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True self-avoiding walks on a percolation cluster

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Abstract. We investigate by Monte Carlo simulations the critical behaviour of true self-avoiding walks (TSAWs) on a percolation cluster performed very close to the percolation threshold. Specifically we generate TSAWs on a site-percolated incipient 'infinite cluster', for various values of the self-avoidance parameter $g > 0$. We found that such walks exhibit critical behaviour different from that of ordinary-self-avoiding walks and also from that of random walks of no constraint. The Flory exponent obtained was $\nu = 0.432 \pm 0.005$ for all $g > 0$, which agrees well with the Flory-type formula suggested by Rammal.

Recently Amit *et al* (1983) presented a certain type of random walk as the problem of a walk which steps randomly but tries to avoid the previously visited sites. They called this a true self-avoiding walk (TSAW). This model was motivated from the theoretical interest because of its unusual critical properties, and the physical realisation of it was subsequently described in the statistics of linear polymers in an extremely polydispersed solution with a broad distribution of chain sizes (Family and Daoud 1984).

The TSAW is a kinetic process in which the probability $p_{j\to i}$ of moving from site j to its nearest-neighbour site i depends on the number of previous visits n_i on the site i by

$$p_{j\to i} = \exp(-gn_i)\left(\sum_k \exp(-gn_k)\right)^{-1} \tag{1}$$

where the sum in the normalisation factor runs over all nearest-neighbour sites of j and the parameter g defines the strength of self-avoidance; the extreme limit of $g = 0$ corresponds to ordinary random walks (RWs). For any $g > 0$, the excluded-volume effect of TSAWs is known to be different from the standard self-avoiding walks (SAWs) even for the case of $g = \infty$. Amit *et al* (1983) have shown by renormalisation calculation that the upper marginal dimension of TSAWs is two instead of four. Thus for lattice dimensionality above two, this model exhibits the critical behaviour similar to the classical RW and below two dimensions it is expected to be different from the RW. The Flory-type formula for TSAWs which characterises the mean-square end-to-end distance (and equivalently radius of gyration) was obtained by a self-consistent approach (Pietronero 1983) and Flory approximation (Family and Daoud 1984) as

$$\nu = 2/(d+2) \tag{2}$$

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where d is the underlying lattice dimensionality. In one dimension, Monte Carlo data indeed show the Flory exponent to be about $\frac{2}{3}$, regardless of the value of $g > 0$ (Rammal *et al* 1984, Bernasconi and Pietronero 1984). For lattice dimensionality between one and two, if exists at all, one can expect that the Flory exponent of TSAWs is greater than the mean field value of $\frac{1}{2}$ but less than the one-dimensional value of $\frac{2}{3}$. Possible candidates of such lattices are the two-dimensional geometrical fractals and the critical percolation clusters.

Various types of random walks have already been studied on various geometrical fractals: the ordinary RW on a Sierpinski gasket exhibits the Flory exponent ν smaller than the normal lattice value of $\frac{1}{2}$ (Havlin 1987 and references therein), while for SAWs ν was found to be greater than the normal lattice value of $\frac{3}{4}$ (Kim and Kahng 1985, Elezovic *et al* 1987). For TSAWs, Angles d'Auriac and Rammal (1984) have redrawn a heuristic argument of Amit *et al* (1983) on a fractal substrate and shown that the self-avoidance may increase the Flory exponent if

$$2 - \tilde{d}/2 - 2\nu_{RW} > 0 \tag{3}$$

where $\nu_{RW} = \bar{d}/2\bar{d}$, and $\tilde{d}$ and $\bar{d}$ are, respectively, spectral and fractal dimensions (Alexander and Orbach 1982, Rammal and Toulouse 1983) of underlying lattices. For a family of Sierpinski gasket, $\bar{d} = \ln(d+1)/\ln 2$ and $\tilde{d} = 2\ln(d+1)/\ln(d+3)$, and thus the condition is satisfied for all d. For an infinite percolation cluster at percolation threshold, if the conjectured value of $\tilde{d} = \frac{4}{3}$ (Alexander and Orbach 1982) is used, then the condition is also satisfied for all $d > 1$. Therefore for both cases, the asymptotic behaviour of TSAWs is expected to be different from that of RWs. Angles d'Auriac and Rammal have also carried out Monte Carlo simulations of TSAWs on a Sierpinski gasket and obtained $\nu = 0.51 \pm 0.02$. This value of ν is slightly greater than both the mean-field value and the RW value on the same lattice but is smaller than (2) would suggest if one merely replaces d by the fractal dimension of the Sierpinski gasket, $\bar{d} = \ln 3/\ln 2$. Interestingly, however, it agrees well with the Flory-type formula for TSAWs on a fractal suggested by Rammal (1984),

$$\nu = \frac{\tilde{d}}{\bar{d}} \frac{2}{\tilde{d}+2}. \tag{4}$$

The next question one might ask is what the value ν would be for TSAWs on a two-dimensional infinite percolation cluster near percolation threshold, which serves as a random fractal substrate with fractal dimension $\bar{d} \simeq 1.896$ (Stauffer 1985). For ordinary RWs the Flory exponent ν was found to be smaller than the normal lattice value (Majid *et al* 1984, Havlin and Ben Abraham 1983), and for SAWs it is still controversial, but seems to be not smaller than the normal lattice value (Kremer 1981, Lee and Nakanishi 1988, Meir and Harris 1989).

Lam (1984) has studied the TSAW on an infinite percolation cluster by cell renormalisation study and estimated the Flory exponent, using the finite-size scaling, as $\nu \simeq 0.58$. This value of ν is greater than that of RWs but smaller than that of TSAWs obtained by the same method on the fully occupied lattice (Nakanishi and Family 1984). In general, however, critical indices obtained by a small-cell renormalisation cannot be trustworthy even when finite-size scaling is employed for several small cell sizes. This can be seen from the result on the fully occupied lattice; whereas the known value of ν is $\frac{1}{2}$, estimated in this way it is about 0.67. Lam also claimed that the statistics of the TSAW is much more easily reflected on a percolation cluster than on a full lattice. This is

because on a percolation cluster the TSAW can easily exhibit its characteristic features of making loops and self-intersections (because of many dead ends) even for a small number of steps, compared to that on a full lattice. Considering these situations, one may conclude that a small-cell renormalisation study cannot clarify whether ν on a percolation cluster is greater or smaller than the full lattice value. Therefore, it is interesting to study the critical behaviour of TSAWs on a percolation cluster by extensive Monte Carlo simulations.

In this paper we study by Monte Carlo simulation TSAWs on an infinite percolation cluster for a square lattice at percolation probability very close to the percolation threshold p_c. We restrict our works to two dimensions because $\bar{d} < d_c$ for two-dimensional percolation clusters. We specifically consider the end-to-end distance and radius of gyration for several selected values of the excluded-volume parameter g. Details of our method are very similar to those of SAWs on a percolation cluster described by Lee *et al* (1989). We generate the site-percolated incipient infinite clusters of linear size $L = 400$ defined as clusters which span the cell along all coordinate directions, and after identifying such clusters, any two opposite edges are connected by periodic boundaries for the purpose of performing TSAWs on them. The starting points of the walks were selected randomly and, for each starting point, a certain predetermined number of walks were generated for walk averages for a given starting point. The disorder average was also carried out for many different starting points and over many different disorder configurations. We have generated 200 walks for each direction of nearest-neighbour undiluted sites from the starting point and 200 starting points were selected for each cluster. Our walks are of 400–800 steps. For this value, we found that walks can never return to the starting point after going out of the cell through one edge and coming into the cell from the opposite edge, thus wrapping around the cell by periodic boundary conditions. This guarantees that TSAWs are fully confined in a fractal region even when we employ the periodic boundaries.

The mean-square end-to-end distance $\langle R_N^2 \rangle$ of the TSAW at upper marginal dimension d_c was found by renormalisation calculations (Amit *et al* 1983) to have the form of

$$\langle R_N^2 \rangle = AN^{2\nu} (\ln N)^{\alpha} \left(1 + B \frac{\ln(\ln N)}{\ln N} + \dots \right) \tag{5}$$

with $\nu = \frac{1}{2}$. For lattice dimensionality below d_c, one can expect that $\langle R_N^2 \rangle$ has the form of

$$\langle R_N^2 \rangle \propto A' N^{2\nu} \tag{6}$$

with Flory exponent $\nu > \frac{1}{2}$. In any of these cases, it would be very difficult to find the critical exponent ν accurately, because of the existing correction terms, by using the usual method of plotting $\langle R_N^2 \rangle$ against N in a double logarithmic scale and estimating the slope of the plot. We instead express ν in terms of its effective value determined by TSAWs of up to N steps, denoted by ν_N, defined by

$$\nu_N = \frac{N \langle R_N^2 \rangle}{\langle R_1^2 \rangle + \langle R_N^2 \rangle + 2 \sum_{i=2}^{N-1} \langle R_i^2 \rangle} - \frac{1}{2}. \tag{7}$$

If $\langle R_N^2 \rangle$ is of the form (5), then the asymptotic expression for ν_N should be

$$\nu_N = \nu + \tfrac{1}{2} [\alpha - (2\nu + 1) B \ln(\ln N)] \frac{1}{\ln N} + \dots . \tag{8}$$

If $\langle R_N^2 \rangle$ is of the form (6), then

$$\nu_N = \nu + f(N^{-1}) \tag{9}$$

where $f(N^{-1})$ is a certain function which depends on the correction terms neglected in (6) and vanishes as $N \to \infty$. Thus the intercept on the ordinate in the plot of ν_N against N^{-1} gives the Flory exponent ν.

We have first carried out simulations for $p = 0.7$. Since it is known that the percolation cluster shows a Euclidian lattice structure for p away from p_c where the best known p_c is $p_c = 0.592\,745 \pm 0.000\,002$ (Ziff and Sapoval 1986), one can expect that the TSAW exhibits a critical behaviour similar to that on the normal lattice. Data for $g = \infty$ averaged over 35 clusters are plotted in figure 1 in terms of their effective values of ν, obtained from the mean-square radii of gyration, as a function of N^{-1}. The inset is the plot of ν_N as a function of $1/\ln N$. If we assume $B \ll 1$ in (5), thus neglecting all corrections except the leading logarithmic one, then ν_N must show a linear behaviour in the inset. As is clear from the plot, data indeed show such behaviour for a wide range of $N \geq 60$, indicating that the leading correction of $\langle R_N^2 \rangle$ is indeed logarithmic. The intercept on the ordinate is the Flory exponent ν and the slope $\alpha/2$. Estimated in this way are $\nu = 0.497 \pm 0.005$ and $\alpha = 0.676 \pm 0.002$, where the quoted errors are those associated with linear regression and there may be additional statistical errors not accounted for. This value of ν is indeed very close to the known value of the TSAW on the normal lattice, indicating that the lattice dilution does not affect the critical behaviour as long as the concentration of the undiluted sites is not critical. Our estimate of α is also comparable to the normal lattice value. Although the renormalisation calculation indicates $\alpha \simeq 1$ (Obukhov and Peliti 1983), our Monte Carlo data of 10^5 walks up to 1000 steps for $g = \infty$, performed on a regular square lattice, produce the best fit with $\nu = \frac{3}{4}$ and $\alpha \simeq 0.7$ (not shown). In fact, the data for $p = 0.7$ are not very

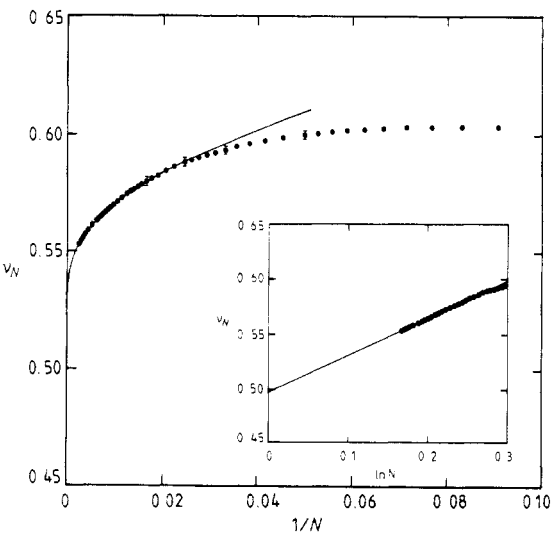

Figure 1. The effective exponent ν_N of (7) against $1/N$ from the mean-square radius of gyration of TSAWs on a percolation cluster for $p = 0.7$ and $g = \infty$. The full line indicates the numerical fit using the leading logarithmic correction in (8) with the estimated values of ν and α from the inset, and the error bars were calculated from seven batches of data set, each of which was averaged over five clusters.

different from the corresponding data on a regular lattice, and the plots of ν_N for the two cases nearly overlap one another over the wide range of N.

We have also studied in a similar way with the mean-square end-to-end distance and the results were found to be essentially the same as those for radius of gyration except the larger fluctuations, as expected from the concept of universality.

Simulations for $p = 0.592\,77$ were also carried out for several selected values of g, $g = 1.0$, 2.0, and $g = \infty$. Plotted in figure 2 are the effective values of ν up to 400 steps, obtained from the mean-square radius of gyration, averaged over 40–65 clusters depending on g. Since the infinite cluster near p_c is known to show the fractal structure with its fractal dimension $\bar{d} < d_c$ ($\bar{d} = 91/48$, Stauffer 1985), then one can expect that the TSAW exhibits its mean end-to-end distance in the form of (6) with Flory exponent ν larger than $\frac{1}{2}$. Surprisingly, however, our Monte Carlo data indicate that ν is smaller than the normal lattice value for all $g > 0$, as shown in the figure. For $N = 400$, estimated values of ν_N are already less than 0.47 and they seem to decrease, as N increases, far below the normal lattice value. Data for all three cases exhibit large corrections to scaling and, in addition, they appear to show asymptotic behaviour rather similar to the case for $p = 0.7$, indicating that the leading correction to scaling might be logarithmic. In fact, data seem to fit well with the expression in (5) for $N \geqslant 200$. The full curves in the figure are logarithmic fits with the fitting parameters ν and α obtained in the same way as in the inset in figure 1. The values of (ν, α) used are (0.354, 1.30), (0.32, 1.76) and (0.32, 1.90), for $g = 1.0$, 2.0 and ∞, respectively. However, we claim that such logarithmic fits cannot be accepted in at least two respects. Firstly, the estimated ν and α appear to depend on the self-avoidance parameter g. Since ν and α are the universal critical exponents, they are not supposed to depend upon the details of the model such as the parameter g, as long as $g > 0$. Nevertheless, similar studies with mean-square end-to-end distance also result in different values of α.

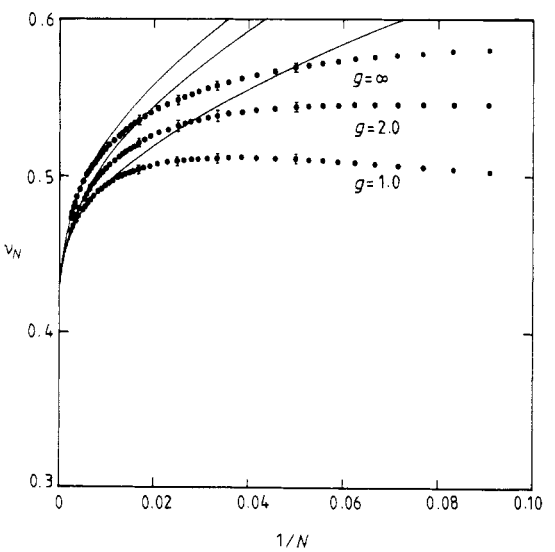

Figure 2. The effective exponent ν_N of (7) against $1/N$ from the mean-square radius of gyration of TSAWs on a percolation cluster for $p = 0.592.77$. Points are the Monte Carlo data and the full curves are the numerical fit using the logarithmic correction in (8). The errors were calculated from 9–13 batches of data set, each of which was averaged over 5 clusters.

Secondly, the critical exponent ν estimated from such a logarithmic fit appears to be smaller than the ordinary RW value ($\nu_{RW} \simeq 0.35$, Havlin and Ben-Abraham 1983). For any $g > 0$, TSAWs in general tend to avoid the previously visited sites. The effect of such a trend is known to enhance the end-to-end distance and, therefore, the Flory exponent of the TSAWs is not expected to be smaller than that of the RWs. In addition, the condition in (3) suggests that the TSAW exhibits a Flory exponent larger than the RW value.

As the corrections to scaling are unexpectedly large for relatively large values of g ($g \geq 1.0$), it seems rather difficult to estimate the Flory exponent from the plots in figure 2. For sufficiently large values of g, the TSAWs behave like the SAWs for the first several steps and, therefore, ν_N's are similar to those for the SAWs for small N. As $N \to \infty$, however, ν_N must eventually cross over to TSAW behaviour, thus exhibiting a sharp decrease, as shown in figure 2. On the other hand, for sufficiently small but positive g, one can expect that ν_N for the TSAWs is not very different from that of the RWs for small N and increases, as $N \to \infty$, to the asymptotic value of ν_{TSAW}, assuming that $\nu_{TSAW} > \nu_{RW}$. Thus one may expect that there might be a moderate value of g, for which the corrections to scaling might be unimportant. We therefore carried out additional simulations for $g = 0$ and 0.1.

Our simulation results for $g = 0$, and 0.1 up to 800 steps are shown in figure 3 together with those for $g = 1.0$ and $g = \infty$. Plotted in the figure are the ν_N calculated from the mean-square end-to-end distance. (Note that we have plotted the large-N region in this plot.) For $g = 0$, i.e. for RWs, our data indicate that $\nu_{RW} = 0.36 \pm 0.01$, which is reasonably close to the previous estimates, $\nu_{RW} \simeq 0.35$ (Havlin and Ben-Abraham 1983, Majid *et al* 1984). Data for $g = 0.1$ are nearly flat over the wide range of N, suggesting that the correction terms are unimportant for this value of g. As is clear from the plot, data for all $g > 0$ indicate the same asymptotic ν, as expected from the universality. The estimated value of ν is

$$\nu = 0.432 \pm 0.005$$

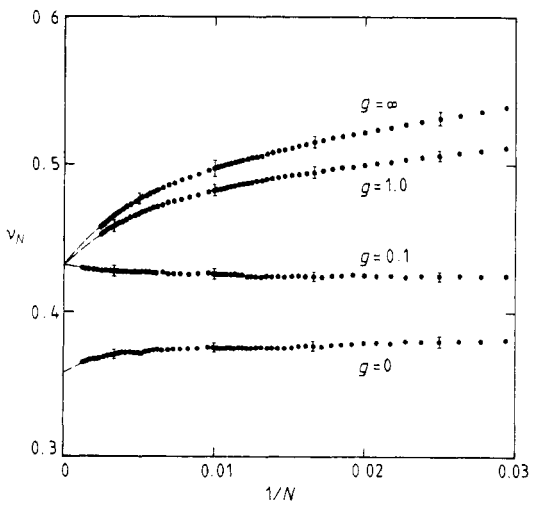

Figure 3. The effective exponent ν of (7) against $1/N$ from the mean-square end-to-end distance of TSAWs on a percolation cluster for $p = 0.592\,77$. The errors were calculated from 5-13 batches of data set, each of which were averaged over 5 clusters.

which is considerably smaller than that obtained by the cell renormalisation study but much larger than that of the ordinary RW on a percolation cluster. Interestingly, this value of ν agrees well with the Flory-type formula in (4). If we use the conjectured value of $\tilde{d} \simeq 4/3$ (Alexander and Orbach, 1981) and $\tilde{d} = 91/48$, then (4) would be $\nu \simeq 0.422$, which is reasonably close to our estimation.

Shown in figure 4 is the double logarithmic plot of mean-square end-to-end distance as a function of N for several different values of g. Points are the simulation data and the full lines for each set of data are those with the slopes of 2ν for each g, i.e. slope of 0.7 for $g = 0$ and of about 0.86 for all $g > 0$. As is clear from the figure, simulation data for $g = 0.1$ fit well with the full line for the entire region of N, indicating that the exponent ν is indeed close to 0.43. For $g = 1.0$ and $g = \infty$, slopes are larger than 2ν for small N and decrease as N increases. Up to 400 steps, the asymptotic slope of 2ν ($\simeq 0.86$) was not reached for both cases; however, they seem to show an eventual crossover to the slope similar to that of full lines for N much larger than we obtained in our simulation.

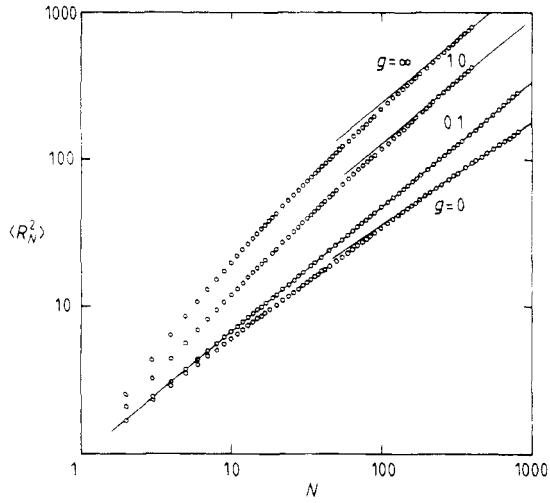

Figure 4. Plots of $\ln\langle R_N^2 \rangle$ against $\ln N$ for TSAWs on a percolation cluster near percolation threshold for various values of g. Points are the simulation data and the full lines are those with the asymptotic slope 2ν, where $\nu \simeq 0.35$ for $g = 0$ and 0.43 for all $g > 0$.

We have also studied the mean number of distinct sites S_N visited during N steps by the TSAW. This quantity is also known to satisfy the power law $S_N \sim N^s$. The exponent s was numerically studied from the Monte Carlo data of S_N in a similar way to that of ν, with s_N defined similarly to (7). The s_N shows large corrections for large and small values of g and, for $g = 1.0$, corrections to scaling appears to be nearly unimportant. The estimated value of s is $s = 0.79 \pm 0.02$, which appears to be nearly twice as big as ν. This value is also reasonably close to but slightly greater than that of TSAWs on a Sierpinski gasket (Angeles d'Auriac and Rammal 1984).

In summary, we have carried out Monte Carlo simulations for TSAWs performed on a site-percolated two-dimensional percolation cluster for the square lattice. For $p = 0.7$, the critical behaviour of TSAWs was found to be rather similar to that on the fully occupied lattice, as expected. For p close to p_c, on the other hand, the critical behaviour of TSAWs is different from that on the fully occupied lattice and also from

that of RWs. The Flory exponent was found to be $\nu \simeq 0.432 \pm 0.005$, which is considerably smaller than that on the normal lattice. The smaller value of ν on a percolation cluster may be explained as follows. Since the percolation cluster generated near p_c contains many dangling bonds and blobs, the dilution may effectively trap the walk and induce self-intersections or immediate returns (backscattering). The occurence of this effect increases as the length of walks increases. The disorder average of this effect favours shorter end-to-end distance and it reflects the smaller value of ν. This kind of effect is very similar to the case of RWs, where the Flory exponent is also considerably smaller than that on the regular lattice. However, for TSAWs, since the self-avoidance parameter g enhances the end-to-end distance, the Flory exponent ν seems to be greater than the RW value, as expected from (3).

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