{D}_1$ provided that $K(\widetilde{k}_{+})$ is replaced by the appropriate analytic continuation formula (see Horiguchi 1972).

3. Elliptic modular transformations

In this section we shall review *briefly* the theory of the elliptic modular transformation of order n. Particular attention will be given to the case of the cubic transformation with $n = 3$.

We begin by introducing the elliptic modular function (Whittaker and Watson 1927)

$$k^2(q) = \frac{\vartheta_2^4(0,q)}{\vartheta_3^4(0,q)} = 16q\prod_{m=1}^{\infty}\left(\frac{1+q^{2m}}{1+q^{2m-1}}\right)^8, \tag{3.1}$$

where $\vartheta_k(0,q)$ is a theta function and $0 < q < 1$. The complementary modular function associated with (3.1) is given by

$$[k'(q)]^2 = 1 - k^2(q) = \frac{\vartheta_4^4(0,q)}{\vartheta_3^4(0,q)} = \prod_{m=1}^{\infty}\left(\frac{1-q^{2m-1}}{1+q^{2m-1}}\right)^8. \tag{3.2}$$

It is possible to write the inverse of the function (3.1) in the form

$$\ln q = -\pi\frac{K'(k)}{K(k)}, \tag{3.3}$$

where $k = k(q)$ and $K'(k)$ denotes the complementary complete elliptic integral of the first kind.

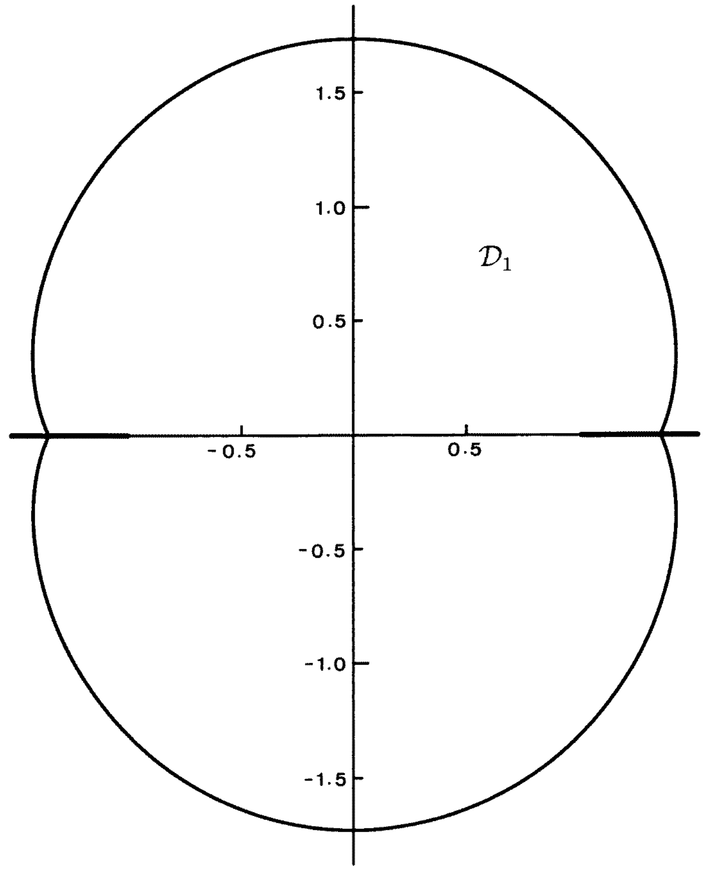

Figure 1. The region of validity $\mathcal{D}_1$ in the cut z plane for the formula (2.22).

Next we replace the parameter q in (3.1) and (3.2) by q^n and define the transformed functions

$$k_n^2(q) \equiv k^2(q^n), \tag{3.4}$$

$$\left[k_n'(q)\right]^2 \equiv \left[k'(q^n)\right]^2, \tag{3.5}$$

where $n = 1, 2, \ldots$. If we make the substitution $q \mapsto q^n$ in equation (3.3) we see that

$$\frac{K'(k_n)}{K(k_n)} = n\,\frac{K'(k_1)}{K(k_1)}, \tag{3.6}$$

where $k_n = k_n(q)$ and $k_1 = k_1(q)$. It is also known that the functions $k_1^2(q)$ and $k_n^2(q)$, with $n \geqslant 2$, satisfy an equation of the type (see Borwein and Borwein 1987, p 125)

$$W_n\left[k_1^2(q), k_n^2(q)\right] = 0, \tag{3.7}$$

where $W_n(x, y)$ is a polynomial in the variables x and y with integer coefficients. The equation (3.7) is called the *modular equation of order* n.

We can derive the $n = 3$ modular equation by first using (3.1), (3.2), (3.4) and (3.5) to eliminate the theta functions from the identity (see Hardy 1940, p 218)

$$\vartheta_3(0, q)\vartheta_3(0, q^3) - \vartheta_4(0, q)\vartheta_4(0, q^3) = \vartheta_2(0, q)\vartheta_2(0, q^3). \tag{3.8}$$

In this manner we obtain Legendre's *algebraic* modular relation

$$\left[k_1(q)k_3(q)\right]^{1/2} + \left[k_1'(q)k_3'(q)\right]^{1/2} = 1. \tag{3.9}$$

From this result it is readily shown that the modular equation of order 3 is

$$\begin{aligned} W_3(x, y) = x^4 - 4y(33 - 96y + 64y^2)x^3 + 6y(64 - 127y + 64y^2)x^2 \\ - 4y(64 - 96y + 33y^2)x + y^4 = 0, \end{aligned} \tag{3.10}$$

with $x = k_1^2(q)$ and $y = k_3^2(q)$. When $k_1(q) = k_3'(q)$ we also have $k_1'(q) = k_3(q)$ and it follows from (3.6) with $n = 3$ and (3.9) that we must have

$$\frac{K'(k_3)}{K(k_3)} = \sqrt{3} \tag{3.11}$$

and

$$16k_3^2(1 - k_3^2) = 1, \tag{3.12}$$

respectively. The particular value of $k_3 \in (0, 1)$ which satisfies equation (3.11) is called the *singular value* of order 3 and will be denoted by $k[3]$. We can determine the value of $k[3]$ by finding the appropriate root of equation (3.12). Hence we obtain

$$k[3] = \frac{\sqrt{3} - 1}{2\sqrt{2}}. \tag{3.13}$$

The modulus k which occurs in the Watson formula (1.5) for the fcc lattice is just the singular value $k[3]$, while the moduli in equations (1.4) and (1.6) are the singular values $k[1]$ and $k[6]$ respectively.

An alternative purely *algebraic* approach to the $n = 3$ modular transformation which is based on the transformation properties of elliptic integrals was first developed in 1825 by Legendre. In 1829 Jacobi continued the investigation of the case $n = 3$ and extended the algebraic analysis to the case $n = 5$. Cayley (1874, 1895) gives a full account of this early work and also discusses various higher-order transformations with $n > 5$. From the results for the cubic transformation we find that the following *rational* parametric forms:

$$k_1^2(\alpha) = \alpha(2 + \alpha)^3/(1 + 2\alpha)^3, \tag{3.14}$$

$$k_3^2(\alpha) = \alpha^3(2 + \alpha)/(1 + 2\alpha), \tag{3.15}$$

$$\left[k_1'(\alpha)\right]^2 = (1 + \alpha)(1 - \alpha)^3/(1 + 2\alpha)^3, \tag{3.16}$$

$$\left[k_3'(\alpha)\right]^2 = (1 - \alpha)(1 + \alpha)^3/(1 + 2\alpha). \tag{3.17}$$

where $0 \leqslant \alpha < 1$, also satisfy the $n = 3$ modular relation (3.9) with the parameter q *formally* replaced by the parameter α. From (3.14) and (3.15) it follows that

$$\alpha^8 = k_3^6(\alpha)/k_1^2(\alpha). \tag{3.18}$$

If the α and q parametric representations both give the *same* values of k_1^2 and k_3^2 then it is clear from (3.18) that we must have

$$\alpha = \left[k_3^3(q)/k_1(q)\right]^{\frac{1}{4}}, \tag{3.19}$$

where $k_n(q)$ is defined by equations (3.1) and (3.4).

It is also known that

$$\frac{K(k_1(\alpha))}{K(k_3(\alpha))} = \frac{1}{M_3(\alpha)}, \tag{3.20}$$

where

$$M_3(\alpha) = (2\alpha + 1)^{-1} \tag{3.21}$$

is called the *multiplier of order* 3. When $\alpha = \frac{1}{2}(\sqrt{3} - 1)$ we have $k_1(\alpha) = k_3'(\alpha)$ and the important result (3.20) reduces to the singular value equation (3.11). If we use (3.21) to eliminate the parameter α from (3.14) it is found that the multiplier $M_3 = M_3(k_1)$ is an algebraic function which satisfies the quartic equation

$$27M_3^4 - 18M_3^2 + 8(2m_1 - 1)M_3 - 1 = 0, \tag{3.22}$$

where $m_1 = k_1^2$. It is interesting to note that equation (3.22) plays an important role in the exact solutions of the Ising model with pure triplet interactions on the triangular lattice (Baxter and Wu 1973, 1974; Joyce 1975a, b) and the hard-hexagon model (Baxter 1980, 1982; Joyce 1988).

The application of the Lagrange inversion formula to (3.22) enables one to express $M_3(k_1)$ in the explicit hypergeometric form (see Joyce 1975a)

$$M_3(k_1) = \left[{}_2F_1\left(\frac{1}{2}, -\frac{1}{6}; \frac{2}{3}; m_1\right)\right]^2, \tag{3.23}$$

where $m_1 = k_1^2$ and $0 \leqslant m_1 \leqslant 1$. It is also possible to use (3.22) to obtain an algebraic formula for $M_3(k_1)$. The final result is

$$M_3(k_1) = \pm\frac{1}{3}(1 - Y)^{\frac{1}{2}} + \frac{1}{3}\left(2 + Y + 2\sqrt{1 + Y + Y^2}\right)^{\frac{1}{2}}, \tag{3.24}$$

where

$$Y = [4m_1(1 - m_1)]^{\frac{1}{3}}, \tag{3.25}$$

and the upper and lower signs in (3.24) are valid for $0 \leqslant m_1 \leqslant \frac{1}{2}$ and $\frac{1}{2} \leqslant m_1 \leqslant 1$, respectively.

4. Application of the cubic modular transformation to the fcc and sc lattice Green functions

The main aim in this section is to show that the cubic transformation formula (3.20) can be used to simplify the expressions (2.6) and (2.22) for the fcc and sc Green functions respectively. First we apply the bilinear transformation

$$\alpha = 2\xi/(1 - \xi) \tag{4.1}$$

to equations (3.14) and (3.15), where $0 \leqslant \xi < \frac{1}{3}$. In this manner we obtain the new parametric representation

$$k_1^2(\xi) = \frac{16\xi}{(1 - \xi)(1 + 3\xi)^3}, \tag{4.2}$$

$$k_3^2(\xi) = \frac{16\xi^3}{(1 - \xi)^3(1 + 3\xi)} \tag{4.3}$$

for the cubic modular transformation. We can also use (4.1) to write (3.20) in the alternative form

$$\frac{K\,(k_1(\xi))}{K\,(k_3(\xi))} = \frac{1 + 3\xi}{1 - \xi}. \tag{4.4}$$

In the derivation of (4.4) it has been assumed that $\xi \in [0, \frac{1}{3})$. However, it is clear from the theory of analytic continuation that the formula (4.4) will remain valid for complex ξ

in the neighbourhood of the origin $\xi = 0$ provided that $k_1^2(\xi)$ and $k_3^2(\xi)$ do not take values in the interval $(1, +\infty)$. To investigate the possibility that $k_1^2(\xi)$ has values in this interval we use (4.2) to obtain the algebraic equation

$$27\xi^4 - 18\xi^2 + 8\left(\frac{2}{m_1} - 1\right)\xi - 1 = 0, \tag{4.5}$$

where $m_1 = k_1^2$. When $m_1 \in (1, +\infty)$ we can solve the quartic equation (4.5) by using the results obtained earlier for the multiplier equation (3.22). In particular, we find that the four solutions $\{\xi_j = \xi_j(m_1);\ j = 1, 2, 3, 4\}$ are expressible in the hypergeometric form

$$\xi_1(m_1) = \left[{}_2F_1\left(\frac{1}{2}, -\frac{1}{6}; \frac{2}{3}; \frac{1}{m_1}\right)\right]^2, \tag{4.6}$$

$$\xi_2(m_1) = -\frac{1}{3}\left[{}_2F_1\left(\frac{1}{2}, -\frac{1}{6}; \frac{2}{3}; \frac{1}{m_1}\right) + (2m_1)^{-\frac{1}{3}}{}_2F_1\left(\frac{5}{6}, \frac{1}{6}; \frac{4}{3}; \frac{1}{m_1}\right)\right]^2, \tag{4.7}$$

$$\xi_3(m_1) = -\frac{1}{3}\left[{}_2F_1\left(\frac{1}{2}, -\frac{1}{6}; \frac{2}{3}; \frac{1}{m_1}\right) - e^{+i\pi/3}(2m_1)^{-\frac{1}{3}}{}_2F_1\left(\frac{5}{6}, \frac{1}{6}; \frac{4}{3}; \frac{1}{m_1}\right)\right]^2, \tag{4.8}$$

$$\xi_4(m_1) = -\frac{1}{3}\left[{}_2F_1\left(\frac{1}{2}, -\frac{1}{6}; \frac{2}{3}; \frac{1}{m_1}\right) - e^{-i\pi/3}(2m_1)^{-\frac{1}{3}}{}_2F_1\left(\frac{5}{6}, \frac{1}{6}; \frac{4}{3}; \frac{1}{m_1}\right)\right]^2, \tag{4.9}$$

where $m_1 \in (1, +\infty)$. The set of complex numbers $\{\xi_3(m_1);\ 1 < m_1 < \infty\}$ forms a curve $\mathcal{B}_2$ in the upper half of the ξ plane, while the set $\{\xi_4(m_1);\ 1 < m_1 < \infty\}$ gives the complex conjugate curve $\mathcal{B}_2^*$. These curves enclose a finite region $\mathcal{D}_2$ in the ξ plane which is shown in figure 2. The sets of real numbers $\{\xi_1(m_1);\ 1 < m_1 < \infty\}$ and $\{\xi_2(m_1);\ 1 < m_1 < \infty\}$ lie outside the region $\mathcal{D}_2$ and form the intervals $(\frac{1}{3}, 1)$ and $(-1, -\frac{1}{3})$ respectively. From a similar analysis of equation (4.3) we also find that $k_3^2(\xi)$ only takes values in the interval $(1, +\infty)$ for points ξ which are *outside* the region $\mathcal{D}_2$. It follows, therefore, that (4.4) is valid for all $\xi \in \mathcal{D}_2$.

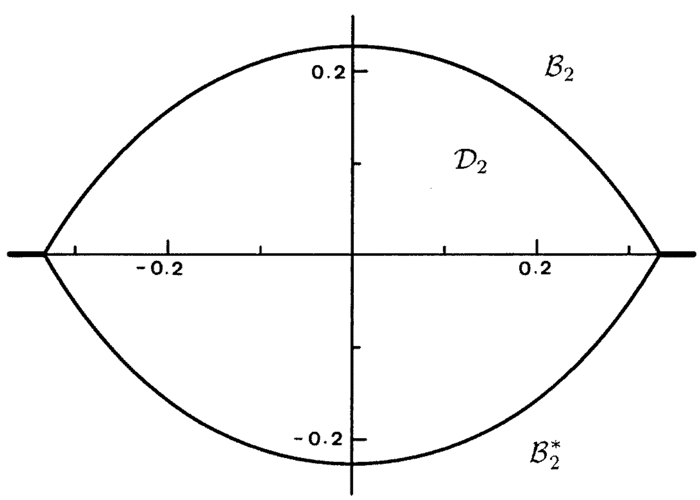

Figure 2. The boundary curves $\mathcal{B}_2$ and $\mathcal{B}_2^*$ in the cut ξ plane and the region of validity $\mathcal{D}_2$ for the formula (4.4).

We can now apply equation (4.4) with $k_1(\xi) = k_+(\xi)$ and $k_3(\xi) = k_-(\xi)$ to the product form (2.6) for the fcc Green function. Hence, we obtain the simplified formula

$$P(z)_{\rm fcc} = \frac{(1+3\xi^2)^2}{(1-\xi)^3(1+3\xi)} \left[\frac{2}{\pi} K(k)\right]^2, \tag{4.10}$$

where

$$k^2 = k^2(\xi) = \frac{16\xi^3}{(1-\xi)^3(1+3\xi)}, \tag{4.11}$$

$$\xi = \xi(z) = \left(1+\sqrt{1-z}\right)^{-1}\left(-1+\sqrt{1+\frac{z}{3}}\right). \tag{4.12}$$

It should be stressed that this basic result can be used to calculate $P(z)_{\rm fcc}$ at *any* point in the z plane provided that cuts are made along the real axis from $z=-\infty$ to $z=-3$, and from $z=1$ to $z=+\infty$. For the special case $z=1$ the formula (4.10) reduces directly to Watson's result (1.5).

In a similar manner we can use (4.4) with $k_1(\xi) = \widetilde{k}_+(\xi)$ and $k_3(\xi) = \widetilde{k}_-(\xi)$ to express the sc Green function formula (2.22) in the reduced form

$$P(z)_{\rm sc} = \frac{(1-9\xi^4)}{(1-\xi)^3(1+3\xi)} \left[\frac{2}{\pi} K(k)\right]^2, \tag{4.13}$$

where

$$k^2 = k^2(\xi) = \frac{16\xi^3}{(1-\xi)^3(1+3\xi)}, \tag{4.14}$$

$$\xi = \xi(z) = \left(1+\sqrt{1-z^2}\right)^{-\frac{1}{2}}\left(1-\sqrt{1-\frac{z^2}{9}}\right)^{\frac{1}{2}}. \tag{4.15}$$

This result enables one to determine the value of $P(z)_{\rm sc}$ at *any* point in the z plane provided that cuts are made along the real axis from $z=-\infty$ to $z=-1$, and from $z=1$ to $z=+\infty$.

When $z=1$ it is found from (4.14) and (4.15) that equation (4.13) can be written as

$$P(1)_{\rm sc} = \frac{3\sqrt{6}}{4}\left(\sqrt{2}+1\right) k_0^2 \left[\frac{2}{\pi} K(k_0)\right]^2, \tag{4.16}$$

where

$$k_0^2 = \left(\sqrt{2}-1\right)^2\left(\sqrt{3}-1\right)^2\left(\sqrt{3}+\sqrt{2}\right). \tag{4.17}$$

If the general quadratic transformation formula (Erdélyi *et al* 1953)

$$K(k) = \frac{2}{k^2}(2-k^2-2k')^{\frac{1}{2}} K\left(\frac{2-k^2-2k'}{k^2}\right), \tag{4.18}$$

where k' denotes the complementary modulus, is applied to (4.16) we find that

$$P(1)_{\rm sc} = 3\sqrt{6}\left(\sqrt{2}+1\right) k_6 \left[\frac{2}{\pi} K(k_6)\right]^2, \tag{4.19}$$

where

$$k_6 \equiv k[6] = \left(2-\sqrt{3}\right)\left(\sqrt{3}-\sqrt{2}\right) \tag{4.20}$$

is the singular value of order 6. This result is in agreement with Watson's formula (1.6).

From the analysis in this section it is seen that the formulae for $k^2_\pm(\eta)$ given in equations (2.3) and (2.11) are basically just *well-disguised* algebraic parametric representations for the elliptic modular transformation of order 3! Finally, it should be noted that an alternative derivation of (4.13) has also been given by Joyce (1994). In this earlier work a rather *complicated* procedure was used which did *not* involve the theory of elliptic modular transformations.

5. Concluding remarks on the related Green function $Q(w)$

In many applications of lattice Green functions it is necessary to consider the transformed Green function (see Katsura *et al* 1971)

$$Q(w) \equiv w^{-1} P(\Delta/w) = Q_R(u, v) + \mathrm{i}\, Q_I(u, v), \tag{5.1}$$

where $w = u + \mathrm{i}v$ is a complex variable in the (u, v) plane which is cut along the real axis from $u = u_{\min}$ to $u = u_{\max}$, and Δ is a constant which takes the values $\Delta_{\mathrm{bcc}} = 1$ and $\Delta_{\mathrm{fcc}} = \Delta_{\mathrm{sc}} = 3$. The values of $(u_{\min}, u_{\max})$ for the bcc, fcc and sc lattices are given by $(-1, 1)$, $(-1, 3)$ and $(-3, 3)$ respectively. We can calculate the numerical values of $Q(w)_{\mathrm{bcc}}$, $Q(w)_{\mathrm{fcc}}$ and $Q(w)_{\mathrm{sc}}$ at any point w in the cut w plane by using the formulae (2.1), (4.10) and (4.13) respectively, with $z = \Delta/w$.

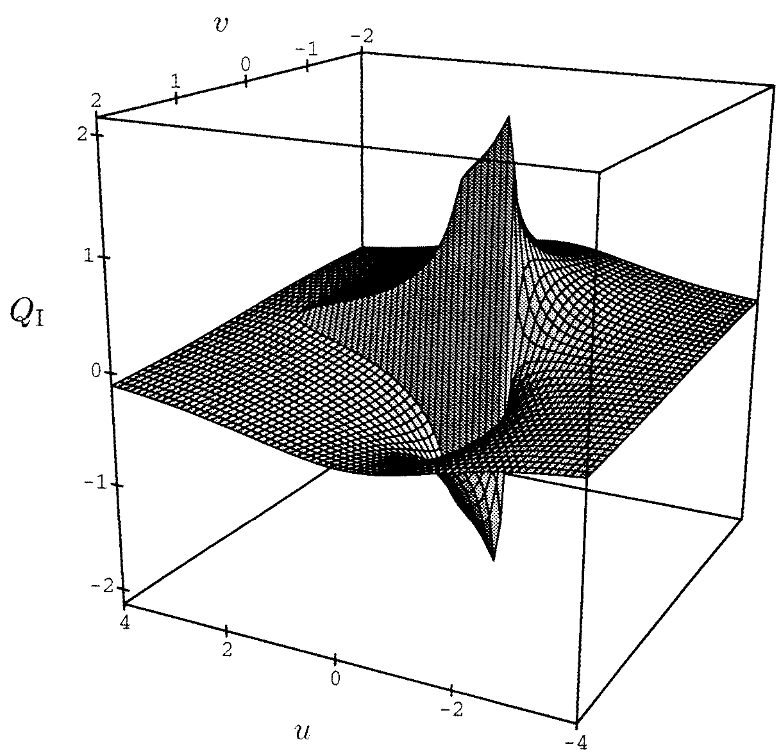

Figure 3. Surface for the imaginary part $Q_I(u, v)$ of the fcc lattice Green function (5.1) plotted above the (u, v) plane.

In figure 3 we give a surface representation of $Q_I(u, v)$ for the fcc lattice which was constructed by making a direct application of *Mathematica* (Wolfram 1991) to equations

(4.10)–(4.12). The profiles of the discontinuities along the upper and lower edges of the cut in the (u, v) plane are given by

$$\lim_{v \to 0\pm} Q_{\rm I}(u, v) \equiv \mp D(u), \tag{5.2}$$

where $-1 < u \leqslant 3$. The limiting function $D(u)$ is directly related to the density of states function for a variety of elementary excitations in the fcc lattice with nearest-neighbour interactions (see Jelitto 1969).

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