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LETTER TO THE EDITOR

Lattice Green function for the simple cubic lattice†

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Abstract. A particular lattice Green function for the simple cubic lattice is evaluated exactly as a square of a Heun function, and as a product of two complete elliptic integrals of the first kind. Applications of these results in lattice statistics are briefly described.

The lattice Green function

$$P(\boldsymbol{l}, z) \equiv P(l_1, l_2, l_3; z)$$
$$= \frac{1}{\pi^3} \int\int\int_0^{\pi} \frac{\cos l_1 x_1 \cos l_2 x_2 \cos l_3 x_3}{1 - \frac{1}{3}z(\cos x_1 + \cos x_2 + \cos x_3)} \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 \tag{1}$$

where l_1, l_2, l_3 are integers, is frequently encountered in the study of lattice statistics on the simple cubic (SC) lattice with isotropic nearest neighbour interactions‡. For example, $P(\boldsymbol{l}, z)$ occurs in the statistical theories of ferromagnetism such as the spherical model (Berlin and Kac 1952, Joyce 1972), and Heisenberg model (Dyson 1956a, 1956b, Dalton and Wood 1967). In the theory of random walks (Montroll and Weiss 1965, Domb and Joyce 1972) on the SC lattice $P(\boldsymbol{l}, z)$ is an integral representation for the basic probability generating function

$$P(\boldsymbol{l}, z) = \sum_{n=0}^{\infty} P_n(\boldsymbol{l}) z^n \qquad |z| \leqslant 1 \tag{2}$$

where $P_n(\boldsymbol{l})$ is the probability that a random walker, starting at the origin $\boldsymbol{l} = \boldsymbol{0}$, will reach the lattice site $\boldsymbol{l}$ after a walk of n steps. The main purpose of this letter is to give an exact general expression for $P(z) \equiv P(\boldsymbol{0}, z)$ in terms of complete elliptic integrals of the first kind.

The procedure used to evaluate $P(z)$ is rather complicated and will be described in detail elsewhere. The basic aim of the analysis is to prove that the Green function $P(z)$ can be written in the form

$$P(z) = [F(9, -\tfrac{3}{4}; \tfrac{1}{4}, \tfrac{3}{4}, 1, \tfrac{1}{2}; z^2)]^2 \tag{3}$$

where $F(a, b; \alpha, \beta, \gamma, \delta; x)$ denotes a Heun function §. It is then shown, using standard quadratic and bilinear transformation formulae for Heun functions (Snow 1952),

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‡ For a recent review on lattice Green functions see Katsura *et al* (1971a).

§ For a detailed account of the properties of Heun functions see Snow (1952).

that $P(z)$ can be directly related to the corresponding lattice Green function for the *face-centred cubic* lattice (Iwata 1969, Joyce 1971). In this manner we obtain the following product formula for the SC lattice Green function:

$$P(z) = (1-\tfrac{3}{4}x_1)^{1/2}(1-x_1)^{-1}(2/\pi)^2 K(k_+)K(k_-) \tag{4}$$

where

$$k_\pm{}^2 = \tfrac{1}{2} \pm \tfrac{1}{4}x_2(4-x_2)^{1/2} - \tfrac{1}{4}(2-x_2)(1-x_2)^{1/2} \tag{5}$$

$$x_1 = \tfrac{1}{2} + \tfrac{1}{6}z^2 - \tfrac{1}{2}(1-z^2)^{1/2}(1-\tfrac{1}{9}z^2)^{1/2} \tag{6}$$

$$x_2 = x_1/(x_1-1) \tag{7}$$

and $K(k)$ is a complete elliptic integral of the first kind. By inspection of this result it is readily seen that $P(z)$ displays branch point singularities in the z^2 plane at $z^2 = 1, 9$ and ∞. Thus the Green function $P(z)$ is a single-valued analytic function in the z^2 plane cut along the real axis from $+1$ to $+\infty$.

We can check the validity of equation (4) by considering particular values of z^2. When $z^2 = 1$ we find that

$$P(1) = \left(\frac{6\sqrt{2}}{\pi^2}\right) K(k_+)K(k_-) \tag{8}$$

where

$$k_\pm{}^2 = -\tfrac{1}{2}(2\sqrt{3}-1 \pm \sqrt{6}). \tag{9}$$

Next we apply the standard transformation formula (Erdélyi *et al* 1953)

$$\left(\frac{2}{\pi}\right) K(k) = {}_2F_1(\tfrac{1}{2},\tfrac{1}{2};1;k^2) = (1-k^2)^{-1/2}{}_2F_1(\tfrac{1}{2},\tfrac{1}{2};1;k^2/k^2-1) \tag{10}$$

to the elliptic integrals in equation (8). This procedure yields

$$P(1) = \left(\frac{12\sqrt{2}}{\pi^2}\right)(2-\sqrt{3})K(k_+)K(k_-) \tag{11}$$

where

$$k_\pm{}^2 = \frac{2\sqrt{3}-1 \pm \sqrt{6}}{2\sqrt{3}+1 \pm \sqrt{6}} = (2-\sqrt{3})^2(\sqrt{3} \pm \sqrt{2})^2. \tag{12}$$

If the relation

$$K(k_+) = (\tfrac{3}{2})^{1/2}(1+k_-)K(k_-) \tag{13}$$

is substituted in equation (11) we finally obtain

$$P(1) = \left(\frac{12}{\pi^2}\right)(18+12\sqrt{2}-10\sqrt{3}-7\sqrt{6})[K(k_-)]^2 \simeq 1{\cdot}516\,386\,059\,151\,978 \tag{14}$$

where $k_- = (2-\sqrt{3})(\sqrt{3}-\sqrt{2})$. This result is in complete agreement with that obtained previously by Watson (1939).

In order to evaluate $P(z) \equiv \tilde{P}(z^2)$ along the edges of the branch cut in the z^2 plane we must replace z^2 in equation (6) by $z^2 \pm i\epsilon$, and use the formula

$$\{1-(\xi \pm i\epsilon)\}^{1/2} = \mp i(\xi - 1 \pm i\epsilon)^{1/2} \tag{15}$$

where $1 < \xi < \infty$ and $\epsilon \gtrsim 0$. For large values of z^2 a considerable simplification occurs, and equation (4) gives

$$\lim_{\epsilon\to 0+} \tilde{P}(z^2 \pm i\epsilon) = \pm i(9/z^2)^{1/2}(2/\pi^2)K(k_+)K(k_-) \tag{16}$$

as $z^2 \to +\infty$, where

$$k_\pm{}^2 = \tfrac{1}{4}(2 \pm \sqrt{3}). \tag{17}$$

This result agrees with that derived by Katsura *et al* (1971b). The general expression (4) has also been used to determine the real and imaginary parts of $\tilde{P}(z^2 \pm i\epsilon)$ as $\epsilon \to 0+$, for $z^2 = 9$ and $z^2 = 9/5$. In both these special cases agreement was found with the work of Katsura *et al* (1971b).

The detailed behaviour of $P(z)$ in the neighbourhood of the branch point $z^2 = 1$ may be readily established by applying a suitable analytic continuation formula (Snow 1952) to the Heun function in equation (3). It is found that

$$\begin{aligned}[P(z)]^{1/2} &= [P(1)]^{1/2}F\left(-8, \frac{9}{16}; \frac{1}{4}, \frac{3}{4}, \frac{1}{2}, \frac{1}{2}; 1-z^2\right) \\ &\quad -\left(\frac{3\sqrt{3}}{4\pi}\right)[P(1)]^{-1/2}(1-z^2)^{1/2}F\left(-8, \frac{69}{16}; \frac{5}{4}, \frac{3}{4}, \frac{3}{2}, \frac{1}{2}; 1-z^2\right)\end{aligned} \tag{18}$$

where $|\arg(1-z^2)| < \pi$, and $|\arg z^2| < \pi$. If this analytic continuation is developed as a Taylor series in powers of $(1-z^2)^{1/2}$ we obtain

$$\begin{aligned}P(z) = P(1) &- \frac{3\sqrt{3}}{2\pi}(1-z^2)^{1/2} + \frac{9}{32}\left(P(1) + \frac{6}{\pi^2 P(1)}\right)(1-z^2) \\ &- \frac{3\sqrt{3}}{4\pi}(1-z^2)^{3/2} + \frac{1}{1024}\left(175P(1) + \frac{1242}{\pi^2 P(1)}\right)(1-z^2)^2 \\ &- \frac{21\sqrt{3}}{40\pi}(1-z^2)^{5/2} + \ldots\end{aligned} \tag{19}$$

where $|1-z^2| < 1$. Maradudin *et al* (1960) and Montroll and Weiss (1965) have calculated the numerical value of the coefficient of $1-z^2$ in this expansion as 0·692381. However, their result is not in agreement with the exact value

$$\frac{9}{32}\left(P(1) + \frac{6}{\pi^2 P(1)}\right) \simeq 0{\cdot}539\,238\,175\,081\,581. \tag{20}$$

The expansion (19) has several applications in lattice statistics. For example, it enables one to carry out a detailed analysis of the critical properties of the spherical model for the SC lattice (Joyce 1972), while in the theory of random walks it can be used to derive the following asymptotic formula for the expected number S_n of *distinct* lattice sites visited in an n step random walk on the SC lattice (Vineyard 1963, Montroll and Weiss 1965):

$$\begin{aligned}S_n \sim [P(1)]^{-1}n\Bigg\{1 &+ \left(\frac{3}{\Delta}\right)\left(\frac{6}{\pi n}\right)^{1/2} + \left(\frac{1}{16\Delta^2}\right)(162+7\Delta^2)n^{-1} \\ &+ \left(\frac{9}{16\Delta^3}\right)(18+\Delta^2)\left(\frac{6}{\pi n^3}\right)^{1/2} + \ldots\Bigg\}\end{aligned} \tag{21}$$

as $n \to \infty$, where $\Delta \equiv \pi P(1)$. Recently, Domb and Joyce (1972) have shown that the expansion (19) is also of considerable importance in the theory of selfavoiding random walks.

Finally, we note that expansions for $P(z)$ about the branch points $z^2 = 9$ and ∞ can be derived from equation (3) by applying standard transformation formulae (Snow 1952). The detailed properties of these expansions are currently being investigated.

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References

Berlin T H and Kac M 1952 *Phys. Rev.* **86** 821–35
Dalton N W and Wood D W 1967 *Proc. Phys. Soc.* **90** 459–74
Domb C and Joyce G S 1972 *J. Phys. C: Solid St. Phys.* **5** 956–76
Dyson F J 1956a *Phys. Rev.* **102** 1217–30
—— 1956b *Phys. Rev.* **102** 1230–44
Erdélyi A, Magnus W, Oberhettinger F and Tricomi F G 1953 *Higher Transcendental Functions* vol 1 (New York: McGraw-Hill) p 64
Iwata G 1969 *Natl. Sci. Rep., Ochanomizu University, Tokyo* **20** 13–8
Joyce G S 1971 *J. Phys. C: Solid St. Phys.* **4** L53–6
—— 1972 *Phase transitions and critical phenomena* vol 2 eds C Domb and M S Green (London: Academic Press) p 375
Katsura S *et al* 1971a *J. math. Phys.* **12** 892–5
Katsura S, Inawashiro S and Abe Y 1971b *J. math. Phys.* **12** 895–9
Maradudin A A *et al* 1960 *Green's Functions for Monoatomic Simple Cubic Lattices* (Bruxelles: Académie Royale de Belgique)
Montroll E W and Weiss G H 1965 *J. math. Phys.* **6** 167–81
Snow C 1952 *Hypergeometric and Legendre functions with applications to Integral Equations of Potential Theory, Applied Mathematics Series* 19 (Washington: National Bureau of Standards,) pp 109–27
Vineyard G H 1963 *J. math. Phys.* **4** 1191–3
Watson G N 1939 *Q. J. Math., Oxford* **10** 266–76