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LETTER TO THE EDITOR

Exact evaluation of the Green function for the anisotropic simple cubic lattice

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Abstract

The lattice Green function at the origin of the simple cubic lattice with anisotropic nearest-neighbour interactions is evaluated exactly in terms of a product of two complete elliptic integrals of the first kind.

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The lattice Green function

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

where $\{l, m, n\}$ denotes a set of integers, $w = u + \mathrm{i}v$ is a complex variable in the (u, v) plane and α is a real parameter, is of frequent occurrence in many lattice statistical problems which involve the simple cubic lattice with partially anisotropic nearest-neighbour interactions (Berlin and Kac 1952, Berlin and Thomsen 1952, Duffin 1953, Montroll and Potts 1955, Isihara 1957, Maradudin *et al* 1960, Montroll and Weiss 1965, Katsura *et al* 1971a). It will be assumed, without loss of generality, that $l \geqslant m \geqslant 0$, $n \geqslant 0$ and $0 < \alpha < \infty$. In this Letter we shall focus our attention on the exact evaluation of the lattice Green function at the origin $G(\alpha, w) \equiv G(0, 0, 0; \alpha, w)$.

It can be shown that $G(\alpha, w)$ defines a single-valued analytic function in the complex (u, v) plane provided that a cut is made along the real axis from $w = -2-\alpha$ to $w = 2+\alpha$, where $\alpha > 0$. In many applications one requires the limiting behaviour of $G(\alpha, w)$ as w approaches the real u axis. It is convenient, therefore, to introduce the further definitions

$$G^{\pm}(\alpha,u) \equiv \lim_{\epsilon\to 0+} G(\alpha, u \pm \mathrm{i}\epsilon) \equiv G_{\mathrm{R}}(\alpha,u) \mp \mathrm{i}G_{\mathrm{I}}(\alpha,u) \tag{2}$$

where $-\infty < u < \infty$ and ϵ is an infinitesimal positive number. When $|u| \geqslant 2+\alpha$ the imaginary part of $G^{\pm}(\alpha, u)$ is always equal to zero. It should also be noted that $G_{\mathrm{R}}(\alpha, u)$ and $G_{\mathrm{I}}(\alpha, u)$ are odd and even functions of u, respectively. We can use $G_{\mathrm{I}}(\alpha, u)$ to express $G(\alpha, w)$ in the alternative form

$$G(\alpha,w) = \int_{-2-\alpha}^{2+\alpha} \frac{\rho(\alpha,u)}{w-u}\,\mathrm{d}u \tag{3}$$

where $\rho(\alpha, u) = (1/\pi)G_I(\alpha, u)$ is a density-of-states function (see Wolfram and Callaway 1963, Katsura *et al* 1971a).

Most of the known exact results for $G(\alpha, w)$ have been obtained for the isotropic case $\alpha = 1$. Watson (1939) proved that

$$G(1,3) = \left(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}\right)\left[\frac{2}{\pi}K(k)\right]^2 \tag{4}$$

where

$$k = \left(2 - \sqrt{3}\right)\left(\sqrt{3} - \sqrt{2}\right) \tag{5}$$

and $K(k)$ denotes the complete elliptic integral of the first kind with a modulus k. An exact formula for the *general* isotropic Green function $G(1, w)$ was first derived by Joyce (1972, 1973). In particular, it was found that

$$wG(1,w) = (1-\eta)^{\frac{1}{2}}\left(1 - \frac{1}{4}\eta\right)^{\frac{1}{2}}\left(\frac{2}{\pi}\right)^2 K(k_+)\,K(k_-) \tag{6}$$

where

$$k_\pm^2 = \tfrac{1}{2}\left[1 \pm \eta\sqrt{1 - \tfrac{1}{4}\eta} - (1 - \tfrac{1}{2}\eta)\sqrt{1-\eta}\right] \tag{7}$$

$$\eta = -16z\left(\sqrt{1-z} + \sqrt{1-9z}\right)^{-2} \tag{8}$$

and $z = 1/w^2$. This result can be used to calculate $G(1, w)$ at *any* point in the (u, v) plane provided that a cut is made along the real axis from $w = -3$ to $+3$. More recently, Joyce (1994, 1998) has shown that the moduli $k_\pm = k_\pm(\eta)$ in (7) are related by the cubic modular transformation of order 3 (see Borwein and Borwein 1987). This remarkable connection enables one to express the formula (6) in terms of the square $[K(k_-)]^2$.

Montroll (1956) extended the work of Watson (1939) and established an exact formula for the *anisotropic* Green function $G(\alpha, 2+\alpha)$. His final result can be written as

$$G(\alpha, 2+\alpha) = \frac{\sqrt{2}}{\alpha}\left(\sqrt{2}\sqrt{1+\alpha} - \sqrt{2+\alpha}\right)\left(\frac{2}{\pi}\right)^2 K[k_+(\alpha)]\,K[k_-(\alpha)] \tag{9}$$

where

$$k_\pm(\alpha) = \frac{1}{\alpha}\left(\sqrt{2}\sqrt{1+\alpha} - \sqrt{2+\alpha}\right)\left(\sqrt{2+\alpha} \pm \sqrt{2}\right) \tag{10}$$

and $0 < \alpha < \infty$. When $\alpha = 1$ we can simplify (9) using the transformation formula

$$K[k_+(1)] = \left(\tfrac{3}{2}\right)^{\frac{1}{2}}[1 + k_-(1)]\,K\,[k_-(1)]. \tag{11}$$

In this manner, we recover the Watson formula (4). It appears that (9) is the *only* exact elliptic function formula currently available in the literature for the Green function at the origin $G(\alpha, w)$ which is valid for *arbitrary* values of the anisotropy parameter α.

The main purpose in this Letter is to show that it is possible to express the *general* Green function $G(\alpha, w)$ in terms of a product of two complete elliptic integrals of the first kind. This new result enables one to calculate the value of $G(\alpha, w)$ for *any* $w = u + \mathrm{i}v$ in the cut (u, v) plane and for *any* $\alpha \in (0, \infty)$. Explicit elliptic integral formulae are also established for $G_R(\alpha, u)$ and $G_I(\alpha, u)$ at the branch-point singularities $u = \alpha$ and $|2-\alpha|$, where $\alpha \in (0, \infty)$.

In the first stage of the analysis we write $G(\alpha, w) \equiv G(0, 0, 0; \alpha, w)$ in the alternative form (Maradudin *et al* 1960)

$$G(\alpha, w) = \int_0^\infty \exp(-wt)\,I_0^2(t)\,I_0(\alpha t)\,\mathrm{d}t \tag{12}$$

where $I_0(t)$ denotes a modified Bessel function of the first kind and $|w| \geqslant 2+\alpha$ with $\alpha > 0$. Next we derive a differential equation for $G(\alpha, w)$ by applying the methods developed by Iwata (1979) to the integral (12). In this manner, we find that the function

$$y_G(\alpha, z) \equiv wG(\alpha, w) \tag{13}$$

where $z = 1/w^2$, is a solution of the linear fourth-order differential equation

$$\mathrm{L}_4(y) \equiv \sum_{j=0}^{4} f_j(\alpha, z)\, \mathrm{D}_z^{4-j} y = 0 \tag{14}$$

where

$$f_0(\alpha, z) = 8z^2(1-\alpha^2 z)\big[1-(2-\alpha)^2 z\big]\big[1-(2+\alpha)^2 z\big]\big[3+5(4-\alpha^2)z\big] \tag{15}$$

$$\begin{aligned} f_1(\alpha, z) = 20z\big[&6-5(8+7\alpha^2)z-(224+52\alpha^2-75\alpha^4)z^2 \\ &+3(4-\alpha^2)(96-20\alpha^2+23\alpha^4)z^3-23\alpha^2(4-\alpha^2)^3 z^4\big] \end{aligned} \tag{16}$$

$$\begin{aligned} f_2(\alpha, z) = \big[&96-4(544+233\alpha^2)z-2(448+608\alpha^2-1365\alpha^4)z^2 \\ &+4(4-\alpha^2)(3040-974\alpha^2+811\alpha^4)z^3-1350\alpha^2(4-\alpha^2)^3 z^4\big] \end{aligned} \tag{17}$$

$$\begin{aligned} f_3(\alpha, z) = \big[&-72(11+3\alpha^2)+6(736+8\alpha^2+177\alpha^4)z \\ &+3(4-\alpha^2)(1760-1076\alpha^2+589\alpha^4)z^2-975\alpha^2(4-\alpha^2)^3 z^3\big] \end{aligned} \tag{18}$$

$$f_4(\alpha, z) = \big[36(10+\alpha^2+\alpha^4)+3(4-\alpha^2)(40-104\alpha^2+31\alpha^4)z-75\alpha^2(4-\alpha^2)^3 z^2\big] \tag{19}$$

and $\mathrm{D}_z = \mathrm{d}/\mathrm{d}z$. This differential equation is of the Fuchsian type with six regular singular points at $z = 0$,

$$\begin{aligned} z_1 &= \frac{1}{(2+\alpha)^2} \\ z_2 &= \frac{1}{\alpha^2} \\ z_3 &= \frac{1}{(2-\alpha)^2} \\ z_4 &= \frac{3}{5(\alpha^2-4)} \end{aligned} \tag{20}$$

and ∞. The singular point z_4 is particularly interesting because the *general* solution of $L_4(y) = 0$ is *analytic* at $z = z_4$. This unusual type of regular singular point is known as an *apparent* (or *accidental*) singularity (Ince 1927, p 406).

It can be shown that any solution of $L_4(y) = 0$ can be written in the product form

$$y(\alpha, z) = \frac{1}{z}\left[\prod_{i=1}^{3}\left(1-\frac{z}{z_i}\right)^{-1/2}\right]\left(1-\frac{z}{z_5}\right)^{1/2} H_1(\alpha, z)\, H_2(\alpha, z) \tag{21}$$

where $z_5 = 3/(4-\alpha^2)$ and $\{H_j(\alpha, z) : j = 1, 2\}$ are, respectively, solutions of the differential equations

$$\big[\mathrm{D}_z^2 + U_+(\alpha, z)\big]y = 0 \tag{22}$$

$$\big[\mathrm{D}_z^2 + U_-(\alpha, z)\big]y = 0. \tag{23}$$

The functions $U_{\pm}(\alpha, z)$ in these second-order equations are given by

$$
\begin{aligned}
U_{\pm}(\alpha, z) = {} & \frac{7(2+\alpha^2)}{12z} + \frac{1}{4z^2} + \frac{\alpha^4(16-19\alpha^2)}{64(1-\alpha^2)(1-\alpha^2 z)} + \frac{3\alpha^4}{16(1-\alpha^2 z)^2} \\
& + \frac{(2-\alpha)^4(8+32\alpha-23\alpha^2-5\alpha^3)}{128\alpha(1-\alpha)[1-(2-\alpha)^2 z]} + \frac{3(2-\alpha)^4}{16[1-(2-\alpha)^2 z]^2} \\
& - \frac{(2+\alpha)^4(8-32\alpha-23\alpha^2+5\alpha^3)}{128\alpha(1+\alpha)[1-(2+\alpha)^2 z]} + \frac{3(2+\alpha)^4}{16[1-(2+\alpha)^2 z]^2} \\
& - \frac{(4-\alpha^2)^2(40-31\alpha^2)}{192(1-\alpha^2)[3-(4-\alpha^2)z]} - \frac{3(4-\alpha^2)^2}{8[3-(4-\alpha^2)z]^2} \\
& \pm \frac{(\alpha^2-1)\,[3+5(4-\alpha^2)z]}{2z\,[3-(4-\alpha^2)z]^2\sqrt{(1-\alpha^2 z)\,[1-(2-\alpha)^2 z]\,[1-(2+\alpha)^2 z]}}.
\end{aligned} \tag{24}
$$

It is necessary to introduce the extra singularity z_5 in equation (21) in order to ensure that the differential equations for $\{H_j(\alpha, z) : j = 1, 2\}$ are in normal form.

Next we define $x = x_{\pm}(\alpha, z)$ to be transformation functions which reduce equations (22) and (23), respectively, to the normal form of the Gauss hypergeometric equation

$$
\left[\mathrm{D}_x^2 + N(a, b; c; x)\right] y = 0 \tag{25}
$$

where

$$
N(a, b; c; x) = \frac{1}{4x^2(1-x)^2}\left\{c(2-c) - 2[2ab + c(1-a-b)]x + [1-(a-b)^2]x^2\right\}. \tag{26}
$$

It can be proved that the functions $x_{\pm}(\alpha, z)$ must satisfy the non-linear equations

$$
\frac{1}{2}\{x_{\pm}, z\} + \left(\frac{\mathrm{d}x_{\pm}}{\mathrm{d}z}\right)^2 N(a, b; c; x_{\pm}) = U_{\pm}(\alpha, z) \tag{27}
$$

respectively, where

$$
\{x, z\} \equiv \frac{x'''(\alpha, z)}{x'(\alpha, z)} - \frac{3}{2}\left[\frac{x''(\alpha, z)}{x'(\alpha, z)}\right]^2 \tag{28}
$$

is the Schwarzian derivative of $x(\alpha, z)$ with respect to z. When $a = \frac{1}{8}$, $b = \frac{3}{8}$ and $c = 1$ the Schwarzian equations (27) have algebraic solutions $x_{\pm}(\alpha, z)$ which satisfy the simple polynomial equation

$$
\begin{aligned}
& \left[1+(4-\alpha^2)z\right]^4 x^2 - 32z\left[2-(16+5\alpha^2)z + 4(8+2\alpha^2+\alpha^4)z^2 - \alpha^2(4-\alpha^2)^2 z^3\right]x \\
& \quad + 256\alpha^4 z^4 = 0.
\end{aligned} \tag{29}
$$

It follows from these results that the Green function can be expressed in the product form

$$
wG(\alpha, w) = \left[1+(4-\alpha^2)z\right]^{-1/2} {}_2F_1\left(\frac{1}{8}, \frac{3}{8}; 1; x_+\right) {}_2F_1\left(\frac{1}{8}, \frac{3}{8}; 1; x_-\right) \tag{30}
$$

where

$$
\begin{aligned}
x_{\pm} \equiv x_{\pm}(\alpha, z) = {} & \frac{16z}{[1+(4-\alpha^2)z]^4}\Big\{\left[1-(4+\alpha^2)z\right] \\
& \pm \left[1-(2+\alpha)^2 z\right]^{\frac{1}{2}}(1-\alpha^2 z)^{\frac{1}{2}}\left[1-(2-\alpha)^2 z\right]^{\frac{1}{2}}\Big\}^2
\end{aligned} \tag{31}
$$

and $z = 1/w^2$. The formula (30) has a very *limited* region of validity in the neighbourhood of the origin $z = 0$. In particular, the result (30) cannot be used directly to calculate the correct value for the Montroll integral $G(\alpha, 2+\alpha)$. Fortunately, this difficulty can be overcome by applying the relation (Erdélyi *et al* 1953, p 111)

$$ {}_2F_1\left(\frac{1}{8}, \frac{3}{8}; 1; x\right) = \left(\frac{1}{2} + \frac{1}{2}\sqrt{1-x}\right)^{-1/4} \left(\frac{2}{\pi}\right) K(k) \tag{32} $$

where

$$ k^2 = \frac{1}{2} - \frac{1}{2}\left(\frac{1}{2} + \frac{1}{2}\sqrt{1-x}\right)^{-1/2} \tag{33} $$

to equation (30).

In this manner, we obtain the required elliptic integral formula

$$ wG(\alpha, w) = \frac{2}{\sqrt{1-(2-\alpha)^2 z} + \sqrt{1-(2+\alpha)^2 z}} \left(\frac{2}{\pi}\right)^2 K(k_+)\, K(k_-) \tag{34} $$

where

$$ \begin{aligned} k_\pm^2 \equiv k_\pm^2(\alpha, z) = {} & \frac{1}{2} - \frac{1}{2}\left[\sqrt{1-(2-\alpha)^2 z} + \sqrt{1-(2+\alpha)^2 z}\,\right]^{-3} \\ & \times \left[\sqrt{1+(2-\alpha)\sqrt{z}}\sqrt{1-(2+\alpha)\sqrt{z}} + \sqrt{1-(2-\alpha)\sqrt{z}}\sqrt{1+(2+\alpha)\sqrt{z}}\,\right] \\ & \times \left\{ \pm 16z + \sqrt{1-\alpha^2 z}\left[\sqrt{1+(2-\alpha)\sqrt{z}}\sqrt{1+(2+\alpha)\sqrt{z}} \right.\right. \\ & \left.\left. + \sqrt{1-(2-\alpha)\sqrt{z}}\sqrt{1-(2+\alpha)\sqrt{z}}\,\right]^2 \right\} \end{aligned} \tag{35} $$

and $z = 1/w^2$. If the variable $z = 1/w^2$ is allowed to trace out any path $\mathcal{P}$ which lies in a complex plane that is cut along the real axis from $z = 1/(2+\alpha)^2$ to $+\infty$, then it is found that the functions $k_\pm^2(\alpha, z)$ map the path $\mathcal{P}$ into two associated paths which do not cross the straight line formed by the real interval $[1, \infty)$. From this result it follows that the basic formula (34) should be valid for *all* values of $w = u + \mathrm{i}v$ which lie in the (u, v) plane, provided that a cut is made along the real axis from $w = -2-\alpha$ to $2+\alpha$.

The formula (35) and the analytic continuations of the result (30) have been used to investigate the behaviour of $G_\mathrm{R}(\alpha, u)$ and $G_\mathrm{I}(\alpha, u)$ in the neighbourhood of the branch-point singularity at $u = \alpha$. In particular, we have found that

$$ G_\mathrm{R}(\alpha, \alpha) = \frac{2}{\pi^2}\left(1 + k_1^2\right) K^2(k_1) \tag{36} $$

$$ G_\mathrm{I}(\alpha, \alpha) = \frac{2}{\pi^2}\left(1 + k_1^2\right) K'(k_1)\, K(k_1) \tag{37} $$

provided that $0 < \alpha \leqslant 1$, where $K'(k_1)$ denotes the complementary complete elliptic integral of the first kind and

$$ k_1 \equiv k_1(\alpha) = \frac{1}{\alpha^2}\left(\sqrt{2}\sqrt{1-\sqrt{1-\alpha^2}} - \alpha\right)\left(1 + \sqrt{1-\alpha^2}\,\right). \tag{38} $$

When $\alpha = 1$ these results are in agreement with the work of Katsura *et al* (1971b) and Joyce (1973). For the more difficult case $1 < \alpha < \infty$ we obtain

$$ G_\mathrm{R}(\alpha, \alpha) = \frac{1}{2\pi^2}\left(1 + k_1^2\right)\left\{2K^2(k_1) + [K'(k_1)]^2\right\} \tag{39} $$

$$ G_\mathrm{I}(\alpha, \alpha) = \frac{1}{2\pi^2}\left(1 + k_1^2\right)\left\{4K'(k_1)K(k_1) - 2\mathrm{i}K^2(k_1) + \mathrm{i}[K'(k_1)]^2\right\}. \tag{40} $$

The modulus $k_1 = k_1(\alpha)$ in (39) and (40) can still be defined using equation (38), provided that the radical $\sqrt{1-\alpha^2}$ is replaced by its principal value $+\mathrm{i}\sqrt{\alpha^2-1}$. It should be stressed that (39) and (40) are *real*-valued functions of α, even though the modulus $k_1(\alpha)$ is a *complex*-valued function for $\alpha \in (1, \infty)$.

A similar analysis has also been carried out in the neighbourhood of the branch-point singularity at $u = |2-\alpha|$. In this manner, we find that

$$G_{\mathrm{R}}(\alpha, \alpha-2) = 0 \tag{41}$$

$$G_{\mathrm{I}}(\alpha, \alpha-2) = -\frac{\mathrm{i}}{\pi^2}\left(1+2k_2-k_2^2\right) K'(k_2)\, K(k_2) \tag{42}$$

where

$$k_2 \equiv k_2(\alpha) = \frac{\mathrm{i}}{\alpha}\left(\sqrt{2}\sqrt{\alpha-1}-\sqrt{\alpha-2}\right)\left(\sqrt{2}+\mathrm{i}\sqrt{\alpha-2}\right) \tag{43}$$

and $\alpha \in (2, \infty)$. For the case $1 < \alpha \leqslant 2$ we have the alternative formulae

$$G_{\mathrm{R}}(\alpha, 2-\alpha) = \frac{1}{2\pi^2}\left(1+2k_2-k_2^2\right)\left\{2K'(k_2)K(k_2)+2\mathrm{i}K^2(k_2)-\mathrm{i}[K'(k_2)]^2\right\} \tag{44}$$

$$G_{\mathrm{I}}(\alpha, 2-\alpha) = \frac{1}{2\pi^2}\left(1+2k_2-k_2^2\right)\left\{[K'(k_2)]^2+2K^2(k_2)\right\} \tag{45}$$

where $k_2 = k_2(\alpha)$ is given by (43), with the radical $\sqrt{\alpha-2}$ replaced by its principal value $+\mathrm{i}\sqrt{2-\alpha}$. Finally, when $0 < \alpha \leqslant 1$ it is found that

$$G_{\mathrm{R}}(\alpha, 2-\alpha) = \frac{1}{\pi^2}\left(1+2k_2-k_2^2\right) K'(k_2)\, K(k_2) \tag{46}$$

$$G_{\mathrm{I}}(\alpha, 2-\alpha) = \frac{2}{\pi^2}\left(1+2k_2-k_2^2\right) K^2(k_2) \tag{47}$$

where $k_2 = k_2(\alpha)$ is now defined by equation (43), with both radicals replaced by their principal values.

We conclude with a brief discussion on the possibility of evaluating the Green function $G(l, m, n; \alpha, w)$ at lattice points $\{l, m, n\}$ which are not at the origin. For the isotropic case $\alpha = 1$ it is known from the work of Morita (1975) and Horiguchi and Morita (1975) that the Joyce formula (6) can be used, at least in principle, to express $G(l, m, n; 1, w)$ as a sum of products of complete elliptic integrals of the first and second kinds for *arbitrary* values of l, m and n. In order to achieve a similar result for the general anisotropic case $\alpha \neq 1$ it would be necessary to have complete elliptic integral formulae for the Green functions $G(0, 0, 0; \alpha, w)$ *and* $G(1, 0, 0; \alpha, w)$. Unfortunately, the exact evaluation of the nearest-neighbour Green function $G(1, 0, 0; \alpha, w)$ has not yet been done for $\alpha \neq 1$. However, it is possible to use the methods developed by Iwata (1979) to evaluate the anisotropic Green function (1) at the lattice points (1, 0, 1), (1, 1, 0) and (1, 1, 1) in terms of $G(\alpha, w)$ and its first three derivatives with respect to w.

A detailed account of the various stages in the derivation of the basic formula (34) and a full analysis of the analytic properties of $G(\alpha, w)$ will be published elsewhere.

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