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COMMENT

Statistics of spiral lattice site animals with loops

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Abstract. For spiral lattice site animals embedded in the square lattice we conjecture a relation $\theta_i = \theta_0 - \alpha c$ where θ_i is the animal number exponent for animals with c loops, θ_0 is the exponent for trees and α is a numerical constant of approximate value 1.62. This result is different from the relation $\theta_i = \theta_0 - c$ which holds true for both undirected and directed animals.

Recently, a new type of lattice animal known as the spiral lattice animal has been defined (Li and Zhou 1985, Bose and Ray 1987, Bose *et al* 1988a, b) which belongs to a new universality class different from those of undirected and directed lattice animals. In a spiral animal the constraint is such that each site of the cluster is attached to the origin through at least one spiral path. In the spiral path, connection is either in the forward direction or in a specific rotational direction, say clockwise. For rooted spiral trees it has been shown that a dimensional reduction by four occurs in the problem (Bose *et al* 1988a). Another interesting result that has been obtained is that spiral lattice animals and spiral lattice trees belong to different universality classes, i.e. loops have a non-trivial effect on spiral lattice animal statistics (Bose *et al* 1988b). In this comment, we present some new results on the asymptotic cluster properties of spiral lattice site animals with c loops (c = 0, 1, 2, 3, 4) defined on the square lattice. Improved estimates of some previously calculated animal exponents are also given.

We concentrate on the following two types of asymptotic relations describing cluster properties. The first relation states that in the asymptotic $n \rightarrow \infty$ limit, where n is the number of sites in the animal, the total number of animals a_n goes as

$$a_n \xrightarrow[n \to \infty]{} \lambda^n n^{-\theta} \tag{1}$$

where λ is a constant for a particular lattice and is known as the 'growth parameter' because asymptotically $a_n/a_{n-1} \rightarrow \lambda$. The animal number exponent θ is universal and changes only if the lattice dimension d changes. For animals with c loops the corresponding relation is

$$a_{nc} \xrightarrow{} \lambda_{c}^{n} n^{-\theta}.$$
⁽²⁾

The second relation shows how the average radius of gyration R_n scales with size n:

$$R_n \underset{n \to \infty}{\sim} n^{\nu} \tag{3}$$

where ν is the radius of gyration exponent. R_n is defined as

$$\boldsymbol{R}_{n} = \left\langle \left(\sum_{i=1}^{n} r_{i}^{2} / n \right)^{1/2} \right\rangle$$
(4)

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where r_i is the distance of a cluster site *i* from the centre of mass of the cluster and $\langle \ldots \rangle$ denotes the average over all animals. For animals with *c* loops the relation corresponding to (3) is

$$R_{nc} \underset{n \to \infty}{\sim} n^{\nu}.$$
⁽⁵⁾

In order to calculate the exponents θ , ν , θ_c , ν_c and the parameters λ , λ_c for spiral animals as well as spiral animals with *c* loops, exact enumeration of cluster properties has been performed. The computer algorithm used generates undirected animals and then checks each animal for spiral connection. Besides spiral lattice animals, spiral animals with *c* loops (c = 0, 1, 2, 3, 4) have also been separately counted. All these enumeration data along with the exact data for radii of gyration are listed in tables 1 and 2. The data for animals and animals with *c* loops have been extended by three and two more terms, respectively, from the two previously reported expansions (Bose *et al* 1988a, b). Also, the results for *c*-loop animals for $c \ge 2$ are new. The number of loops *c* in an animal has been determined through the following relations:

$$b = \frac{1}{2} \sum_{i=1}^{4} iq(i) \qquad c = b - n + 1$$
(6)

where b is the number of bonds in the animal and q(i) is the number of sites in the animal which have *i* nearest-neighbour occupied sites. Figure 1 shows the variation of the ratio $r_n = a_n/a_{n-1}$ with 1/n for both animals and trees (c = 0). Extrapolation of the last few points to $n \to \infty$ can be performed by employing standard numerical procedures (Gaunt and Guttmann 1974). The intercept on the y axis gives λ and the exponent θ is determined from the slope. The linear extrapolants $r'_n = nr_n - (n-1)r_{n-1}$ and their averages $r''_n = (r'_n + r'_{n-1})/2$ should approach λ as $n \to \infty$. The crosses in figure 1 indicate the estimated values of λ and λ_0 . The exponent θ is calculated from the sequence of biased estimates

$$\theta(n) = n(1 - r_n/\lambda') \tag{7}$$

Table 1. Total number of spiral lattice site animals a_n and spiral lattice site animals with c loops, a_n , of size n on the square lattice.

n	<i>a</i> ,,	a_m					
		c = 0	<i>c</i> = 1	<i>c</i> = 2	<i>c</i> = 3	<i>c</i> = 4	
1	1	1					
2	2	2					
3	6	6					
4	17	16	1				
5	49	41	8				
6	140	104	34	2			
7	396	262	112	22			
8	1114	648	344	116	6		
9	3 134	1 577	1 032	452	72	1	
10	8 824	3 790	2 986	1 590	428	30	
11	24 924	9 0 1 4	8 384	5 3 2 6	1 888	304	
12	70 618	21 242	23 011	16 936	7 438	1 838	
13	200 810	49 676	61 924	51 662	27 448	8 684	
14	573 136	115 406	163 678	153 040	95 216	36 742	
15	1641 924	266 536	426 060	442 612	314 328	144 588	

	R _n	R _{nt}			
n		c = 0	c = 1	<i>c</i> = 2	
1	0.000 000	0.000 000	0.000 000	0.000 000	
2	0.500 000	0.500 000	0.000 000	0.000 000	
3	0.716 660	0.716 660	0.000 000	0.000 000	
4	0.910 290	0.923 000	0.707 000	0.000 000	
5	1.078 040	1.113 878	0.894 370	0.000 000	
6	1.231 843	1.291 327	1.066 030	0.957 500	
7	1.374 336	1.454 111	1.242 450	1.095 680	
8	1.506 745	1.608 090	1.412 910	1.237 630	
9	1.629 771	1.756 120	1.568 150	1.387 330	
10	1.744 838	1.898 981	1.712 813	1.538 150	
11	1.852 868	2.037 250	1.850 760	1.681 340	
12	1.954 931	2.171 439	1.983 384	1.817 950	
13	2.052 397	2.301 900	2.111 800	1.949 923	
14	2.145 651	2.429 000	2.236 866	2.078 000	
15	2.235 525	2.553 062	2.359 000	2.201 691	

Table 2. Exact radius of gyration data for spiral lattice site animals (R_n) and spiral lattice site animals with c loops (R_n) .





where λ' is the best estimate of λ . For trees, λ' is given by the best estimate of λ_0 . For both animals and trees, the convergence of $\theta(n)$ has been found to be good. The λ and θ values obtained are

$$\lambda = 3.002 \pm 0.02 \qquad \theta = 0.69 \pm 0.1$$

$$\lambda_0 = 2.123 \pm 0.004 \qquad \theta_0 = -1.318 \pm 0.02.$$
(8)

With a longer animal series available, the value of the animal number exponent θ is considerably changed from that previously reported. The value of θ_0 is, however, approximately the same.

For animals with c loops (c = 1, 2, 3, 4) we have found on extrapolation that the growth parameter λ_c is independent of the number of loops c and tends to λ_0 , the growth parameter for trees. The exponent θ_c has been calculated for c = 1 and c = 2 from the sequence of biased estimates similar to (7) and putting $\lambda' = \lambda_0$, the best estimate for the growth parameter of c-loop animals. The convergence of $\theta(n)$ in both cases is not good and θ has been estimated by extrapolating the plot of $\theta(n)$ against 1/n. The values obtained are

$$\theta_1 = -2.8 \pm 0.2$$
 $\theta_2 = -4.3 \pm 0.2.$ (9)

From (8) and (9) the exponents θ_c and θ_0 appear to satisfy the relation

$$\theta_{c} = \theta_{0} - \alpha c \tag{10}$$

where the constant α has an approximate value 1.5 ± 0.2 . For both undirected and directed lattice animals the corresponding relation is

$$\theta_c = \theta_0 - c \tag{11}$$

(Whittington *et al* 1983, Lam 1987, Duarte 1985). Soteros and Whittington (1988) have given a proof of (11) for undirected weakly embeddable animals (bond animals) in the square lattice. Universality demands that the same relation be true for strongly embeddable (site) animals. Whittington *et al* (1983) have derived the inequality

$$\theta_{\iota} \ge \theta_{\iota+1} \ge \theta_{\iota} - 1 \tag{12}$$

for the animal number exponents of animals with loops. The inequality is derived from another inequality involving lattice animal numbers

$$a_{n+3,c} \leq a_{n,c+1} \leq 2dna_{nc} \tag{13}$$

where $a_{nc} \sim n^{-\theta} \lambda_{i}^{n}$ and λ_{i} is independent of number of loops c_{i} all the λ_{i} being equal to λ_{0} , the growth parameter for trees. For spiral lattice site animals an inequality similar to the first half of the inequality in (13) can be proved. Let the vertices or sites of the spiral animals have coordinates (x_{i}, y_{i}) , i = 1, 2, ..., n. Following Whittington *et al* (1983) the top (bottom) vertex is defined as the vertex having maximum (minimum) x coordinate and, in case of ambiguity, the vertex in this subset having maximum (minimum) y coordinate. Consider any c-loop animal belonging to the set W_{nc} of animals with n sites and c loops. The number of such animals is a_{nc} . Let t be the top vertex of the animal with coordinates (x_{i}, y_{i}) . The top vertex can be approached in three ways:

(i) from the vertex $(x_i - 1, y_i)$ if it is occupied

(ii) from the vertex $(x_i, y_i - 1)$ if it is occupied

(iii) from both the vertices $(x_i - 1, y_i)$ and $(x_i, y_i - 1)$ if both are occupied.

In cases (ii) and (iii), add four vertices v_1 , v_2 , v_3 , v_4 with coordinates $(x_t + 1, y_t)$, $(x_t + 1, y_t - 1)$, $(x_t + 2, y_t)$ and $(x_t + 3, y_t)$, respectively. For lattice site animals, addition of a new site implies that the bonds between this site and its nearest occupied neighbours automatically exist. Addition of four new sites leads to an increase in the number of bonds by five. The number of loops therefore increases by one. The new animal obtained is also spirally connected and so belongs to the set $W_{n+4,c+1}$ of animals with c+1 loops. In case (i) there are two possibilities, either the vertex $(x_t, y_t - 1)$ is occupied

or unoccupied. If the first possibility is true, add four vertices with the same coordinates as in the case of (ii) and (iii) to get a spiral animal of n + 4 sites and c + 1 loops. If the second possibility is true, add vertices with coordinates $(x_i + 1, y_i)$, $(x_i + 2, y_i)$, $(x_i + 1, y_i - 1)$ and $(x_i + 2, y_i - 1)$ generating a spiral animal of n + 4 sites and c + 1 loops. Thus for each animal belonging to the set W_{nc} of animals, an animal belonging to the set $W_{n+4,c+1}$ can be generated, i.e. $a_{nc} \le a_{n+4,c+1}$ or, $a_{n-4,c} \le a_{n,c+1}$.

The proof given by Whittington *et al* (1983) for the second half of the inequality fails in the case of spiral animals. For undirected weakly embeddable animals, an upper limit to a_{nc} is $2dna_{n,c-1}$ as there are *n* vertices and at each vertex an edge can be added in 2d ways, addition of an edge (bond) implying an increase in the number of loops by 1. Thus $a_{nc} \leq 2dna_{n,c-1}$, or $a_{n,c+1} \leq 2dna_{nc}$, the second half of the inequality in (13) is obtained. In the case of spiral lattice animals, animals with *c* loops can be generated not only from spiral animals with c-1 loops but also from undirected animals with c-1 loops which are not spirally connected but which on the addition of an edge (bond) become spirally connected with *c* loops. Thus a simple relation like $a_{m} \leq 2dna_{n,c-1}$ cannot be written down for spiral lattice animals.

For spiral lattice site animals we have proved the inequality

$$a_{nc} \le a_{n+4,c+1}. \tag{14}$$

The asymptotic form of a_{nc} is given in (2). Taking logarithms on both sides of (14), dividing by *n* and letting *n* go to infinity leads to the result log $\lambda_c \leq \log \lambda_{c+1}$. As already mentioned, numerical evidence suggests that λ_c is independent of *c* and hence log $\lambda_c = \log \lambda_{c+1} = \ldots = \log \lambda_0$. Another piece of evidence for this result is as follows. From (2),

$$\frac{a_{n,c+1}}{a_{nc}} = \frac{b_{c+1}}{b_c} n^{-(\theta_{c+1}-\theta_{c+1})} \left(\frac{\lambda_{c+1}}{\lambda_c}\right)^n$$
(15)

where the bs are multiplicative constants. If λ_c is independent of c, then the plot of $\log(a_{n,c+1}/a_{nc})$ against $\log n$ should be a straight line. We have verified that this is the case for n = 14, 15 and c = 0, 1, 2, 3. Thus the growth parameter λ_c does not depend on c. If this is so, then from (14), one derives the inequality $\theta_c \ge \theta_{c+1}$ which, as (8) and (9) show, is true. In order to prove that the numerical constant α in (10) is not 1, unlike in the cases of undirected and directed lattice animals, we have plotted in figure 2 three sets of curves for undirected, directed and spiral lattice site animals



Figure 2. Plot of $-\Delta\theta(n)$ against 1/n for undirected (u), directed (d) and spiral (s) lattice site animals; $-\Delta\theta(n)$ is given by (16). The crosses denote intercepts of the extrapolated straight lines.

embedded in the square lattice. The data for undirected and directed lattice animals have been taken from published tables (Whittington *et al* 1983, Lam 1987, Duarte 1985). From (15) we obtain

$$\frac{y_{n+1}}{y_n} = \left(\frac{n+1}{n}\right)^{-\left(\theta_{n+1} - \theta_n\right)}$$
(16)

where $y_n = a_{n,c+1}/a_{nc}$.

So, $-\Delta\theta(n) = -(\theta_{c+1} - \theta_c) = \log(y_{n+1}/y_n)/\log[(n+1)/n]$. In figure 2, $-\Delta\theta(n)$ has been plotted against 1/n for c = 0. As expected, the plot is a straight line for all three types of animals: undirected, directed and spiral. For undirected and directed animals the difference $\theta_1 - \theta_0$ tends to 1 whereas for the spiral animals the difference tends towards 1.62 with an error bar of ± 0.05 . Similar conclusion can be drawn from plots of $-\Delta\theta(n)$ against 1/n for c = 1, 2, ... The above result is in support of the conjecture put forward in (10). The radius of gyration data have been analysed using a sequential fit to the form

$$\log R_{nc} = \nu_c \log(n+\delta) + B \tag{17}$$

the parameter δ being chosen in the range of values which gives a satisfactory convergence of the successive estimates of ν_c . The values of ν_c obtained are

$$\nu = 0.50 \pm 0.02 \qquad \nu_0 = 0.67 \pm 0.02 \nu_1 = 0.66 \pm 0.02 \qquad \nu_2 = 0.67 \pm 0.02.$$
(18)

Within the limits of error it appears that the radius of gyration exponent ν_c is independent of the number of loops c. The radius of gyration exponent ν for spiral animals is, however, different and the value 0.5 indicates that spiral animals are compact in structure.

To sum up, for spiral lattice site animals embedded in the square lattice, we have conjectured the relation $\theta_c = \theta_0 - \alpha c$ for the animal number exponents for animals with c loops. The numerical constant α has a value around 1.62 ± 0.05 . This result is different from that for undirected and directed lattice animals for which $\alpha = 1$. The growth parameter λ_c and radius of gyration exponent ν_c have values independent of loop number c. The values of λ_c , ν_c are $\lambda_c = \lambda_0$ and $\nu_c = \nu_0$ where λ_0 , ν_0 are the corresponding values for trees. This result is similar to what one finds in the cases of undirected and directed lattice animals.

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