IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Exact series studies of self-avoiding walks on two-dimensional critical percolation clusters

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1990 J. Phys. A: Math. Gen. 23 L831

(http://iopscience.iop.org/0305-4470/23/16/010)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 129.252.86.83
The article was downloaded on 01/06/2010 at 08:42

Please note that terms and conditions apply.

J. Phys. A: Math. Gen. **23** (1990) L831-L836. Printed in the UK

LETTER TO THE EDITOR

Exact series studies of self-avoiding walks on two-dimensional critical percolation clusters

P M Lam†

Fachbereich Physik, Universität Essen, 4300 Essen 1, Federal Republic of Germany

Received 21 June 1990

Abstract. We present results of exact series studies of self-avoiding walks on percolation clusters on the square lattice performed very close to the percolation threshold and estimate the critical exponents ν and γ defined by the disorder averages of the mean square radius of gyration or the end-to-end distance and the number of self-avoiding walks, respectively. The self-avoiding walk configurations are enumerated exactly up to 35 steps. The result for ν indicates a large increase compared with the self-avoiding walks on fully occupied lattice. The result for γ, however, indicates a behaviour similar to that on a fully occupied lattice. The result for ν is completely different from that of Lee, Nakanishi and Kim.

In this letter we treat the problem of self-avoiding random walks (SAWs) confined to clusters of the percolation problem in two dimensions. This problem is a direct analogue of the problem of linear-chain polymers trapped in a porous medium where excluded regions can occur with the length scales of the order of the persistence length of the chain.

According to the Harris criteria [1], since the specific heat exponent α is positive, the critical behaviour of SAWs on a randomly diluted lattice would be expected to be different from that of an ordinary SAW for any amount of disorder. On the other hand, Harris [2] himself argued that the disorder average is very trivial and all critical exponents remain unchanged for any $p > p_c$, where p represents the concentration of non-impurity sites and p_c is the percolation threshold. Also, a modified analysis of his criteria [2] indicates that the critical behaviour of an SAW is not affected by lattice dilution even though α is positive. This was partially supported by field theoretic calculations [3].

Later Lyklema and Kremer [4] presented an argument that randomness is irrelevant except at the percolation threshold. This was supported by Monte Carlo results [5] and real-space renormalization studies [6-8]. Recently, however, Lee and Nakanishi [9] and Lee *et al* [10] pointed out an error in the data analysis of the Monte Carlo result of [5] and presented new Monte Carlo data of their own. They calculated the exponent ν_N, as a function of the number of steps N, for an SAW on the infinite percolation cluster at $p = p_c$. On the square lattice in two dimensions, with $p = 0.59273$, they found that up to the 25th step, ν_N was monotonically increasing and beyond that it seems to emerge to the full lattice result. A similar behaviour was also found for three dimensions.

† Present address: Physics Department, Emory University, Atlanta, GA 30322, USA.

0305-4470/90/160831+06$03.50 © 1990 IOP Publishing Ltd

This crossover behaviour of ν_N appears to us to be somewhat unusual since at $p = p_c$, the correlation length on the infinite cluster is infinite and the cluster structure is self-similar at all length scales. This crossover effect seems to indicate some sort of finite-size effect. Moreover we believe that the real-space renormalization group result [6-8] with the appearance of a new disorder fixed point right at $p = p_c$ should be qualitatively correct. The purpose of this paper is to check the calculations of [9] and [10] with an exact enumeration method. It turns out that since the number of SAW configurations on the infinite critical percolation clusters are much fewer than those on the fully occupied lattice, it is in fact possible to enumerate exactly all the self-avoiding walk configurations on the infinite cluster on the square lattice up to 35 steps. This is ten steps beyond the point where ν_N, in [9] and [10], starts to cross over into the fully occupied lattice value. Therefore this is sufficient to check their results and in our case we have here only a disorder average over the different infinite percolation clusters.

The infinite clusters are generated by the Leath [11] cluster growth method. The centre site of the square lattice is taken as an occupied site and all the other sites are empty. Each of the growth sites of this occupied site are the four neighbour sites. In the next step, each of these four growth sites becomes either occupied or blocked randomly with probability p or $(1-p)$ respective, where $p = 0.592\,73$. In each subsequent step, the cluster sites are the occupied sites and the growth sites are the perimeter sites of this cluster which are at the same time unblocked, i.e. empty. The growth sites are then changed randomly into occupied or blocked sites respectively with probability p or $(1-p)$. Thus at each step, the cluster can continue to grow in shells around the initial centre site, as long as the number of growth sites is finite. If at a certain step the number of growth sites becomes zero, the process has to restart again with one single occupied site at the centre of the lattice and all the other sites being empty. Only those clusters that are grown after more than 35 steps are kept. For each cluster, the SAWs always start from the centre site of the lattice, i.e. the first starting occupied site of the cluster. All SAW configurations on the generated cluster of occupied sites, starting from this centre site are enumerated using the backtracking method [12]. We have checked our results by setting $p = 1$. In that case we obtain the known averaged squared radius of gyration and end-to-end distance of the fully occupied lattice up to $N = 18$. Our results for the average values of the squared radius of gyration G_N^2, the end-to-end distance E_N^2 and the number of SAW configurations C_N are shown in table 1. In table 1 of [10], the values of the average radius of gyration and the end-to-end distance are given for the square lattice for $N = 20$ to be $3.45 \pm 0.04\%$ and $9.41 \pm 0.05\%$ respectively. These are quite different from our corresponding values 3.303 ± 0.027 and 8.942 ± 0.103 respectively obtained from our table 1.

Let R_N^2 denote either the average squared radius of gyration or the squared end-to-end distance of N-step SAWs. Then asymptotically for large N

$$R_N^2 = AN^{2\nu} \tag{1}$$

where A is a proportionality constant. Taking the logarithm on both sides of equation (1) and then integrating both sides of the resulting equation from M to N one obtains

$$\int_M^N \ln R_n^2 \, dn = (N-M)\ln A + 2\nu(N \ln N - N - M \ln M + M)$$

$$= NR_N^2 - MR_M^2 - 2\nu(N-M). \tag{2}$$

Table 1. The average values of the number of SAW configurations C_N, the squared radius of gyration G_N^2 and the squared end-to-end distance E_N^2 as functions of the number of steps N.

N	C_N	G_N^2	E_N^2
10	261 ± 13	3.854 ± 0.023	26.529 ± 0.259
11	408 ± 23	4.406 ± 0.030	30.538 ± 0.396
12	645 ± 43	4.994 ± 0.038	34.883 ± 0.427
13	998 ± 70	5.617 ± 0.056	39.530 ± 0.681
14	1562 ± 119	6.256 ± 0.078	44.342 ± 0.866
15	2415 ± 187	6.970 ± 0.096	49.746 ± 1.094
16	3760 ± 296	7.696 ± 0.126	55.257 ± 1.357
17	5838 ± 459	8.478 ± 0.136	61.290 ± 1.450
18	9088 ± 691	9.262 ± 0.164	67.292 ± 1.712
19	$(1421 \pm 110) \times 10$	10.010 ± 0.160	73.736 ± 1.618
20	$(2215 \pm 167) \times 10$	10.913 ± 0.178	79.954 ± 1.819
21	$(3480 \pm 274) \times 10$	11.787 ± 0.163	86.603 ± 1.600
22	$(5408 \pm 430) \times 10$	12.626 ± 0.175	92.998 ± 1.773
23	$(8491 \pm 706) \times 10$	13.541 ± 0.157	99.942 ± 1.547
24	$(1314 \pm 115) \times 10^2$	14.427 ± 0.162	106.696 ± 1.684
25	$(2057 \pm 185) \times 10^2$	15.400 ± 0.147	114.190 ± 1.612
26	$(3182 \pm 308) \times 10^2$	16.358 ± 0.140	121.585 ± 1.670
27	$(4970 \pm 486) \times 10^2$	17.403 ± 0.129	129.859 ± 1.929
28	$(7722 \pm 825) \times 10^2$	18.438 ± 0.110	138.038 ± 1.917
29	$(1210 \pm 129) \times 10^3$	19.546 ± 0.125	147.028 ± 2.541
30	$(1891 \pm 223) \times 10^3$	20.646 ± 0.106	155.937 ± 2.429
31	$(2979 \pm 348) \times 10^3$	21.789 ± 0.166	165.288 ± 3.233
32	$(3996 \pm 488) \times 10^3$	23.099 ± 0.223	171.585 ± 3.555
33	$(6297 \pm 843) \times 10^3$	24.262 ± 0.275	180.405 ± 4.286
34	$(9793 \bullet 1455) \times 10^4$	25.617 ± 0.342	191.680 ± 4.574
35	$(1550 \pm 253) \times 10^4$	26.749 ± 0.391	200.020 ± 5.346

Defining the integral on the left-hand side of equation (2) as

$$I(M, N) \equiv \int_M^N \ln R_n^2 \, dn \tag{3}$$

one obtains an N-dependent exponent ν_N as

$$\nu_N = [N \ln R_N^2 - M \ln R_M^2 - I(M, N)]/[2(N-M)]. \tag{4}$$

The integral $I(M, N)$ is calculated using the Simpson rule. The lower limit M is chosen to be either 1 or 2 such that $(N-M)$ is an even integer larger than or equal to four as required for the Simpson rule quadrature. The resulting ν_N obtained from using both the average squared radius of gyration and the squared end-to-end distance are shown in figure 1, plotted against $1/N$. These data are obtained averaging over 500 percolation clusters. The error bars are obtained by grouping the data into ten sets and calculating the standard deviations. Also shown in figure 1 are the results for ν_N for the case of the fully occupied lattice. These data are obtained using a Monte Carlo method called the incomplete enumeration method [13–18] up to 100 steps on the square lattice. The ν_N values obtained from both the averaged square radius of gyration and the end-to-end distance for the case of the fully occupied lattice approach asymptotically the exact value $\nu = 0.75$ in the limit $N \to \infty$ in a monotonic fashion. For the case of a SAW on the infinite percolation cluster, the ν_N values obtained from

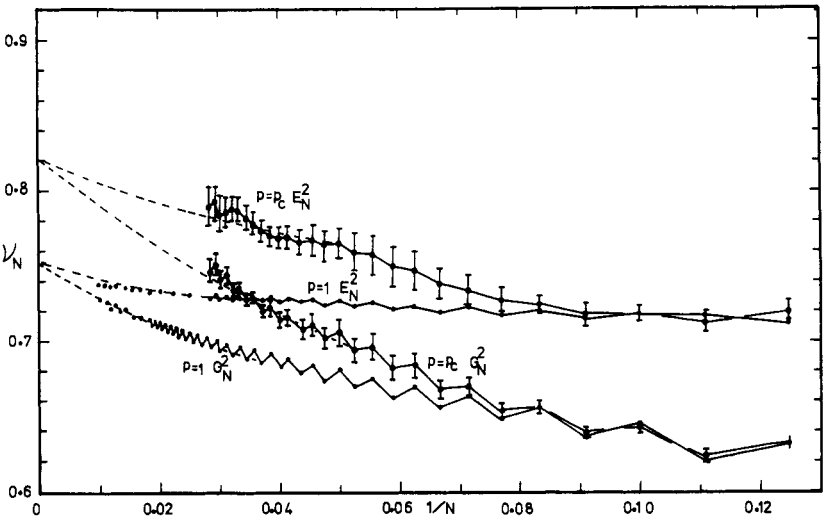

Figure 1. The exponent ν_N plotted against $1/N$ for the fully occupied lattice ($p = 1$) and the infinite percolation cluster ($p = p_c$), obtained using average squared radius of gyration (G_N^2) and average squared end-to-end distance (E_N^2).

both the average squared radius of gyration and the squared end-to-end distance increase monotonically with $1/N$ up to $N = 35$ and seem to approach asymptotically the value $\nu \equiv \nu_\infty = 0.81 \pm 0.03$. In both cases of G_N and E_N the values ν_N are always above the corresponding full lattice values for all N above 10. Up to $N = 35$ there is no crossover effect in the ν_N values. From our result we have to conclude that the crossover observed in [9] and [10] must be spurious.

The average number of walks of N steps C_N is given asymptotically by

$$C_N = BN^{\gamma-1}\mu^N \tag{5}$$

with B a proportionality constant, γ a universal exponent and μ a lattice dependent constant. Let Q_N be defined as

$$Q_N \equiv \ln(C_N/C_{N-1}). \tag{6}$$

Then integrating equation (6) from M to N and using equation (5) we can determine the N-dependent exponent γ_N and the lattice dependent constant μ_N

$$\gamma_N = 1 + \frac{J(M, N) - NQ_N + MQ_M}{\ln(N-1) - \ln(M-1)} \tag{7}$$

$$\ln \mu_N = \{J(M, N) - (Q_N - Q_M)f(M, N)\}/(N - M) \tag{8}$$

where

$$J(M, N) \equiv \int_M^N Q_n \, \mathrm{d}n \tag{9}$$

and

$$f(M, N) \equiv \frac{N \ln N - (N-1)\ln(N-1) - M \ln M + (M-1)\ln(M-1)}{\ln N - \ln(N-1) - \ln M + \ln(M-1)}.$$

Just as for the calculation of the exponent ν_N, we choose M here to be either 2 or 3 such that $(N-M)$ is an even integer and the integral $J(M, N)$ is evaluated using the Simpson rule. The resulting values of γ_N and μ_N are shown in figure 2 for both the full ($p=1$) and the diluted ($p=p_c$) lattices, plotted against $1/N$. We find in the full lattice case $\gamma \equiv \gamma_\infty = 1.30 \pm 0.05$ and $\mu \equiv \mu_\infty = 2.67 \pm 0.03$. For the diluted lattice, we have $\gamma = 1.30 \pm 0.1$ and $\mu = 1.53 \pm 0.05$. Since μ corresponds to an effective coordination number for the SAWs, it is the small value of μ in the disorder case that enables us to enumerate the SAW configurations up to large number of steps $N = 35$.

We can conceive of two sources that can cause the discrepancy between our result for ν and that of [9] and [10]. One is of course that we have enumerated our SAW configurations exactly while in [9] and [10] they have a disorder average over the percolation clusters and another configurational average over the Monte Carlo generated SAW configurations. A second source of discrepancy is the following. In [9] and [10], the critical percolation cluster is first generated on a fixed cell of size $L \times L$, where L is the linear size of the cell. The SAWs are started on randomly chosen sites on this cluster and periodic boundary conditions are imposed on the $L \times L$ cell in both directions for the case that the SAWs get outside of the original cell. The validity of such a procedure is not clear.

We have purposely used a relatively small number of SAW steps $N = 35$, and low spatial dimensions $d = 2$, but exact enumeration for the SAW configurations to make a clear comparison with [9] and [10]. Our results clearly show that the crossover effect of the correlation length exponent ν into the fully occupied lattice value found in those references is spurious. The exponent ν for an SAW on the infinite percolation cluster is in fact different and larger than that on the fully occupied lattice. We find in two dimensions, $\nu = 0.81 \pm 0.03$, compared with the exact value $\nu = 0.75$ on the full lattice. We believe that our results presented here are the only clear numerical evidence so far on the controversial problem of SAWs on disorder media. To get a better estimate

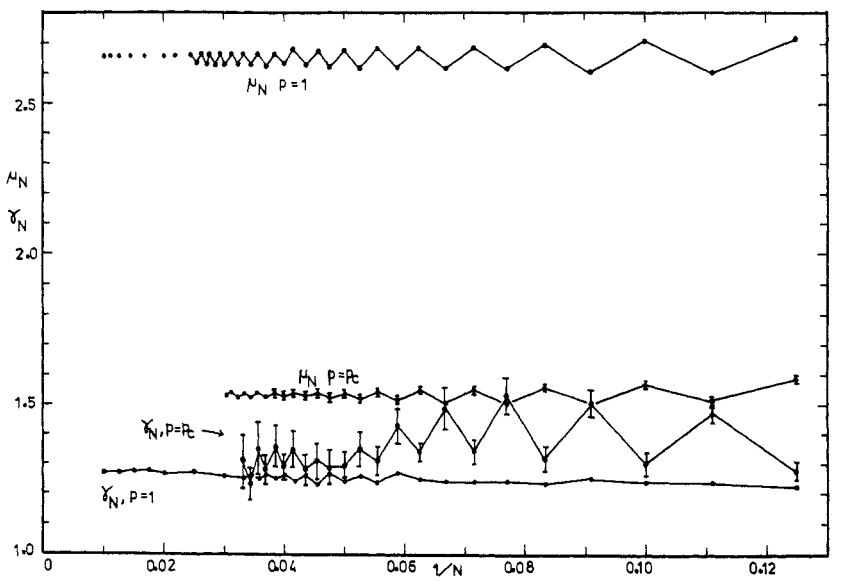

Figure 2. The exponent γ_N and the lattice dependent constant μ_N plotted against $1/N$ for the fully occupied lattice ($p_0 = 1$) and the infinite percolation cluster ($p = p_c$).

of the exponent ν one has to use SAWs of larger step numbers, i.e. by Monte Carlo methods. Also one has to calculate this exponent in three dimensions. The incomplete enumeration method [13-18] is most suited for this purpose. Work in this direction is in progress and will be reported elsewhere.

Finally we want to point out that, very recently, Meir and Harris [19] also confirmed that SAWs on diluted lattices belong to a different universality class than on a pure lattice, using a cumulant real-space renormalization group and ε-expansion.

This work has been supported by the Sonderforschungsbereich 237 *Unordnung and große Fluktuationen* of the Deutsche Forschungsgemeinschaft.

References

[1] Harris A B 1974 *J. Phys. C: Solid State Phys.* 7 1671
[2] Harris A B 1982 *Z. Phys.* B **49** 348
[3] Kim Y. 1987 *J. Phys. C: Solid State Phys.* **20** 1293
[4] Lyklema J W and Kremer K 1984 *Z. Phys.* B **55** 41
[5] Kremer K. 1981 *Z. Phys.* B **45** 149
[6] Roy A K and Chakrabarti B K 1982 *Phys. Lett.* **91A** 393
[7] Sahimi M 1984 *J. Phys. A: Math. Gen.* **17** L379
[8] Lam P M and Zhang Z Q 1984 *Z. Phys.* B **56** 155
[9] Lee S B and Nakanishi H 1988 *Phys. Rev. Lett.* **61** 2022
[10] Lee S B, Nakanishi H and Kim Y 1989 *Phys. Rev.* B **39** 9561
[11] Leath P L 1976 *Phys. Rev. Lett.* **36** 921; 1976 *Phys. Rev.* B **14** 5046
[12] Redner S 1982 *J. Stat. Phys.* **29** 309
[13] Yang Y S and Lam P M 1985 *Commun. Theor. Phys., China* **4** 497
[14] Dhar D and Lam P M 1986 *J. Phys. A: Math. Gen.* **19** L1057
[15] Lam P M 1986 *Phys. Rev.* A **34** 2399
[16] Lam P M 1987 *Phys. Rev.* A **35** 349
[17] Lam P M and Hansen A 1988 *J. Stat. Phys.* **52** 447
[18] Lam P M unpublished
[19] Meir Y and Harris A B 1989 *Phys. Rev. Lett.* **25** 2819