Lower bounds on the numbers of lattice animals

1978 J. Phys. A: Math. Gen. 11 1449

(http://iopscience.iop.org/0305-4470/11/7/031)

J. Phys. A: Math. Gen., Vol. 11, No. 7, 1978. Printed in Great Britain

COMMENT

Lower bounds on the numbers of lattice animals

S G Whittington†‡ and D S Gaunt§

† Department of Chemistry, University of Bristol, Bristol BS8 1TL UK
§ Wheatstone Physics Laboratory, King's College, Strand, London WC2R 2LS, UK

Received 13 March 1978

Abstract. Rigorous lower bounds on the connective constants for site and bond animals have been derived for d-dimensional simple hypercubic lattices. These bounds establish for arbitrary d that the connective constants for site and bond animals are strictly greater than the connective constant for self-avoiding walks.

In this note we present some exact results concerned with the derivation of bounds on the numbers of site and bond lattice animals. The enumeration problem on lattices of two, three and higher dimensions, and the subsequent analysis of data is of interest in the theory of percolation and has been the subject of several recent papers (Sykes and Glen 1976, Sykes *et al* 1976, Gaunt *et al* 1976, Gaunt and Ruskin 1978). We consider the square lattice as an example and define a_n, b_n and c_n to be, respectively, the numbers of site animals, bond animals and self-avoiding walks weakly embeddable in the lattice, per lattice site. The subscript refers to the number of sites for site animals, and the number of bonds for bond animals and self-avoiding walks. Since each (undirected) self-avoiding walk with n bonds is a site animal with $(n+1)$ sites, which is in turn a bond animal with n bonds, we have

$$\tfrac{1}{2}c_n \leqslant a_{n+1} \leqslant b_n. \tag{1}$$

Hammersley (1957) showed that

$$\lim_{n\to\infty} n^{-1} \ln c_n = \inf_{n>0} n^{-1} \ln c_n = \ln \mu \tag{2}$$

say, and Klarner (1967) showed that

$$\lim_{n\to\infty} n^{-1} \ln a_n = \sup_{n>0} n^{-1} \ln a_n = \ln \lambda_s \tag{3}$$

say. An exactly analogous argument can be constructed for the case of the bond animals giving

$$\lim_{n\to\infty} n^{-1} \ln b_n = \sup_{n>0} n^{-1} \ln b_n = \ln \lambda_b \tag{4}$$

say. Hence (1) implies that

$$\mu \leqslant \lambda_s \leqslant \lambda_b. \tag{5}$$

‡ Permanent address: Department of Chemistry, University of Toronto, Toronto, M5S 1A1, Canada.

The number of animals has also been studied under the name of polyominoes (Golomb 1965). The numbers a_n correspond to *fixed* polyominoes; the numbers of *free* polyominoes p_n correspond to an enumeration of space types (Domb 1960). It is easily proved that free and fixed polyominoes have the same limit λ_s (Klarner 1967). For example, on the square lattice

$$8p_n \geqslant a_n \geqslant p_n \tag{6}$$

which implies that

$$\lim_{n\to\infty} n^{-1} \ln p_n = \lim_{n\to\infty} n^{-1} \ln a_n = \ln \lambda_s. \tag{7}$$

The factor of 8 in (6) is the maximum count per lattice site of any particular space type. (For a general simple hypercubic lattice of dimensionality d this factor should be replaced by $2^d d!$) Furthermore, if we *assume* asymptotic forms of the kind

$$a_n \sim an^{-\theta}\lambda_s^n, \qquad p_n \sim pn^{-\tau}\lambda_s^n \tag{8}$$

then it follows from (6) that $\tau = \theta$.

Although a_n and p_n have the same form asymptotically, the initial coefficients of a_n behave quite differently from the initial coefficients of p_n. For the square lattice, the number of animals is given by Sykes and Glen (1976) through a_{19} and the number of polyominoes through p_{18} by Lunnon (1971). We have analysed both of these sequences by the ratio method (Gaunt and Guttmann 1974) and find (not surprisingly, we feel) that the a_n are considerably smoother and attain their asymptotic behaviour much faster than do the p_n. We conclude that for the purpose of numerical estimation of the growth parameter λ_s and the critical exponent θ *from the first few terms of the series*, the a_n are to be preferred to the p_n. However, by $n = 18$ we find $a_n = 7{\cdot}99919\ldots p_n$, so there is little to choose between the two sequences. Lunnon (1971) has proved that asymptotically $a_n \sim 8p_n$ for the square lattice.

There is now a good deal of exact enumeration data available for a_n, b_n and c_n which has allowed good estimates to be made of the limits λ_s, λ_b and μ, respectively. Although these estimates suggest very strongly that all of the inequalities in (5) are strict for all lattices, they involve assumptions (see (8), for example) about the ways in which the limits are approached and are therefore non-rigorous. One of the consequences of our results is that two of the three inequalities in (5) can be made strict for a general simple hypercubic lattice of dimensionality d.

An exactly known value of a_m, for example, for some particular m, allows one to establish a rigorous lower bound on λ_s since

$$m^{-1} \ln a_m \leqslant \ln \lambda_s \tag{9}$$

for any m. For instance, using $a_{19} = 5940\,738\,676$ (Sykes and Glen 1976), gives $\lambda_s \geqslant 3{\cdot}2689\ldots$, for the square lattice. We shall show how this can be improved to give $\lambda_s \geqslant 3{\cdot}3904\ldots$, which is still well below the best numerical estimate of $4{\cdot}065 \pm 0{\cdot}005$ (Guttmann and Gaunt 1978), and also below the best lower bound of $\lambda_s \geqslant 3{\cdot}72$ (Klarner 1967). However, our technique readily generalises to site and bond animals on simple hypercubic lattices of dimensionality d, for which problems we give explicit lower bounds for all $d \leqslant 7$.

For each site animal on the square lattice we define the top (bottom) site as the left-most (right-most) site in the top (bottom) row of sites, and the left (right) site as the top (bottom) site in the left-most (right-most) column of sites. Let the coordinates of the top, bottom, left and right sites of a particular m-animal be (x_T, y_T), (x_B, y_B), (x_L, y_L) and (x_R, y_R) and those of a second m-animal be (x'_T, y'_T), etc. If each m-animal is joined to each other m-animal by translating so that

$$\text{(i)}\quad x'_B = x_T, \qquad y'_B = y_T + 1$$

$$\text{(ii)}\quad x'_L = x_R + 1, \qquad y'_L = y_R$$

and a bond is added joining the appropriate pair of adjacent vertices, the resulting graphs will be animals with $2m$ sites, and moreover, these animals will be distinct. Hence,

$$a_{2m} \geqslant 2a_m^2. \tag{10}$$

Now fix m and write $n = mp + q$ with $0 \leqslant q < m$. Successive application of (10) gives

$$\begin{aligned} a_n &\geqslant 2^{p-1} a_m^p \{2a_q\}, \qquad a_0 = \tfrac{1}{2} \\ &\geqslant 2^{p-1} a_m^p. \end{aligned} \tag{11}$$

Taking logarithms, dividing by n, and letting $n \to \infty$, gives

$$\lim_{n\to\infty} n^{-1} \ln a_n \geqslant m^{-1} \ln(2a_m) \tag{12}$$

which yields, on using $a_{19}(2)$, $\lambda_s \geqslant 3{\cdot}3904\ldots$ for the square lattice.

Similar arguments apply to the case of a d-dimensional simple hypercubic lattice. In this case there is one way of joining in each dimension, so that

$$\ln \lambda_s(d) \geqslant m^{-1} \ln[da_m(d)]. \tag{13}$$

Using $a_{13}(3) = 3322\,769\,129$, $a_{11}(4) = 3178\,474\,308$, $a_{10}(5) = 3648\,115\,531$, $a_9(6) = 1398\,295\,989$ and $a_9(7) = 5933\,702\,467$ from Gaunt *et al* (1976), we find the following lower bounds for $\lambda_s(d)$: $5{\cdot}8765\ldots$ ($d = 3$), $8{\cdot}2903\ldots$ ($d = 4$), $10{\cdot}6194\ldots$ ($d = 5$), $12{\cdot}6659\ldots$ ($d = 6$), $15{\cdot}1295\ldots$ ($d = 7$).

We have also deduced from the data of Gaunt *et al* (1976) that for all d

$$\begin{aligned} a_9(d) = \binom{d}{1} + 9908\binom{d}{2} + 1\,123\,143\binom{d}{3} + 20\,762\,073\binom{d}{4} + 125\,055\,400\binom{d}{5} \\ + 313\,921\,008\binom{d}{6} + 343\,901\,376\binom{d}{7} + 136\,048\,896\binom{d}{8} \end{aligned} \tag{14}$$

which may be used to obtain lower bounds for $d > 7$. In addition, it can be shown using (13) and (14), that for any particular d

$$\lambda_s(d) > 2d - 1. \tag{15}$$

(It should be noted that the bound (9) is too weak to prove this result for any $d \geqslant 6$ with the data presently available.) Since it is well known that

$$\mu(d) \leqslant 2d - 1 \tag{16}$$

we have that *for all d*

$$\lambda_s(d) > \mu(d) \tag{17}$$

and hence from (5)

$$\lambda_b(d) > \mu(d). \tag{18}$$

These results are of some interest since there appears to be a wide class of connected graphs which have the same connective constant, for a given lattice (see e.g. Guttmann and Whittington 1978). The interesting difference is probably that, as n increases, new *types* of graph (for example, graphs with higher cyclomatic index) contribute to the number of animals.

Similar reasoning, in which for instance the bottom site of a bond cluster is made to coincide with the top site of a second bond cluster, can be given for bond animals, and we obtain

$$\ln \lambda_b(d) \geq m^{-1} \ln[d b_m(d)]. \tag{19}$$

For the square and simple cubic lattices, $b_{15}(2) = 1880\,580\,352$ (Sykes and Glen 1976, unpublished) and $b_{11}(3) = 2375\,037\,477$ (Sykes *et al* 1976, unpublished), which yield $\lambda_b(2) \geq 4{\cdot}3486\ldots$ and $\lambda_b(3) \geq 7{\cdot}8651\ldots$, respectively. For $d \geq 4$ we may obtain bounds by using the result

$$\begin{aligned} b_{10}(d) = \binom{d}{1} &+ 730\,532\binom{d}{2} + 255\,716\,421\binom{d}{3} + 8\,975\,840\,816\binom{d}{4} \\ &+ 95\,175\,488\,385\binom{d}{5} + 442\,224\,105\,756\binom{d}{6} \\ &+ 1048\,268\,558\,064\binom{d}{7} + 1326\,024\,805\,120\binom{d}{8} \\ &+ 853\,070\,397\,696\binom{d}{9} + 219\,503\,494\,144\binom{d}{10} \end{aligned} \tag{20}$$

which we have deduced from the work of Gaunt and Ruskin (1978) and is valid for all d. This gives $\lambda_b(4) \geq 11{\cdot}4873\ldots$, $\lambda_b(5) \geq 15{\cdot}3219\ldots$, $\lambda_b(6) \geq 19{\cdot}2308\ldots$, $\lambda_b(7) \geq 23{\cdot}2044\ldots$ and so on.

For the d-dimensional simple hypercubic lattices, Gaunt and Ruskin (1978) have shown that

$$\lambda_b - \lambda_s = \lambda_B[\tfrac{3}{2}\sigma^{-1} + O(\sigma^{-3})] \tag{21}$$

where $\sigma = 2d - 1$ and $\lambda_B = \sigma^\sigma/(\sigma-1)^{\sigma-1}$ is the Bethe approximation for the growth parameter λ of either bond or site clusters. This expansion which is probably asymptotic in nature suggests that $\lambda_b > \lambda_s$ for all d. Numerical estimates of λ_b and λ_s support this conjecture for $d = 2$ to 6 (Gaunt *et al* 1976, Gaunt and Ruskin 1978). For the square lattice ($d = 2$), the best upper bound we know of is $\lambda_s < 4{\cdot}5$ due to Conway and Guy (see Lunnon 1971). Unfortunately, our best lower bound of $\lambda_b \geq 4{\cdot}3486\ldots$ is just too weak for us to prove rigorously that $\lambda_b > \lambda_s$ for the square lattice. However, we note that our lower bound on $\lambda_b(2)$ *is* greater than the best numerical estimate of $\lambda_s(2)$ which further supports this conjecture.

Acknowledgments

We would like to thank Professor R W Robinson for the hospitality of the Mathematics Department at the University of Newcastle, NSW, Australia, where this work was begun. We have also benefited from conversations with a number of members of the Mathematics Department at Newcastle especially Professor A J Guttmann. SGW is also grateful to Professor D H Everett for his hospitality at the University of Bristol, UK, where some of this work was also carried out, and to Professor J B Wilker for helful conversations.

References

Domb C 1960 *Phil. Mag. Suppl.* **9** 149–361
Gaunt D S and Guttmann A J 1974 *Phase Transitions and Critical Phenomena* vol 3 ed C Domb and M S Green (New York: Academic Press) pp 181–243
Gaunt D S and Ruskin H 1978 *J. Phys. A: Math. Gen.*, **11** 1369–80
Gaunt D S, Sykes M F and Ruskin H 1976 *J. Phys. A: Math. Gen.* **9** 1899–911
Golomb W S 1965 *Polyominoes* (New York: Scribner's)
Guttmann A J and Gaunt D S 1978 *J. Phys. A: Math. Gen.* **11** 949–53
Guttmann A J and Whittington S G 1978 *J. Phys. A: Math. Gen.* **11** 721–9
Hammersley J M 1957 *Proc. Camb. Phil. Soc.* **53** 642–5
Klarner D A 1967 *Can. J. Math.* **19** 851–63
Lunnon W F 1971 *Computers in Number Theory* eds A O L Atkin and B J Birch (London: Academic Press) pp 347–72
Sykes M F, Gaunt D S and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 1705–12
Sykes M F and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 87–95