Restricted valence site animals on the simple cubic lattice

D S Gaunt†, J L Martin†, G Ord‡, G M Torrie‡ and S G Whittington‡

† Wheatstone Physics Laboratory, King's College, University of London, Strand, London WC2R 2LS, UK
‡ University of Toronto, Toronto M5S 1A1, Canada

Abstract. Exact values of the numbers of connected clusters of n sites, each site having valence no larger than ν, are presented for the simple cubic lattice for $\nu = 2, 3, 4, 5$ and 6 for small values of n. Assuming a plausible asymptotic form for the dependence of these numbers on n and ν we show rigorously that the exponent τ characterising the dominant singularity in the generating function is negative for $\nu = 2$ but positive for $\nu \geqslant 3$. Series analysis techniques suggest that the *same* value of τ obtains for *all* $\nu \geqslant 3$.

A lattice (site) animal is a cluster of sites of the lattice (of coordination number Q) such that adjacent sites are joined by a bond and every site in the cluster can be reached from every other site in the cluster by a path along these bonds, i.e. a site animal is a connected section graph of the lattice. Lattice animals are of interest in the theory of percolation processes (Sykes and Glen 1976). It has been shown rigorously (Klarner 1967) that if the number of site animals with n sites, per lattice site, is a_n then

$$0 < \lim_{n \to \infty} n^{-1} \ln a_n \equiv \ln \lambda < \infty \tag{1}$$

and a plausible assumption would seem to be

$$a_n \sim C n^{-\tau} \lambda^n \qquad (n \to \infty). \tag{2}$$

Making use of exact enumerations of lattice animals for small n, series analysis techniques have yielded estimates of λ, the exponent τ and the amplitude C (Sykes and Glen 1976, Sykes *et al* 1976, Guttmann and Gaunt 1978). It is found that both λ and C are lattice-dependent whereas the exponent τ is a dimensional invariant. These conclusions are consistent with the universality hypothesis.

More recently, attention has been focused (Gaunt *et al* 1979, Whittington *et al* 1979) on a generalisation of this problem in which the valence of each site in a cluster is not allowed to exceed some pre-assigned number ν, i.e. the number of bonds meeting at a site cannot exceed $\nu \leqslant Q$. If the number of animals on the square lattice with n sites having no vertex of degree greater than ν is $a_n(\nu)$, Gaunt *et al* (1979) showed rigorously that $a_n(\nu)^{1/n}$ approaches a limit $\lambda(\nu)$, say, for all ν and, assuming that

$$a_n(\nu) \sim C(\nu) n^{-\tau(\nu)} \lambda(\nu)^n \qquad (n \to \infty) \tag{3}$$

they showed that $\tau(2) < 0$ but $\tau(\nu) > 0$ for $\nu \geqslant 3$. In addition, they presented numerical evidence that $\tau(3) = \tau(4) = 1$. Subsequently, this work was extended to the triangular and honeycomb lattices by Whittington *et al* (1979). They concluded that for site

clusters on the triangular, square and honeycomb lattices the exponent τ changes between $\nu = 2$ and $\nu = 3$ from $\tau(2) \simeq -\frac{1}{3}$ to $\tau(3) = 1$, and is then independent of ν for all larger values of ν.

The above results are interesting in that they extend the universality class of site animals on two-dimensional lattices to include the cases $3 \le \nu \le Q$, and show that $\nu = 2$ animals belong to a different universality class. Of course, it is also of interest to consider the corresponding problem on three-dimensional lattices. Consequently, we shall consider here the simple cubic lattice site animals with $\nu = 2, 3, 4, 5$ and 6. Some exact enumeration data are presented in table 1. The values for $\nu = 6$ up to $n = 13$ are reproduced from Gaunt *et al* (1976). For $\nu = 3, 4$ and 5 we have obtained the numbers of clusters with up to 12, 11 and 11 vertices, respectively. For $\nu = 2$, the number of clusters with n vertices is the sum of the number of strongly embedded simple chains with $n - 1$ edges, $[n - 1]_c$, and the number of strongly embedded polygons with n edges, $[n]_0$,

$$a_n(2) = [n - 1]_c + [n]_0. \tag{4}$$

Table 1. Numbers of clusters $a_n(\nu)$ with maximum valence ν and simple chains $[n - 1]_c$, having n sites and strongly embeddable in the simple cubic lattice.

n	$[n - 1]_c$	$a_n(2)$	$a_n(3)$	$a_n(4)$	$a_n(5)$	$a_n(6)$
1	1	1	1	1	1	1
2	3	3	3	3	3	3
3	15	15	15	15	15	15
4	63	66	86	86	86	86
5	267	267	519	534	534	534
6	1107	1111	3247	3475	3481	3481
7	4623	4623	20807	23399	23501	23502
8	19071	19098	136393	161641	162895	162913
9	78987	78987	911439	1139421	1152639	1152870
10	324543	324789	6189701	8163899	8292218	8294738
11	1337511	1337511	42596055	59284095	60469374	60494549
12	5483235	5485642	296398781			446205905
13	22527315	22527315				3322769129
14	92200455					
15	377965479					
16	1544925891					
17	6322891707					

We have enumerated $a_n(2)$ up to $n = 13$ and $[n - 1]_c$ up to $n = 17$. Values of $[n - 1]_c$ were previously available only through $n = 14$ (Fisher and Hiley 1961, Hioe 1967). As pointed out by Gaunt *et al* (1979), the dominant asymptotic behaviour of $a_n(2)$ will be the same as $[n - 1]_c$, the number of $(n - 1)$ step undirected neighbour-avoiding walks (NAWS).

Before presenting the analysis of these data, we shall extend the arguments of Gaunt *et al* (1979) for the square lattice to show that $\tau(3) > 0$ for the simple cubic lattice.

The basic argument in that paper rested on joining two animals together to form a larger animal, without violating the restricted valence criterion. Gaunt *et al* (1979)

showed that, for the d-dimensional hypercubic lattice,

$$a_n(\nu)a_m(\nu) \leq a_{n+m}(\nu) \tag{5}$$

for all n and m, when $\nu \geq d+1$. That is, for the square lattice $a_n(\nu)$ is a supermultiplicative function of n for $\nu \geq 3$ and, assuming the functional form (3), it follows that $\tau(\nu) \geq 0$ for $\nu \geq 3$. For the simple cubic lattice, this argument only shows that $a_n(\nu)$ is supermultiplicative for $\nu \geq 4$ and hence that $\tau(\nu) \geq 0$ for $\nu \geq 4$. The argument used by Gaunt *et al* to show that $\tau(2) < 0$ for the square lattice will also work for the cubic lattice, so that the only remaining case is $\nu = 3$. For this value of ν the 'joining construction' used by Gaunt *et al* would not necessarily yield animals with no vertices with degree greater than three and we must seek an alternative proof.

We first need a definition and a lemma.

Definition. For a site animal (A) on the cubic lattice, with all vertices of degree less than or equal to three, the *top set* of vertices $T(A)$ consists of the set of vertices with largest z coordinate.

Lemma. $T(A)$ cannot consist entirely of articulation points of degree three.

The proof of this lemma is rather complicated and we shall defer it until the remainder of the proof has been outlined. In the same way that we can define a top set of vertices of an animal, we can define a *bottom set* $B(A)$, all of which have smallest z coordinate. Clearly the lemma will also apply to the bottom set B, and we shall construct an animal by joining a vertex in $T(A)$ to a vertex in $B(A')$ where A and A' are animals with, respectively, n and m vertices. If $T(A)$ and $B(A')$ both contain a vertex of degree two or less they can be joined as follows. Suppose that these vertices are σ and σ', then translate A' so that the x and y coordinates of σ' are the same as those of σ and the z coordinate of σ' is $z_0 + 2$, where z_0 is the z coordinate of σ. By adding a vertex σ'', between σ and σ' (with z coordinate $z_0 + 1$) and adding two edges (σ, σ'') and (σ', σ'') the resulting animal is a section graph of the lattice, has $(n+m+1)$ vertices and all vertices have degree less than or equal to three. (Notice that it is necessary to insert this additional vertex, σ'', since otherwise a degree-three vertex in A or A' might become adjacent to a vertex in the other animal, thus becoming a degree-four vertex.) If $T(A)$ does not contain a vertex of degree two or less (e.g. A might consist of the vertices of a cube) then, by the above lemma, at least one vertex in $T(A)$ must not be an articulation point. On removing this vertex (and its incident edges) a neighbouring vertex in $T(A)$ must be reduced to degree two. The same procedure can be used for $B(A')$ or for $T(A)$ and $B(A')$ together, and the above construction can be used. This leads to the following inequality:

$$a_n(3)a_m(3) \leq a_{n+m+1}(3) + a_{n+m}(3) + a_{n+m-1}(3) \leq 3a_{n+m+1}(3). \tag{6}$$

Defining $b_n(3) = a_n(3)/3$ gives

$$b_n(3)b_m(3) \leq b_{n+m+1}(3) \tag{7}$$

and, since $a_n(3) \leq a_n(6)$ and $\lim_{n \to \infty} a_n(6)^{1/n}$ exists and is finite, we know that $b_n(3)^{1/n}$ is bounded above. Hence (Wilker and Whittington 1979) $\lim_{n \to \infty} b_n(3)^{1/n}$ exists and is finite and so $\lim_{n \to \infty} a_n(3)^{1/n}$ exists and is finite. If the value of this limit is $\lambda(3)$ then it also follows (Wilker and Whittington 1979) that

$$a_n(3) \leq 3\lambda(3)^{n+1} \tag{8}$$

and, combining this result with the plausible asymptotic form (3), we obtain

$$\tau(3) \geqslant 0. \tag{9}$$

Proof of lemma. Suppose the contrary to be true. Consider an arbitrary animal, A, having no vertex of degree greater than three. Choose an arbitrary vertex $\sigma \in T(A)$. By hypothesis σ is an articulation point of degree three and is therefore either connected to three vertices σ', σ'', $\sigma''' \in T(A)$, in which case we say that σ is of type 1, or to two vertices σ', $\sigma'' \in T(A)$ and to a third vertex σ''' which is not a member of $T(A)$, in which case we say that σ is of type 2.

On deleting σ and its incident edges, A decomposes into two or three sub-animals which we label A', A'' and possibly A'''. If σ was a type-1 vertex, choose A' such that $T(A')$ contains only one of σ', σ'', $\sigma'''(\sigma'$, say). If σ was a type-2 vertex, choose A' such that it contains *either* both of σ' and σ'' *or* only one of these (σ', say) and not σ'''.

Now replace σ and all edges incident on σ and on a vertex in A', and call this new animal B. All vertices in $T(A')$ will be of degree three and will be articulation points of B and, in particular, this will be true of σ'. On removing σ' and all edges incident on σ', B will decompose into two or more sub-animals B', B'', and perhaps B'''.

We now wish to show that one of these (B', say) has the following properties:

(i) $\sigma \notin B'$,

(ii) $T(B')$ contains a vertex $\sigma^* \in T(B)$ which is a neighbouring lattice point to σ'.

From the geometry of the cubic lattice σ' must have at least two neighbours which are members of $T(B)$ and one of these will be σ. If σ was of type 1 in A or if it was of type 2 in A but A' did not contain both σ' and σ'' then σ is connected to other vertices in B only through σ'. Hence, when σ' is deleted from B, σ must form a separate sub-animal and there must be another sub-animal, B', not containing σ but containing a vertex $\sigma^* \in T(B')$ which was directly connected to σ' in B. The remaining possibility is that σ was of type 2 in A but A' contained both σ' and σ''. Then σ' must be type 1 (otherwise σ''' would also be in B) so σ' must have three neighbouring vertices in $T(B)$. Hence there must be a sub-animal (B') of B which does not contain σ but which contains a vertex $\sigma^* \in T(B')$ which is a neighbour of σ' on the lattice.

We now form an animal C from B' by replacing σ' and all edges incident on σ' and on a vertex in B'. This procedure can be continued, forming a sequence of animals $A \supset B \supset C \supset \ldots X \supset \ldots$ Since X is a proper sub-graph of the preceding members of the sequence, eventually we must obtain an animal (X, say) with only two vertices in $T(X)$. Both of these will be, at most, of degree two but the above argument shows that one must be of degree three (and an articulation point). Therefore we have a contradiction and the lemma is proved.

Remark. The *triangular lattice* has a similar difficulty in that the Gaunt *et al* (1979) proof works only for $\nu \geqslant 4$. However, for $\nu = 3$, it is possible to construct a very simple argument as follows. If the *bottom vertex*, σ (see Gaunt *et al* (1979) for definitions), of an animal is of degree three then two of its neighbouring vertices in the animal (σ' and σ'') must be connected through the third neighbour (σ''') so that σ''' is directly connected to each of σ, σ' and σ''. Hence, since $\nu = 3$, σ''' cannot be directly connected to any other vertices and cannot be an articulation point. σ''' can then be deleted so that σ becomes of degree two, and can be directly connected to the *top vertex* of a second animal. This leads to the inequality

$$a_n(3)a_m(3) \leqslant a_{n+m}(3) + a_{n+m-1}(3) + a_{n+m-2}(3) \leqslant 3a_{n+m}(3) \tag{10}$$

from which the existence of the limit

$$\lim_{n \to \infty} n^{-1} \ln a_n(3) = \ln \lambda(3) < \infty \tag{11}$$

follows, as does the property that $\tau(3) > 0$.

We now return to the analysis of the data in table 1 and have used standard methods of series analysis (Gaunt and Guttmann 1974) to estimate $\lambda(\nu)$, $\tau(\nu)$ and $C(\nu)$. Our best estimates are given in table 2.

**Table 2.** Estimates of critical parameters for the simple cubic lattice.

ν	$\lambda(\nu)$	$\tau(\nu)$	$C(\nu)$
2	$4\cdot046 \pm 0\cdot003$	$-\frac{1}{6} \pm 0\cdot015$	$0\cdot19 \pm 0\cdot02$
3	$7\cdot85 \ \pm 0\cdot03$	$1\cdot50 \pm 0\cdot05$	$0\cdot26 \pm 0\cdot05$
4	$8\cdot32 \ \pm 0\cdot01$	$1\cdot50 \pm 0\cdot05$	$0\cdot18 \pm 0\cdot05$
5	$8\cdot33 \ \pm 0\cdot03$	$1\cdot50 \pm 0\cdot05$	$0\cdot19 \pm 0\cdot05$
6	$8\cdot33 \ \pm 0\cdot025$	$1\cdot50 \pm 0\cdot05$	$0\cdot19 \pm 0\cdot04$

The values of $\lambda(\nu)$ are 'biased' in the sense that the central values quoted for $\tau(\nu)$ have been used in their estimation. The sensitivity of $\lambda(\nu)$ to small changes in τ is given roughly by $0\cdot25\Delta\tau$ for $\nu = 2$ and $0\cdot4\Delta\tau$ for $3 \leqslant \nu \leqslant 6$, where $\Delta\tau$ represents the change in τ. The estimates of $\lambda(\nu)$ for $\nu = 2$ and $\nu = 6$ are in good agreement with previous work (Hioe 1967, Sykes *et al* 1976, Guttmann and Gaunt 1978). $\lambda(\nu)$ appears to be a monotonic *increasing* function of ν (note that it is easy to *prove* that $\lambda(\nu)$ is monotone non-decreasing).

For $\nu = 2$, there are good theoretical reasons (Watson 1970) for believing that the exponent for NAWS (and hence $a_n(2)$) will be the same as for self-avoiding walks (SAWS), and hence we expect $\tau(2) \simeq -\frac{1}{6}$ (McKenzie 1976). Our estimate supports such a value, as did the work of Hioe (1967). For $\nu = 6$ our estimate of $\tau(6) \simeq 1\frac{1}{2}$ is in good agreement with earlier work (Sykes *et al* 1976, Guttmann and Gaunt 1978). Furthermore our results suggest that $\tau(\nu) \simeq 1\frac{1}{2}$ for all ν such that $3 \leqslant \nu \leqslant 6$. Perhaps our most persuasive evidence for the invariance of $\tau(\nu)$ with ν for $\nu \geqslant 3$ is shown in figure 1. Here, successive estimates, $\tau_n(\nu)$, of $\tau(\nu)$ given by $\tau_n(\nu) = n[1 - (\lambda_n/\lambda'_n)]$, where $\lambda'_n = n\lambda_n - (n-1)\lambda_{n-1}$ and $\lambda_n = a_n(\nu)/a_{n-1}(\nu)$, are plotted against n for $\nu = 3, 4, 5$ and 6. These plots suggest quite strongly the existence of a *common limit*, even though its precise value is rather uncertain. For estimating the limit we confined our attention to the $\nu = 6$ series since (a) it is longest, and (b) suffers very little from interference from sub-dominant singularities (see below).

The amplitudes $C(\nu)$ proved rather difficult to estimate precisely. $C(6)$ is in good agreement with the estimate $C(6) = 0\cdot19 \pm 0\cdot02$ of Guttmann and Gaunt (1978), whose smaller uncertainty does not reflect the uncertainties in λ and τ as do our estimates. It should be noted that the amplitude $C(\nu)$ defined through (3) is not quite the same as the amplitude $A(\nu)$ defined previously (Gaunt *et al* 1979, Whittington *et al* 1979), although they are simply related. We now feel that the present definition is more 'basic', particularly when the animal generating function

$$G(x, \nu) = 1 + \sum_{n \geqslant 1} a_n(\nu)x^n \tag{12}$$
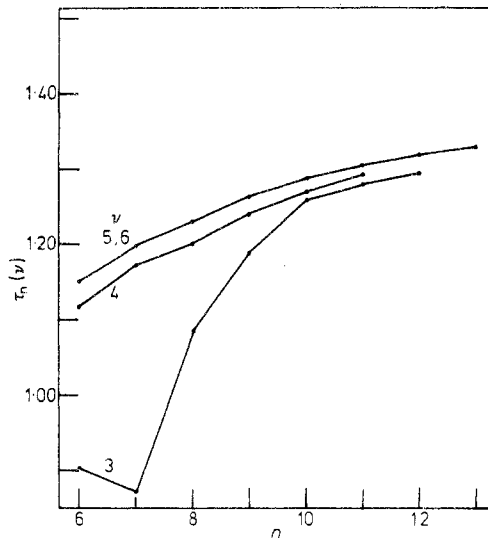
Figure 1. Successive estimates, $\tau_n(\nu)$, of $\tau(\nu)$ plotted against n for $\nu = 3, 4, 5$ and 6 for the simple cubic lattice. On this scale, the plot for $\nu = 5$ ($n \leqslant 11$) coincides with the plot for $\nu = 6$.

has a cusp-like singularity at $x = 1/\lambda(\nu)$ as it will for $\tau > 1$. (Notice that $C(\nu) = A(\nu)$ when $\tau(\nu) = 1$, as it does in two dimensions for $3 \leqslant \nu \leqslant Q$.)

Using Padé approximant techniques we have examined each of the generating functions to try to identify the sub-dominant singularities. For $\nu = 3$ there is a sub-dominant singularity on the negative real axis at about $x \simeq -2/\lambda(3)$, but is further out than $-3/\lambda(\nu)$ for all $\nu > 3$. For $\nu = 2$ and for NAWs it appears to be at $x = -1/\lambda(2)$, and a similar result is known for the SAW generating function (Hioe 1967, Watts 1975). Such symmetrically placed singularities in all three generating functions were also found (Gaunt *et al* 1979, Whittington *et al* 1979) for loose-packed lattices in two dimensions.

In summary, we have shown rigorously that for site clusters on the simple cubic lattice τ must change on going from $\nu = 2$ to $\nu = 3$. Numerical evidence suggests that $\tau(2) \simeq -\frac{1}{6}$ and $\tau(\nu) \simeq 1\frac{1}{2}$ for all $\nu \geqslant 3$. By the universality hypothesis the same result should be true for *all* three-dimensional lattices. The only results available for other three-dimensional lattices are $\tau(2) \simeq -\frac{1}{6}$ (Hioe 1967) and $\tau(6) \simeq 1\frac{1}{2}$ (Sykes *et al* 1976, Guttmann and Gaunt 1978) for the diamond, body-centred cubic and face-centred cubic lattices. Nevertheless, there can be little doubt about the truth of the conjecture in view of the present work and the knowledge that an analogous result appears to hold for all two-dimensional lattices (Gaunt *et al* 1979, Whittington *et al* 1979).

Acknowledgments

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