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# Self-avoiding walk connectivity constant and theta point on percolating lattices

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**Abstract.** *The average connectivity constant $\mu$ of self-avoiding walks (SAWs) is obtained* from exact enumeration of SAWs on Monte Carlo generated percolating clusters in a randomly diluted square lattice. For averages over the (infinite) percolating cluster, $\mu$ decreases almost linearly with bond dilution $(1-p)$, where $p$ is the bond occupation concentation. We find $\mu(p_c) = 1.31 \pm 0.03$ at the percolation threshold $p_c$ and could not detect any significant difference between $\mu(p_c)$ and $p_c\mu(1)$. The variation of $\theta$-point for SAWs on the same lattice with dilution is also estimated, analysing the partition function zeros. Within the limited accuracy of our analysis, its variation with dilution is observed as being quite weak and the $\theta$-point increases somewhat (compared to pure lattice value) near $p_c$; we find a non-vanishing $\theta$-point ($K_\theta(p_c) \cong 0.59$, where $K_\theta = J/k\theta$) on the square lattice percolation cluster at $p_c$.

## 1. Introduction

The statistics of self-avoiding walks (SAWs) on lattices with quenched random impurities is presently being investigated with keen interest (see e.g. [1, 2] for recent reviews). So far, most of the studies investigated the average size of the SAWs by measuring the end-to-end distance of the walks and estimating the associated size exponent on percolation clusters [3].

The statistics of the (lattice) SAW model of linear polymers (in dilute solutions) also involve some less universal or non-universal quantities. For example, the total number of SAW configurations $C_N$, or the total number of SAW loops $L_N$, grow (on perfect lattices) with the step size $N$ as [4].

$$C_N \sim \mu^N N^{\gamma-1} \qquad \text{and} \qquad L_N \sim \mu^N N^{-(2-\alpha)} \tag{1}$$

where $\mu$ is called the SAW connectivity constant which depends on the lattice and $\gamma$ and $\alpha$ are universal exponents [5] dependent only on lattice dimension. The connectivity constants $\mu$ for walks and loops are identical for the perfect lattice [4, 5] and have been estimated accurately on various regular lattices; e.g. $\mu \simeq 2.638$, 4.151, 4.684 for square, triangular and simple cubic lattices respectively [6]. With attractive interaction ($J$) between the nearest-neighbour sites visited by a SAW, the SAWs undergo a collapse transition (average end-to-end distance square $R_N^2 \sim N^{2\nu}$, $\nu = \nu_c = 1/d$ for collapse; $d$ is the lattice dimension) at temperatures below the $\theta$-point and for $T > \theta$ one gets the normal excluded volume (random SAW) phase ($\nu = \nu_{SAW} \simeq 3/(2+d)$ [5]). At $T = \theta$ this

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lattice model is believed [7] to have a 'tricritical' $\theta$-point transition. There have been several attempts to estimate the (lattice) $\theta$-point, using Monte Carlo [8], series analysis [9, 10] etc for various regular lattices; e.g. the existing estimates are $K_\theta$ $(\equiv J/k\theta) = 0.65 \pm 0.03$ and $0.41 \pm 0.13$ for square and triangular lattices respectively [8–11].

As mentioned earlier there have been several attempts to investigate the critical behaviour of the SAW statistics on (quenched) random lattices; specifically in estimating the size exponent $\nu$ ($\nu_{SAW}$ [1–3] and $\nu_\theta$ [12, 13]) and other exponents like $\gamma$ and $\alpha$ [2], for SAWs on the percolating fractal. However, comparable investigations for the variation with disorder of the non-universal quantities like the connectivity constant $\mu$ or of the $\theta$-point etc on quenched random dilute lattice have not been made. Let us consider the SAW statistics on randomly (say, bond) diluted lattices with (bond) occupation probability $p$. On various perfect lattices (at $p = 1$), there exist good estimates for quantities like $\mu$ [4] and $K_\theta$ [9–11] as mentioned before (e.g. $\mu \simeq 2.64$ and $K_\theta \simeq 0.65$ on square lattice). Similarly very accurate estimates for the percolation threshold ($p_c$) of various lattices, beyond which the lattices loose their macroscopic connectivity, are also available [14] (e.g. $p_c = 1/2$ for bond dilute square lattice). It is quite obvious that $\mu$ or $K_\theta$ would be affected by increasing lattice dilution. However, there is not much literature estimating these (connectivity and $\theta$) constants at different $p$ and specifically at $p_c$. Of course, if the SAW is not confined to the percolation cluster alone and if one averages the statistics over all the clusters (including all the finite clusters) of the dilute lattice, then $\mu(p) = p\mu_0$ exactly, where $\mu_0 \equiv \mu$ $(p = 1)$. This is trivial and can be seen straightforwardly: since a SAW does not visit any bond more than once, the occupation operator of each bond (step) is independently averaged (with average value $p$), and thus the effective connectivity $\mu$ of each step renormalizes to $p\mu$. Since, however, each existing bond on the infinite percolating cluster has a non-trivial (correlated) probability of occurrence, a similar argument cannot be applied to the SAWs confined to the infinite or percolating cluster only [1]; although an early enumeration estimate suggested $\mu(p) \simeq p.\mu_0$ up to $p_c$ for SAWs on the percolation cluster alone [15]. It turns out, that this difference from linear relationship, even for infinite or percolating cluster averaging, is subtle and, in particular, the difference between $\mu(p_c)$ and $p_c \cdot \mu_0$ could not be detected. Similarly, the estimates of $\theta(p)$, specially of $\theta(p_c)$ (if non-vanishing), are also quite interesting [12, 13], and are not trivially known from the estimate of $\theta_0$ $(\equiv \theta$ at $p = 1)$ on perfect lattices and the percolation threshold ($p_c$) on the respective lattices. In fact, it is possible to argue that, with the percolation cluster being extremely ramified, the nearest-neighbour (or, of that matter, any finite range) attractive interaction will not support any statistically significant order towards collapse, suggesting $\theta(p_c) = 0$. On the other hand, in an effective $n$-vector field Hamiltonian, with the disorder (averaging) induced replica coupled term being negative and of order $p(1-p)$, and quadratic field (excluded volume) term being proportional to $(T - \theta_0)$, one might expect [16, 17] an increase of $\theta$-point with disorder. Apart from a very weak indication for an initial decrease we find a slight increase in the $\theta$-point value, with increasing lattice dilution near $p_c$.

## 2. Series studies and results

We have studied here the variation of the SAW connectivity constant $\mu$ and the $\theta$-point on the infinite (percolation) cluster, with dilution concentration $p$, on a bond diluted square lattice. The size of the lattice taken in this simulation is $100 \times 100$. For a particular

concentration of bonds ($p \geqslant p_c$), the disordered lattice is first generated using a Monte Carlo program and then the infinite percolating cluster (which spans the lattice in all directions) is isolated. On that infinite cluster, starting from a (suitably chosen) central site, we enumerate exactly all SAW configurations of a given step size $N$ (total number of SAWs $C_N$). Together with that, we have also calculated the total number of loops $L_N$ (SAWs whose end point is a nearest-neighbour of the starting point). For a single disordered lattice configuration, the values of $C_N$ and $L_N$ are typically around $6.9\times10^6$, $1.2\times10^5$ and $8.9\times10^4$, $1.3\times10^3$ for $p=0.9$ and 0.7 respectively for $N=17$. We went up to $N=30$ for $p=p_c=0.5$ where $C_N\simeq2.3\times10^4$ and $L_N\simeq8.3\times10^1$ for $N=29$. In fact, large fluctuations are observed in these quantities from configuration to configuration and these quantities themselves are not self-averaging. We find that the effective connective constants obtained from the ratio $C_N/C_{N-2}$ or $L_N/L_{N-2}$ are quite well behaved and are self-averaging quantities; these are shown in figures 1 and 2. Clearly, the values of $L_N$ being an order of magnitude less than those of $C_N$, the connective constants evaluated from $C_N$ are much more accurate compared to those evaluated from $L_N$ values (see figure 2). It may be noted, from figure 1, that the slopes of the curves $C_N/C_{N-2}$ against $1/N$ seem to have a change of sign near $p\simeq0.65$. The number $C_{NM}$ of $N$-stepped walks with $M$ nearest-neighbour bonds, created by visits to nearest-neighbour sites, is also calculated ($\Sigma_M C_{NM}=C_N$). The values of $\bar{C}_{NM}$ ($\equiv\overline{C_{NM}/C_N}$), for different bond concentrations $p$ are given in table 1. Maximum step size for the enumerated SAWs was fixed between 17 and 30 and the averages were taken over 10 to 150 lattice congfiruations, depending on the lattice occupation concentration ($p$). For this simulation we have used 16 hours CPU time of CYBER and 20 hours of HORIZON-III computer.

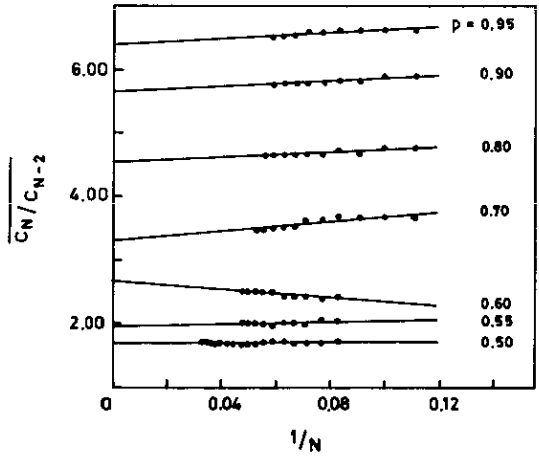


**Figure 1.** Plot of $(\overline{C_N/C_{N-2}})$ (averaged over random configurations) against $1/N$ for SAWs on dilute square lattice. $\mu_w$ values ($N\to\infty$) are obtained by linear fitting of these points.

The total number of SAW configuration $C_N$ and the total number of SAW loops $L_N$ on percolating clusters are fitted to the asymptotic forms as $C_N\sim\mu_w^N N^{\gamma-1}$ and $L_N\sim\mu_L^N N^{-(2-\alpha)}$ in the limit $N\to\infty$. In figure 1 and figure 2 we have plotted the configurationally averaged (over different percolating clusters) values of $\overline{C_N/C_{N-2}}$ and $\overline{L_N/L_{N-2}}$ (for finite steps $N$) respectively against $1/N$. The values of $\mu_W$ and $\mu_L$ in

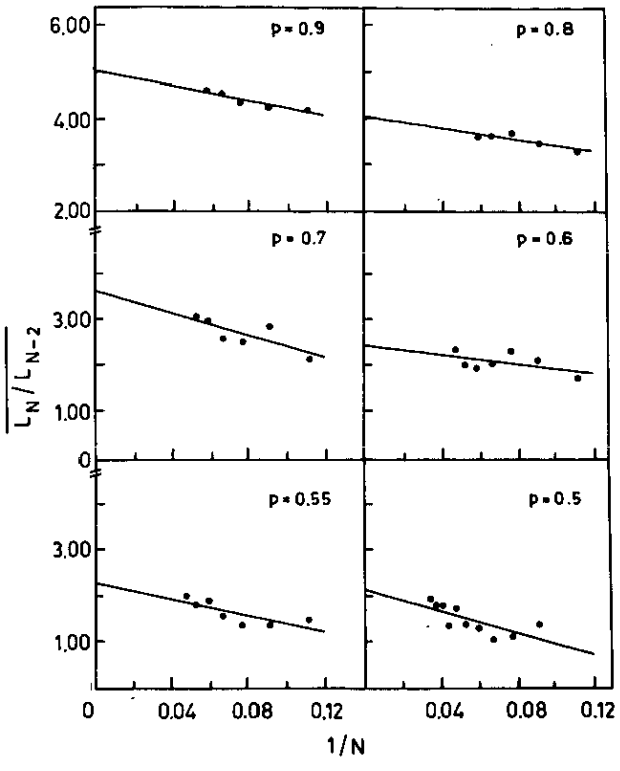


**Figure 2.** Plot of $(\overline{L_N/L_{N-2}})$ (averaged over random configurations) against $1/N$ for loops on dilute square lattice. $\mu_L$ values ($N \to \infty$) are obtained by linear fitting of these points.

the limit $N \to \infty$ were estimated from figure 1 and figure 2 respectively. Similar averages were also investigated earlier and the non-triviality of the these types of average over the percolating cluster are discussed there [15]. In figure 3 we have plotted, against bond dilution $(1-p)$, the (lattice configuration averaged) values $\mu_W$ and $\mu_L$ (for $N \to \infty$). The average connectivity constant decreases almost linearly with decreasing lattice bond concentration. We find $\mu_W(p_c) = 1.307 \pm 0.001$ and $\mu_L(p_c) = 1.4 \pm 0.2$ (compared with $\mu_0 . p_c \simeq 1.319$, with $\mu_0 \simeq 2.638$ [6] and $p_c = 0.5$ [14]). It may be noted here that even with better statistics and larger system size (compared to [15]), no significant difference from the linear relationship (for $\mu(p)$ with $p$) is observed. It may also be noted that because of the presence of (singly connected) links in the infinite percolation cluster at $p_c$, no SAW loop was expected on the $p_c$-cluster [1], suggesting $\mu_L(p) \to 0$ at $p_c$ unlike $\mu_W(p)$ which should remain greater than unity at $p_c$ (as more than one SAW configuration is possible in the percolation cluster). However, we could not detect any significant difference between $\mu_W$ and $\mu_L$ at any $p$.

For estimating, the (lattice) $\theta$-point, we analyse the zeros of the SAW partition function [9], defined as

$$Z_N = \sum_M \bar{C}_{NM} \varepsilon^M \tag{2}$$

where $\varepsilon = \exp(-J/kT)$, $J$ being the interaction between two nearest-neighbour sites visited by a SAW, and the normalized average $\bar{C}_{NM}$ is found out from the configuration averaged values of $C_{NM}/C_N$ which are obtained from the previous simulations (see

**Table 1.** Normalized $(\overline{C_{NM}/C_N})$ for generating the partition function polynomial $Z_N$ in equation (2). $n$ denotes the number of dilute lattice configurations over which the statistics has been averaged.

| $M$ | $p=0.5$ $n=127$ $N=30$ | $p=0.55$ $n=78$ $N=21$ | $p=0.6$ $n=40$ $N=21$ | $p=0.7$ $n=20$ $N=19$ | $p=0.8$ $n=10$ $N=18$ | $p=0.9$ $n=6$ $N=17$ | $p=0.95$ $n=6$ $N=17$ |
|---|---|---|---|---|---|---|---|
| 0 | 0.031 027 | 0.084 803 | 0.075 060 | 0.093 706 | 0.113 514 | 0.113 456 | 0.115 360 |
| 1 | 0.085 721 | 0.173 491 | 0.166 922 | 0.186 509 | 0.211 628 | 0.212 957 | 0.214 366 |
| 2 | 0.153 590 | 0.206 914 | 0.225 175 | 0.220 269 | 0.232 375 | 0.232 024 | 0.232 196 |
| 3 | 0.180 198 | 0.186 898 | 0.197 340 | 0.189 817 | 0.185 632 | 0.183 662 | 0.183 912 |
| 4 | 0.170 312 | 0.141 756 | 0.144 221 | 0.137 715 | 0.124 852 | 0.123 597 | 0.123 407 |
| 5 | 0.136 366 | 0.097 296 | 0.089 360 | 0.085 461 | 0.071 405 | 0.071 111 | 0.070 087 |
| 6 | 0.097 212 | 0.056 124 | 0.053 111 | 0.047 107 | 0.035 699 | 0.037 295 | 0.036 432 |
| 7 | 0.063 912 | 0.029 070 | 0.027 815 | 0.023 424 | 0.016 062 | 0.016 024 | 0.015 243 |
| 8 | 0.038 050 | 0.014 596 | 0.012 224 | 0.010 161 | 0.006 144 | 0.006 862 | 0.006 311 |
| 9 | 0.021 409 | 0.005 669 | 0.005 736 | 0.003 973 | 0.002 132 | 0.002 723 | 0.002 418 |
| 10 | 0.011 388 | 0.002 376 | 0.001 935 | 0.001 543 | 0.000 536 | 0.000 289 | 0.000 267 |
| 11 | 0.006 168 | 0.000 860 | 0.000 750 | 0.000 306 | 0.000 022 | | |
| 12 | 0.002 760 | 0.000 136 | 0.000 320 | 0.000 007 | | | |
| 13 | 0.001 200 | 0.000 010 | 0.000 031 | | | | |
| 14 | 0.000 437 | | | | | | |
| 15 | 0.000 158 | | | | | | |
| 16 | 0.000 058 | | | | | | |
| 17 | 0.000 025 | | | | | | |
| 18 | 0.000 007 | | | | | | |
| 19 | 0.000 001 | | | | | | |
| 20 | 0.000 000 | | | | | | |

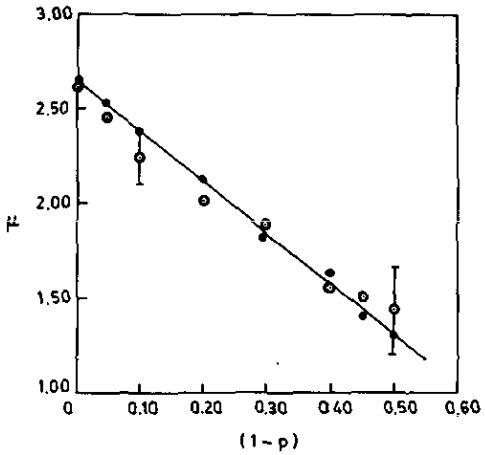


***Figure 3.*** *'Phase diagram' ($\mu_W$ and $\mu_L$ against $(1-p)$) for* SAWs *on a dilute square lattice. The statistical errors in $\mu_W$ are of the symbol (filled circle) size while those for $\mu_L$ (open circle) are indicated. The straight line fit with the filled circles indicates the nature of variation of $\mu$ with dilution.*

table 1). It may be noted from table 1 that the numbers of nearest-neighbour bonds between points visited by SAW on the percolation cluster are considerable even at $p_c$ (fractions are finite). This suggests a possibility of finite $\theta$-point on percolation cluster with attractive interactions between such nearest-neighbour bonds. The transition point can be obtained from knowledge of the zeros of the above partition function in the complex $\varepsilon$-plane (or complex temperature), using the Yang-Lee theorem [10]. We have evluated the zeros using the Lin-Bairstow method. In figure 4 we have plotted all the zeros of $Z_N$ for a number of finite stepped SAWs for each concentration of bond dilution. Also in figure 5 we have plotted a subset of the above zeros formed by the right furthest zeros (with maximum value of the real part) for various bond dilution concentrations. From figure 4 and figure 5 it is evident that, in the limit $N \to \infty$, the zeros of the partition function extrapolates to the positive real axis. In figure 6 we have plotted the real part of the subset of zeros shown in figure 5, as a function of $1/N$ for various concentrations $p$. Within our limits of accuracy, these points can be fitted to linear equations and the extrapolated values of the $\theta$-point can be estimated

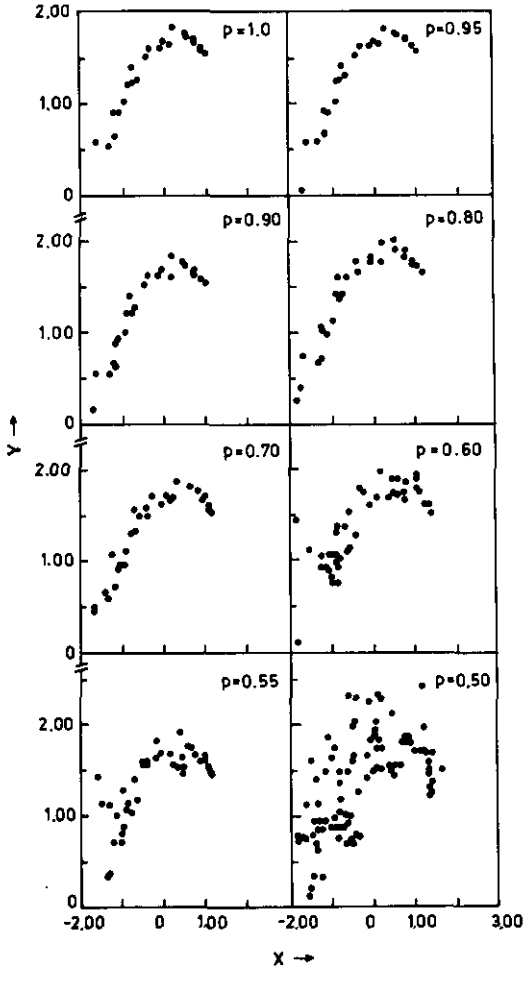


**Figure 4.** All the zeros of $Z_N$ (from equation 2: with simulation results (cf table 1) for $(\overline{C_{NM}/C_N})$) satisfying $x > -2.0$ and $y > 0$.

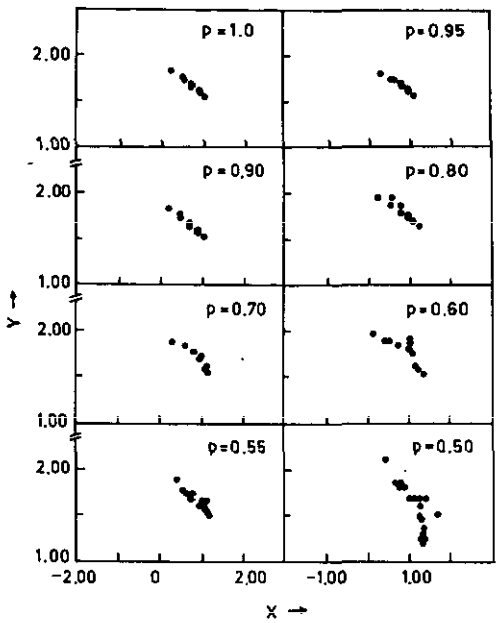


**Figure 5.** Furthest right zeros of $Z_N$ extracted from figure 4.

in the limit $N \to \infty$. This indicates the existence of some unique $\theta$-point for SAWs even on the fractal.

We observe that these (extrapolated) $\theta$-values increase slightly (apart from an initial indication of a decrease) with increasing lattice dilution, and in figure 7 these extrapolated values ($K_\theta \sim \theta^{-1}$) are plotted against dilution concentration. It may be noted that although such an increase in the $\theta$-point value, with increasing lattice dilution, is somewhat unexpected in view of the ramified structure of the percolation cluster, this is not completely unjustified. In fact, as already mentioned before, such behaviour was indeed predicted [16], using an effective field theoretic Hamiltonian for the $n$-vector magnetic model on dilute lattices in the $n \to 0$ limit, using replica trick (cf [18]):

$$\mathcal{H} = \sum_q \sum_\alpha (r + q^2) \boldsymbol{S}_q^\alpha \cdot \boldsymbol{S}_{-q}^\alpha + \sum_{\substack{q_1, q_2, q_3, q_4 \\ \alpha, \beta}} \sum (u\delta_{\alpha\beta} - v) \boldsymbol{S}_{q_1}^\alpha \cdot \boldsymbol{S}_{q_2}^\alpha \boldsymbol{S}_{q_3}^\beta \cdot \boldsymbol{S}_{q_4}^\beta \delta(q_1 + q_2 + q_3 + q_4)$$

Here $\boldsymbol{S}$ is the $n$-component spin vector, $\alpha = 1, 2, \ldots, m$ is the replica index (coming from averaging over quenched randomness) and the limit $m \to 0$ is to be taken, $u$ is a measure of the two body (repulsive) interaction, and $v = g^2 p(1-p)$ term gives the replica coupling due to quenched disorder (with coupling strength $g$). For polymers in solvent $u = (T - \theta_0)/\theta_0$ [5]; $\theta_0$ here refers to the pure lattice $\theta$-point value. As shown by Kim [18], because of the simultaneous appearance of $n$ and $m$ sums for any closed loop which does not contribute in the $n \to 0$ (SAW) and $m \to 0$ (replica averaging) limits, the replica coupling effectively disappears in this $n \to 0$ limit and the excluded volume term $u$ in the above Hamiltonian can be effectively replaced [12] by $u_{\text{eff}} = u - v = [T - \theta_0 - g^2 p(1-p)\theta_0]/\theta_0$. For $u_{\text{eff}} > 0$, one gets the usual SAW critical behaviour [5] in the $n \to 0$ limit and collapse occurs when $u_{\text{eff}} < 0$. The tricritical $\theta$-point behaviour occurs when $u_{\text{eff}} = 0$ and $S^6$ order term determines the fluctuation [5]. $\theta$-point thus effectively increases [16, 17] with dilution; using the above formalism, the estimate is $\theta(p) \sim \theta_0 + g^2 p(1-p)$.

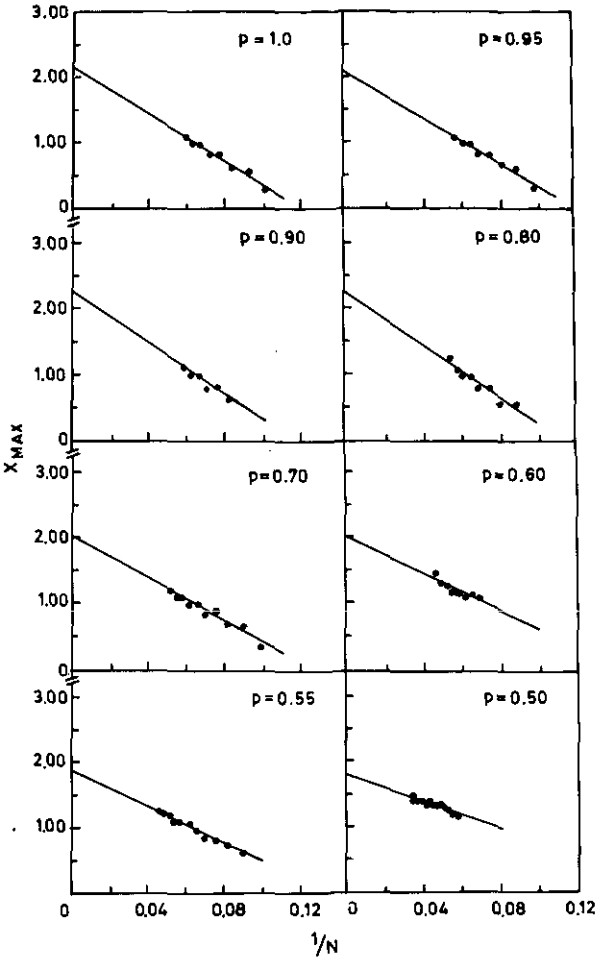


**Figure 6.** Real part of the furthest right zeros (obtained from figure 5) against $1/N$.

## 3. Discussion

Our present study indicates the same value for the self-avoiding walk and loop connectivity constants on a dilute lattice and in particular at $p_c$, where the existence of singly connected links of the percolation cluster would suggest [1] the loop connectivity constant be zero while for SAW, it would be greater than unity. Also, we could not detect any significant difference between $\mu(p_c)$ for the infinite percolating cluster averages and that for all cluster averages which is exactly $p_c\mu_0$. The $\theta$-point has been estimated here on such dilute lattices, analysing the partition function zeros. Our estimate for the $\theta$-point being approximate (even on the perfect lattice), we did not perhaps get a very precise variation of $\theta(p)$. However, there seems to be some indication of an increase in the $\theta$-point value with dilution (a possible justification given in the last section), and we thus find a clearly non-vanishing value of the $\theta$-point on the percolation cluster. In view of the extremely ramified structure of the percolation cluster, we believe this existence (non-zero value) of the $\theta$-point is important and will help to see the effect of percolating fractals on the statistical effects of ($\theta$-point)

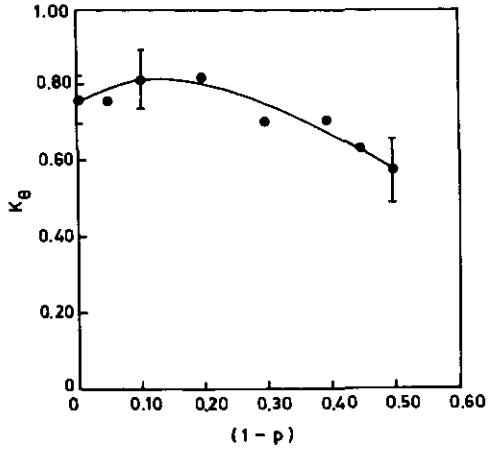


**Figure 7.** $K_\theta$ values obtained from figure 6 are plotted against dilution concentration. Statistical errors are also indicated. The continuous line drawn through the points indicates the overall variation of average $K_\theta$.

excluded volume in linear polymers. The effect of percolation fractal on SAW statistics (for $T > \theta(p_c)$) at $p_c$, is very small and is still being debated [1-3]. It has recently been pointed out [12, 13] that the effect of percolation fractal on the tricritical exponent at $T = \theta(p_c)$ is expected to be quite prominent (e.g. $\nu_\theta = 4/7 \simeq 0.57$ on pure two-dimensional lattices while $\nu_\theta \simeq 0.68$ on two-dimensional percolation clusters [13]). Such effects can be seen only if $\theta(p_c)$ is finite (non-zero), which our present study clearly indicates.

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*Note added in proof.* In the model for estimating the $\theta$-point from the partition function in (2), all the $N$-step SAW configurations (on the percolating cluster only) were enumerated and also the number of configurations with $M$ nearest-neighbour bridges were counted independent of the cluster geometry (even vacant lattice bonds were assumed to convey the monomer-monomer interaction). This gave a slight increase in the $\theta$-point value at $p_c$, as supported by the filled theoretic estimate for the same (discussed in section 2), which also implicitly assumes similar counting.

If one considers the interaction only through the occupied bonds present in the percolating cluster, then we find the $\theta$-point to decrease considerably at $p_c$. Series results for $N$ up to 30 and averaging over 160 clusters at $p_c$ give $K_\theta(p_c) = 1.49 \pm 0.10$, which is still quite large and non-vanishing (the $\theta$-point at $p_c$ is about half of that at $p = 1$).

The linear relation $\mu(p_c) = p_c \mu_0$, observed even on the percolation cluster, gets further support from the newly published data for SAWs on site diluted percolating lattices [19].

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