On the number of spanning trees for the 3D simple cubic lattice

1987 J. Phys. A: Math. Gen. 20 L923

(http://iopscience.iop.org/0305-4470/20/14/005)

J. Phys. A: Math. Gen. **20** (1987) L923–L927. Printed in the UK

LETTER TO THE EDITOR

On the number of spanning trees for the 3D simple cubic lattice†

Anders Rosengren

Condensed Matter Theory Group, Department of Physics, Box 530, Uppsala University, S-751 21 Uppsala, Sweden

Received 13 July 1987

Abstract. The number of spanning trees on a large lattice is evaluated exactly for the 3D simple cubic lattice graph. Similarities to the evaluation of the lattice Green function are pointed out.

If G is a connected graph, then a spanning tree in G is a spanning subgraph of G, which contains no circuits. That a subgraph is spanning means that its vertex set is the same as that of G. For a regular lattice graph of N sites, the number of spanning trees $T(N)$ behaves as $\exp(zN)$ for large N, i.e.

$$z = \lim_{N\to\infty} B^{-1} \ln T(N). \tag{1}$$

This limit was evaluated by Wu (1977) for three planar lattice graphs, namely for the square, triangular and honeycomb lattice graphs. Thereby Wu used the partition function of ice-type models on the related medial lattices. (Note that the medial lattices also are planar.) The method used in this letter enables the calculation of z also when the lattice graph is not planar and the method used by Wu is therefore not applicable. Here we calculate z for the simple cubic lattice graph. We also note the similarities in calculating the number of spanning trees on a lattice and in calculating the lattice Green function.

From graph theory it is known that for a connected graph

$$T(N) = N^{-1} \prod \mu \tag{2}$$

where the product runs through all non-zero eigenvalues μ of the matrix $C = \Delta - A$ where A is the adjacency matrix and Δ is the diagonal matrix, and where each diagonal entry is the valency of the corresponding vertex (Cvetković *et al* 1980). Furthermore, the spectrum of the graph of an $n_1 \times n_2 \times n_3$ cubic lattice is known (see, e.g., Cvetković *et al* 1980), and consists of all numbers of the form

$$2\sum_{j=1}^{3} \cos\left(\frac{\pi}{n_j+1}\nu_j\right)$$

† This work was supported by the Swedish Natural Science Research Council.

where $\nu_j = 1, \ldots, n_j$. If instead we introduce periodic boundary conditions, the spectrum is given by all numbers of the form

$$2\sum_{j=1}^{3}\cos\left(\frac{2\pi}{n_j}\nu_j\right).$$

This together with (2) gives

$$z = \lim_{\min_i n_i \to \infty} N^{-1}\ln T(N) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \ln[2(3-\cos\alpha-\cos\beta-\cos\gamma)]\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}\gamma \tag{3}$$

irrespective of the boundary conditions used. We would here like to point out similarities to the calculation of the lattice Green function, a function frequently encountered in the study of lattice statistics. For the simple cubic lattice it is defined by

$$G(t; l, m, n) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{\cos l\alpha\cos m\beta\cos n\gamma}{t-\cos\alpha-\cos\beta-\cos\gamma}\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}\gamma \tag{4}$$

where l, m and n are integers and t is a parameter (Maradudin *et al* 1960). Much effort has been spent to evaluate this integral. $G(3; 0, 0, 0)$ is one of the famous Watson integrals (Watson 1939). Watson's result seems to have been unnoticed by some members of the physics community as subsequently published numerical tabulations of $G(3; l, m, n)$ reveal. Joyce (1972) showed that $G(t, 0, 0, 0)$ could be expressed as a product of two complete elliptic integrals of the first kind. A few years later Morita (1975) showed that the function $G(t; l, m, n)$ for an arbitrary lattice site (l, m, n) could be expressed in terms of $G(t; 0, 0, 0)$, $G(t; 2, 0, 0)$ and $G(t; 3, 0, 0)$ only. Soon thereafter Horiguchi and Morita (1975) were able to obtain also $G(t; 2, 0, 0)$ and $G(t; 3, 0, 0)$ in closed forms, containing sums of products of complete elliptic integrals of the first and second kind. If we define

$$F(t; l, m, n) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \cos l\alpha\cos m\beta\cos n\gamma \times\ln(t-\cos\alpha-\cos\beta-\cos\gamma)\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}\gamma \tag{5}$$

we obtain

$$z = \ln 2 + F(3; 0, 0, 0). \tag{6}$$

On the other hand

$$\frac{\mathrm{d}F(t; l, m, n)}{\mathrm{d}t} = G(t; l, m, n) \tag{7}$$

so in principle $F(t; l, m, n)$ could be obtained by integration. However, Horiguchi and Morita (1975) derived a simple recurrence relation, which after integration with respect to t gives

$$F(t; l, m, n) = (G(t; l+1, m, n) - G(t; l-1, m, n))/2l. \tag{8}$$

This relation can therefore be used to obtain $F(t; l, m, n)$ for all values of l, m and n except for $l = m = n = 0$, exactly the case of interest here! However, as will be shown below

$$F(3; 0, 0, 0) = \ln 3 - \sum_{n=1}^{\infty}\frac{1}{2n}f(n) \qquad F(3; 1, 0, 0) = -\sum_{n=1}^{\infty}\frac{1}{2n-1}f(n) \tag{9}$$

where

$$f(n)=\frac{1}{6^{2n}}\binom{2n}{n}\sum_{k=0}^{n}\binom{n}{k}^2\binom{2k}{k} \tag{10}$$

so $F(3;0,0,0)$ could be evaluated by means of the known value of $F(3;1,0,0)$ and an estimate of the error obtained by replacing the factor $2n$ by the factor $2n-1$. We will, however, proceed in a more direct way to evaluate $F(3;0,0,0)$. Firstly we write

$$F(3;0,0,0)=\ln 3-\frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi\sum_{n=1}^{\infty}\frac{w^n}{n}\frac{1}{3^n}\,\mathrm{d}\alpha\,\mathrm{d}\beta\mathrm{d}\gamma \tag{11}$$

where $w=A+B+C$, $A=\cos\alpha$, $B=\cos\beta$ and $C=\cos\gamma$. Then we make a trinomial expansion of w^n and note that only even powers of A, B and C contribute to the integral. Further we use the relation

$$\int_0^\pi A^{2j}\,\mathrm{d}\alpha=\frac{(2j-1)!!}{(2j)!!}\pi. \tag{12}$$

These steps together give

$$F(3;0,0,0)=\ln 3-\sum_{n=1}^{\infty}\frac{1}{2n}\frac{1}{6^{2n}}\binom{2n}{n}\sum_{k=0}^{n}\binom{n}{k}^2\sum_{j=0}^{n-k}\binom{n-k}{j}^2. \tag{13}$$

This expression can be further simplified by using

$$\sum_{k=0}^{n}\binom{n}{k}^2=\binom{2n}{n} \tag{14}$$

which gives

$$F(3;0,0,0)=\ln 3-\sum_{n=1}^{\infty}\frac{1}{2n}\frac{1}{6^{2n}}\binom{2n}{n}\sum_{k=0}^{n}\binom{n}{k}^2\binom{2k}{k}. \tag{15}$$

We note that the summand of the inner sum Σ has a narrow maximum of width $\approx 1/\sqrt{n}$ at $k=k_0=\frac{2}{3}n$ and first rewrite Σ by means of Stirling's formula

$$\Sigma=\sum_{k=0}^{n}\binom{n}{k}^2\binom{2k}{k}=\Sigma_1+\Sigma_2+\ldots \tag{16}$$

where

$$\Sigma_1=\sum_{k=0}^{n}\frac{1}{\sqrt{\pi k}}\binom{n}{k}^2 2^{2k}\qquad \Sigma_2=-\sum_{k=0}^{n}\frac{1}{\sqrt{\pi k}}\binom{n}{k}^2 2^{2k}\frac{1}{8k}. \tag{17}$$

Then a Taylor expansion is made around $k=k_0$, giving

$$\Sigma=\Sigma_{11}+\Sigma_{12}+\Sigma_{13}+\Sigma_{21}+\mathrm{O}(n^{-3}) \tag{18}$$

where

$$\Sigma_{11}=\frac{1}{\sqrt{\pi k_0}}\sum_{k=0}^{n}\binom{n}{k}^2 4^k\qquad \Sigma_{12}=-\frac{1}{2\sqrt{\pi}k_0^{3/2}}\sum_{k=0}^{n}\binom{n}{k}^2 4^k(k-k_0)$$
$$\Sigma_{13}=\frac{3}{8\sqrt{\pi}k_0^{5/2}}\sum_{k=0}^{n}\binom{n}{k}^2 4^k(k-k_0)^2\qquad \Sigma_{21}=-\frac{3}{16n}\Sigma_{11}. \tag{19}$$

Then we use that

$$\Sigma_{11}=\frac{1}{\sqrt{\pi k_0}}q_n(4) \tag{20}$$

where

$$q_n(x) = (1-x)^2 P_n((1+x)/(1-x)) \tag{21}$$

and $P_n(x)$ are Legendre polynomials (Riordan 1968). Further, if the asymptotic expansion of $P_n(x)$ for large n is used (Gradshteyn and Ryzhik 1965), one obtains

$$\Sigma_{11} = \frac{3^{2n+3/2}}{4n\pi}\left[1 - \frac{3}{32}\frac{1}{n} + \frac{49}{2048}\frac{1}{n^2} + O\left(\frac{1}{n^3}\right)\right]. \tag{22}$$

The sums Σ_{12} and Σ_{13} are developed in a similar fashion and in total it is found for Σ that

$$\Sigma = \frac{3^{2n+3/2}}{4n\pi}\left[1 - \frac{1}{4}\frac{1}{n} + O\left(\frac{1}{n^2}\right)\right]. \tag{23}$$

This means that

$$F(3; 0, 0, 0) = \ln 3 - \sum_{n=1}^{\infty} a_n \tag{24}$$

where for large n

$$a_n = \frac{3\sqrt{3}}{8\pi\sqrt{\pi}\, n^{5/2}}\left[1 - \frac{3}{8}\frac{1}{n} + O\left(\frac{1}{n^2}\right)\right]. \tag{25}$$

We now rewrite (24) as

$$F(3; 0, 0, 0) = \ln 3 - S_0 - S_1 \tag{26}$$

where

$$S_0 = \sum_{n=1}^{N_0-1} a_n \qquad S_1 = \sum_{n=N_0}^{\infty} a_n. \tag{27}$$

Equations (25) and (27) give

$$S_1 = AS_{11} + BS_{12} + O(N_0^{-7/2}) \tag{28}$$

where

$$S_{11} = \sum_{n=N_0}^{\infty} n^{-5/2} \qquad S_{12} = \sum_{n=N_0}^{\infty} n^{-7/2} \tag{29}$$

and $A = 3\sqrt{3}/(8\pi\sqrt{\pi})$ and $B = -3A/8$. We now use the Riemann zeta function to express S_{11} and S_{12} as

$$S_{11} = \zeta(5/2) - \sum_{n=1}^{N_0-1} n^{-5/2} \qquad S_{12} = \zeta(7/2) - \sum_{n=1}^{N_0-1} n^{-7/2} \tag{30}$$

where the sums are performed simultaneously with the sum S_0, and where $\zeta(5/2)$ and $\zeta(7/2)$ are taken from Gram (1925). In doing so, we obtain that $z = \ln 2 + F(3; 0, 0, 0) \approx 1.673\,3893$.

References

Cvetković D M, Doob M and Sachs H 1980 *Spectra of Graphs* (New York: Academic) pp 39, 75
Gradshteyn I S and Ryzhik I M 1965 *Tables of Integrals, Series and Products* (New York: Academic)
Gram J P 1925 *D. Kgl. Danske Vidensk. Selsk. Skrifter, Naturvidensk. og Mathem. Afd.*, 8 *Roekke* **10** 3
Horiguchi T and Morita T 1975 *J. Phys. C: Solid State Phys.* **8** L232-5
Joyce G S 1972 *J. Phys. A: Gen. Phys.* **5** L65-8
Maradudin A A, Montroll E W, Weiss G H, Herman R and Milnes H W 1960 *Green's Functions for Monoatomic Simple Cube Lattices* (Brussels: Académie Royale de Belgique)
Morita T 1975 *J. Phys. A: Math. Gen.* **8** 478-89
Riordan J 1968 *Combinatorial Identities* (New York: Wiley)
Watson G N 1939 *Q. J. Math.* **10** 266-76
Wu F Y 1977 *J. Phys. A: Math. Gen.* **10** L113-5