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Directed site lattice animals with restricted valence

Y Liu†, Z Q Zhang† and Z R Yang‡

† Institute of Physics, Chinese Academy of Sciences, Beijing, China
‡ Department of Physics, Beijing Normal University, Beijing, China

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Abstract. The critical behaviour of directed site lattice animals having valence no larger than v is studied in the square lattice for the cases of $v = 2$ and 3 by using exact enumerations. We also study the cases where the microscopic restrictions are anisotropic so that the universality hypothesis can be tested for the systems possessing a non-trivial preferred axis. As expected, for both the isotropic and anisotropic restrictions, series analysis together with some exact results show that when $v = 3$ the systems have the same critical behaviour as the unrestricted case while for $v = 2$ the systems belong to the same universality class as directed self-avoiding walks.

1. Introduction

The new lattice animals models with restricted valence have been studied recently by Gaunt *et al* (1979, 1980) and Whittington *et al* (1979). Taking into account the effects of steric hindrance, those authors considered (in the case of site animals) that each animal vertex has valence no larger than a fixed value v. The value of v can vary from 2 to z where z is the coordination number of the lattice. For all the lattices they studied, both in two and three dimensions, they found that when $v \geq 3$ the exponent θ for the generating function is the same as the unrestricted case ($v = z$), while when $v = 2$ a different exponent was found which is believed to be in the same universality class as the neighbour-avoiding walks (Fisher and Hiley 1961).

In recent years, the critical behaviour of systems with a preferred axis has been the focus of many studies. It is well known that the introduction of a preferred axis leads to two independent correlation lengths, one parallel and the other perpendicular to the preferred axis ($\xi_{\parallel}$ and $\xi_{\perp}$), which diverge at the critical point with different exponents $\nu_{\parallel}$ and $\nu_{\perp}$.

The purpose of this work is to consider the restricted valence effects in the direct site lattice animals models. Specifically, we study the cases of $v = 2$ and 3 in a square lattice. Both the microscopically isotropic and anisotropic restrictions to the valence are considered. The reason that we study the anisotropic restrictions is to introduce a non-trivial preferred axis to the system. The explicit studies of the critical behaviour of such a system will enable us to test the universality hypothesis that the critical behaviour is independent of the direction of the preferred axis. Here, we study not only the exponent θ of the generating function but also the correlation length exponents $\nu_{\parallel}$ and $\nu_{\perp}$. Generally, we use the method of exact enumerations together with the standard Padé and ratio analysis to obtain various critical exponents. In one particular case ($v = 2$ with anisotropic restrictions) exact results can be obtained.

2. Directed site animals in a square lattice with restricted valence $v = 3$

First we study the critical behaviour of the fully directed site animals in a square lattice with maximum valence $v = 3$. At each animal vertex we can define v_h and v_s as the number of valences in the horizontal and vertical directions respectively. In the case of $v = 3$, the microscopic configurations at each animal vertex must satisfy the relation $v_h + v_s \leq v = 3$. Here we consider both the microscopically isotropic and anisotropic restrictions. For the isotropic restrictions, the allowed configurations of (v_h, v_s) are $(0, 1)$, $(1, 0)$, $(1, 1)$, $(0, 2)$, $(2, 0)$, $(1, 2)$ and $(2, 1)$. In this case the preferred axis is still the symmetry axis (45° relative to the horizontal axis). For the anisotropic restrictions, the allowed configurations of v_h and v_s are $(0, 1)$, $(1, 0)$, $(1, 1)$, $(0, 2)$, $(2, 0)$ and $(1, 2)$ where the configuration $(2, 1)$ is not allowed. In this case the preferred axis of the system will be some non-trivial direction and it is interesting to see if the critical behaviour still remains unchanged.

The number of directed site animals of size N, W_N, is enumerated by computer. For each N we also calculate the averaged mean-square radii $R_\parallel^2(N)$ and $R_\perp^2(N)$. $R_\parallel^2(N)$ and $R_\perp^2(N)$ are defined by

$$R_\parallel^2(N) = \sum_{i,\boldsymbol{r}(i)} W_N(\boldsymbol{r}(i)) r_\parallel^2(i) \Big/ N \sum_{\boldsymbol{r}(i)} W_N(\boldsymbol{r}(i)), \tag{1}$$

$$R_\perp^2(N) = \sum_{i,\boldsymbol{r}(i)} W_N(\boldsymbol{r}(i)) r_\perp^2(i) \Big/ N \sum_{\boldsymbol{r}(i)} W_N(\boldsymbol{r}(i)), \tag{2}$$

where $W_N(\boldsymbol{r}(i))$ is the number of directed site animals of size N with the ith site at position $\boldsymbol{r}(i)$ from the origin $\mathbf{0}$ (Family 1980). Obviously, we have $\sum_{\boldsymbol{r}(i)} W_N(\boldsymbol{r}(i)) = W_N$. $r_\parallel(i)$ and $r_\perp(i)$ are respectively the parallel and perpendicular projections of $\boldsymbol{r}(i)$ to the preferred axis. For the anisotropic restrictions, the preferred axis of the system is not known. So, for each N, we define the N-dependent preferred axis as the direction from the origin $\mathbf{0}$ to the averaged centre of mass $(X(N), Y(N))$. Thus, for each N, we also have to calculate $(X(N), Y(N))$ using formulae (1) and (2) with $x(i)$ and $y(i)$ replacing $r_\parallel^2(i)$ and $r_\perp^2(i)$. It is expected that the preferred axis of the system is the infinite N limit of the N-dependent preferred axis.

The values of W_N, $R_\parallel(N)$ and $R_\perp(N)$ are given in tables 1 and 2 respectively for the cases of isotropic and anisotropic restrictions. It is easy to prove that the super-multiplicative property (Klarner 1967, Gaunt *et al* 1979) for both cases is satisfied. Hence we expect that, for large N, W_N will behave like

$$W_N \sim N^{-\theta} \lambda^N. \tag{3}$$

For the directed systems, when N is large, we also expect that $R_\parallel^2(N)$ and $R_\perp^2(N)$ will diverge with two different exponents,

$$R_\parallel^2(N) \sim N^{2\nu_\parallel} \qquad \text{and} \qquad R_\perp^2(N) \sim N^{2\nu_\perp}. \tag{4}$$

Let K be the fugacity of each animal. The generating function G and the correlation lengths $\xi_\parallel$ and $\xi_\perp$ can be defined as

$$G(K) = 1 + \sum_{N=1}^{\infty} W_N K^N, \tag{5}$$

$$\xi_\parallel^2(K) = \sum_{N=1}^{\infty} R_\parallel^2(N) W_N K^N / G(K), \tag{6}$$

Table 1. The values of W_N, $R_{\|}(N)$ and $R_{\perp}(N)$ for the case of $v=3$ with isotropic restrictions.

N	W_N	$R_{\|}(N)$	$R_{\perp}(N)$
1	1	0.0000	0.0000
2	2	0.5000	0.5000
3	5	0.8563	0.6831
4	13	1.1929	0.8321
5	35	1.5119	0.9562
6	95	1.8233	1.0703
7	260	2.1284	1.1751
8	716	2.4281	1.2726
9	1986	2.7215	1.3632
10	5542	3.0091	1.4482
11	15 543	3.2914	1.5284
12	43 766	3.5691	1.6046
13	123 646	3.8425	1.6774
14	350 308	4.1123	1.7472
15	994 919	4.3785	1.8143
16	2831 808	4.6416	1.8791
17	8075 507	4.9016	1.9417

Table 2. The values of W_N, $R_{\|}(N)$ and $R_{\perp}(N)$ for the case of $v=3$ with anisotropic restrictions.

N	W_N	$R_{\|}(N)$	$R_{\perp}(N)$
1	1	0.0000	0.0000
2	2	0.5000	0.5000
3	5	0.8563	0.6831
4	12	1.2046	0.8335
5	28	1.5584	0.9673
6	66	1.9080	1.0853
7	158	2.2473	1.1901
8	381	2.5793	1.2860
9	922	2.9063	1.3754
10	2239	3.2288	1.4593
11	5459	3.5461	1.5383
12	13 354	3.8588	1.6132
13	32 759	4.1670	1.6846
14	80 555	4.4714	1.7530
15	198 516	4.7720	1.8186
16	490 152	5.0691	1.8818
17	1212 309	5.3629	1.9430
18	3003 054	5.6537	2.0021
19	7449 333	5.9417	2.0595

$$\xi_{\perp}^2(K)=\sum_{N=1}^{\infty} R_{\perp}^2(N)\,W_N K^N/G(K). \tag{7}$$

Near the critical fugacity $K_c=1/\lambda$, we expect that the above functions will behave like

$$G(K)\sim|K_c-K|^{\theta-1}, \tag{8}$$

$$\xi_{\parallel}^2(K) \sim |K_c - K|^{-2\nu_{\parallel}}, \tag{9}$$

$$\xi_{\perp}^2(K) \sim |K_c - K|^{-2\nu_{\perp}}. \tag{10}$$

It is known that in the directed site lattice animals the correction to scaling exponent Ω_p is equal to 1 (Dhar 1982, 1983, Margolina *et al* 1983). According to the universality concept, we would also expect that this will be the case in the restricted model considered here. Thus we will use the standard Padé and ratio analysis (Gaunt and Guttmann 1974) to extract the values of θ, $\nu_{\parallel}$ and $\nu_{\perp}$ from tables 1 and 2. Since the generating function is only weakly singular, we actually perform the Dlog Padé approximants to the first or second derivative of the generating function. These derivatives are also used in forming the Dlog Padé approximants of $\xi_{\parallel}^2(K)$ and $\xi_{\perp}^2(K)$. For the isotropic restrictions (the first derivative is used) the pole–residue plot of (5) is shown in figure 1. The pole–residue plots of (6) and (7) behave similarly. From

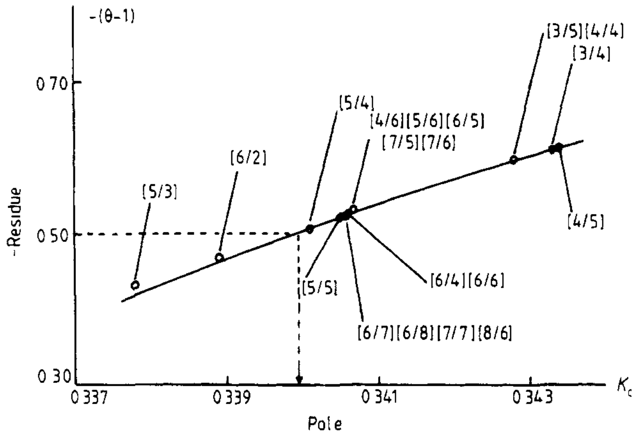

Figure 1. Pole–residue plot for $v = 3$ with isotropic restrictions. The generating function is $G(K)$ where the first derivative is used in the actual calculations.

the universality concept, it is reasonable to assume that θ has the same value 0.5 (Dhar 1982, 1983) as in the unrestricted case. Using this assumption, we can obtain the biased estimate of K_c from figure 1 from which the biased estimates of $\nu_{\parallel}$ and $\nu_{\perp}$ can be obtained. If the assumption is correct, the values of $\nu_{\parallel}$ and $\nu_{\perp}$ so obtained should also agree with the known values of the unrestricted case. We find that the biased estimates of K_c, $\nu_{\parallel}$ and $\nu_{\perp}$ are $K_c = 0.3400 \pm 0.0005$ ($\lambda = 2.941 \pm 0.004$), $\nu_{\parallel} = 0.821 \pm 0.025$ and $\nu_{\perp} = 0.494 \pm 0.025$. A similar procedure is used for the case of anisotropic restrictions where the second derivative of the generating function is used. By assuming $\theta = 0.5$, the biased estimates of K_c, $\nu_{\parallel}$ and $\nu_{\perp}$ are $K_c = 0.3929 \pm 0.0003$ ($\lambda = 2.5451 \pm 0.0021$), $\nu_{\parallel} = 0.832 \pm 0.035$ and $\nu_{\perp} = 0.483 \pm 0.025$. For both cases, the exponents $\nu_{\parallel}$ and $\nu_{\perp}$ found here are in good agreement with the known values of the unrestricted case; $\nu_{\parallel} = 0.8185$ and $\nu_{\perp} = 0.5$ (Nadal *et al* 1982). For the ratio analysis, we use the same method as used by Redner and Yang (1982). We first form the sequence $\lambda_N = W_N/W_{N-1}$. The values of λ and θ are estimated from the limiting values of the sequences $N\lambda_N - (N-1)\lambda_{N-1}$ and $\theta_N = N(1 - \lambda_N/\lambda)$ respectively. To estimate the values of $\nu_{\parallel}$ and $\nu_{\perp}$, we first examine the dependence of $\nu_{\parallel}(N)$ and $\nu_{\perp}(N)$ against N

on a double logarithmic scale. The values of $\nu_\parallel(N)$ and $\nu_\perp(N)$ are calculated from the slope of successive data points. The limiting values of $\nu_\parallel$ and $\nu_\perp$ are extrapolated from $\nu_\parallel(N)$ and $\nu_\perp(N)$ sequences by means of Neville tables. For the case of isotropic restrictions, we find $\lambda = 2.941 \pm 0.005$, $\theta = 0.51 \pm 0.02$, $\nu_\parallel = 0.821 \pm 0.004$ and $\nu_\perp = 0.495 \pm 0.006$. For the case of anisotropic restrictions, we find $\lambda = 2.551 \pm 0.010$, $\theta = 0.53 \pm 0.04$, $\nu_\parallel = 0.821 \pm 0.018$ and $\nu_\perp = 0.486 \pm 0.010$. These results are consistent with the Padé analysis and both indicate that the models considered here (isotropic and anisotropic restrictions) being to the same universality class as the unrestricted lattice animals model. Again, it demonstrates that the direction of the preferred axis is irrelevant to the critical behaviour.

3. Directed site animals in a square lattice with restricted valence $v = 2$

In the case of $v = 2$ we again consider both the isotropic and anisotropic restrictions. For the isotropic restrictions, the allowed configurations of (v_h, v_s) are (0, 1), (1, 0), (1, 1), (0, 2) and (2, 0). The values of W_N, $R_\parallel(N)$ and $R_\perp(N)$ are given in table 3.

Table 3. The values of W_N, $R_\parallel(N)$ and $R_\perp(N)$ for the case of $v = 2$ with isotropic restrictions.

N	W_N	$R_\parallel(N)$	$R_\perp(N)$
1	1	0.0000	0.0000
2	2	0.5000	0.5000
3	5	0.8563	0.6831
4	11	1.2154	0.8394
5	21	1.6183	1.0095
6	44	1.9867	1.1315
7	92	2.3498	1.2386
8	191	2.7124	1.3367
9	393	3.0783	1.4299
10	810	3.4388	1.5152
11	1 662	3.8005	1.5965
12	3 410	4.1590	1.6729
13	6 974	4.5187	1.7463
14	14 262	4.8755	1.8161
15	29 098	5.2334	1.8836
16	59 359	5.5889	1.9482
17	120 873	5.9453	2.0110
18	246 098	6.2996	2.0714
19	500 342	6.6547	2.1303
20	1017 098	7.0080	2.1873
21	2065 158	7.3621	2.2430

Again, we form the Dlog Padé approximants of (5)–(7) where the second derivatives of the generating function are actually used. In this case, we would expect that the critical behaviour might belong to the class of directed self-avoiding walks (DSAWS) where the exact exponents are known; i.e. $\theta = 0$. $\nu_\parallel = 1$ and $\nu_\perp = 0.5$ (Redner and Majid 1983). Thus, by assuming $\theta = 0$, we obtain the biased estimates of K_c, $\nu_\parallel$ and $\nu_\perp$ from the pole–residue plots of (5)–(7). The results are $K_c = 0.4928 \pm 0.005$ ($\lambda = 2.029 \pm 0.002$), $\nu_\parallel = 0.990 \pm 0.02$ and $\nu_\perp = 0.495 \pm 0.025$. These results are consistent with the original assumption that the critical behaviour is in the universality class of DSAWs. However, in this case the Padé approximants show that there exist both defects and other non-physical singularities inside the circle of physical singularity. This makes the ratio analysis rather difficult. Thus we will not give the results of ratio analysis in this case.

For the case of anisotropic restrictions, the allowed configurations of (v_h, v_s) are $(0, 1)$, $(1, 0)$, $(1, 1)$ and $(0, 2)$. In this case, it is easy to show that for $N > 4$, $W_N = a_N + a_{N-3}$ where a_N is the number of DSAWs of N steps with the above anisotropic restrictions. Thus we only have to study the critical properties of DSAWs with anisotropic restrictions. This problem can be solved exactly as follows.

Let x and y be the fugacities of each directed step of the walk in the horizontal and vertical directions respectively. If we let $f(n, m)$ be the number of DSAWs of $(n+m)$ steps ended at site (n, m), the generating function $G(x, y)$ becomes

$$G(x, y) = \sum_{n,m}^{\infty} f(n, m) x^n y^m. \tag{11}$$

Now we define $\langle A(n, m)\rangle$ as the average of any (n, m)-dependent function $A(n, m)$ with

$$\langle A(n, m)\rangle = \sum_{n,m}^{\infty} A(n, m) f(n, m) x^n y^m \Big/ \sum_{n,m}^{\infty} f(n, m) x^n y^m. \tag{12}$$

The correlation lengths $\xi_\parallel$ and $\xi_\perp$ in this case become

$$\xi_\parallel^2(x, y) = \langle R_\parallel^2(n, m)\rangle \qquad \text{and} \qquad \xi_\perp^2(x, y) = \langle R_\perp^2(n, m)\rangle \tag{13}$$

where $R_\parallel(n, m)$ and $R_\perp(n, m)$ are respectively the horizontal and vertical projections of the end vector (n, m) on the preferred axis. The preferred axis is determined by the position of the averaged centre of mass which has the coordinates $(\langle n\rangle, \langle m\rangle)$. Thus the preferred axis has an angle $\varphi = \tan^{-1}(\langle m\rangle/\langle n\rangle)$ relative to the horizontal axis. Let the angle between the end vector (n, m) and the horizontal axis be $\alpha(n, m)$; then we have

$$\alpha(n, m) = \tan^{-1}(m/n), \tag{14}$$

$$R_\parallel^2(n, m) = (n^2 + m^2)\cos^2(\varphi - \alpha), \tag{15}$$

$$R_\perp^2(n, m) = (n^2 + m^2)\sin^2(\varphi - \alpha). \tag{16}$$

Substituting (14)–(16) into (12), after some manipulations, we find

$$\xi_\parallel^2(x, y) = (1 + \tan^2\varphi)^{-1}(\langle n^2\rangle + \langle m^2\rangle \tan^2\varphi + 2\langle nm\rangle \tan\varphi), \tag{17}$$

$$\xi_\perp^2(x, y) = (1 + \tan^2\varphi)^{-1}(\langle n^2\rangle \tan^2\varphi + \langle m^2\rangle - 2\langle nm\rangle \tan\varphi). \tag{18}$$

The generating function of (11) can be evaluated exactly by using the transfer-matrix method of Redner and Majid (1983). In our case the transfer matrix T is given by $\begin{pmatrix} 0 & x \\ y & y \end{pmatrix}$. Thus we have

$$G(x, y) = (1 \;\; 1)(1 - T)^{-1}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1 + x}{1 - y - xy}. \tag{19}$$

Using the relation

$$G(x, y)\langle n^i m^j\rangle = (x\,\partial/\partial x)^i (y\,\partial/\partial y)^j G(x, y) \tag{20}$$

all the averages $\langle n\rangle$, $\langle m\rangle$, $\langle n^2\rangle$, $\langle m^2\rangle$ and $\langle nm\rangle$ can be evaluated using (19). After some straightforward manipulations, we obtain

$$\xi_{\|}^2(x,y)=\frac{x^3(1-y-xy)+y^3(1+x)^6(1+y+xy)+4y^2x^2(1+x)^3}{(1+x)[x^2+(1+x)^4y^2](1-y-xy)^2}, \tag{21}$$

$$\xi_{\perp}^2(x,y)=\frac{xy(1+x)(x+y-x^2y)}{[x^2+(1+x)^4y^2](1-y-xy)}, \tag{22}$$

$$\tan\varphi=(1+x)^2y/x. \tag{23}$$

We can see from (21) and (22) that the critical line is given by $1-y-xy=0$ and the correlation length exponents are $\nu_{\|}=1$ and $\nu_{\perp}=1/2$. For the special case of $x=y=K$, we have $K_c(\sqrt{5}-1)/2$. The number of DSAWS of N steps, a_N, can be evaluated through

$$a_N=\frac{1}{2\pi i}\oint\frac{G(x,x)}{X^{N+1}}\,dx=\frac{1}{\sqrt{5}}\left[\left(\frac{1}{K_c}\right)^{N+2}+(-1)^{N+1}K_c^{N+2}\right]. \tag{24}$$

From (24), we obtain $\lambda=1/K_c$ and $\theta=0$. Thus we have shown rigorously that in the anisotropic case, the $v=2$ model has exactly the same critical behaviour as the DSAWS. We would like to point out that (24) yields the Fibonnaci sequences (Korn and Korn 1968) $(1,2,3,5,8,13,\ldots)$ for a_N $(N=0,1,2,3,\ldots)$. In fact, it is not difficult to show that a_N satisfies the recursion relation $a_{N+1}=a_N+a_{N-1}$, for $N=0,1,2,\ldots$ with $a_{-1}=1$. The relations $W_N=a_N+a_{N-3}$ for $N>4$ yield the Fibonnaci sequences $(16, 26, 42, 68,\ldots)$ for W_N $(N=5,6,7,\ldots)$.

4. Conclusions

We have studied the restricted valence effects on the critical behaviour of directed site lattice animals. Both microscopically isotropic and anisotropic restrictions are considered. In the case of $v=3$, exact enumerations together with Padé and ratio analysis indicate that the critical behaviour remains the same as the unrestricted case. In the case of $v=2$, both series analysis for the isotropic restrictions and exact analysis for the anisotropic restrictions show that they belong to the universality class of DSAWS. These results also show that the direction of the preferred axis is irrelevant to the critical behaviour. All these results are in full agreement with our expectations.

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