Kinetic self-avoiding walks on randomly diluted lattices at the percolation threshold

S. L. Narasimhan
Solid State Physics Division, Bhabha Atomic Research Centre, Bombay 400 085, India
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Survival probability arguments have been developed for obtaining generalized formulas for the end-to-end distance exponents of the self-avoiding walk, the kinetic growth walk (KGW), and the true self-avoiding walk on a percolating cluster. A crossover in the asymptotic behavior of KGW on a two dimensional percolating cluster has been observed at a walk length ≈ 60. This is presented as numerical evidence of the fact that the KGW latches onto a backbone as it grows longer.

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Self-avoiding walks (SAW's) on a randomly diluted lattice have been a subject of great interest because of their relevance to polymers in porous media. Much attention has been focused on studying the effect of lattice dilution on the end-to-end distance exponent ν and the susceptibility exponent γ. It has been demonstrated [1,2] that the exponent ν changes at the percolation threshold to a higher value $\nu_P \approx 3/(d_f+2)$, with d_f representing the fractal dimension of the percolating cluster, whereas the exponent γ does not change at all with lattice dilution. Even though it can be argued that ν_P must be greater than the Flory value $\nu_F = 3/(d+2)$, the question of what the value of ν_P should be has remained controversial [3]. In particular, the exact enumeration studies [4–6] report higher values of ν_P than the Monte Carlo studies [7,8]. The reason for this discrepancy is said [3] to be due to the nature of the unbiased Monte Carlo sampling: The percolating cluster is known to be made up of self-similar blobs which are linked by singly connected paths; it is very difficult for the Monte Carlo method to generate unbiased SAW's through these singly connected paths.

This raises the interesting academic question of whether it is possible to estimate ν_P independently by some other means. For example, the kinetic growth walk (KGW [9]) grows by stepping into one of the unoccupied nearest neighbor (UNN) sites at random, and so cannot miss going from one blob to another through the singly connected channels of a percolating cluster. This walk represents the nonequilibrium conformations of a linear polymer, and is also intimately related to the hull of a percolating cluster [10]. In regular Euclidean spaces, the KGW is known [11,12] to have the same asymptotic behavior as a SAW. Hence a study of whether it is also true on a percolating cluster will throw light on the Monte Carlo as well as the exact enumeration results for SAW's.

A KGW can be viewed as a true self-avoiding walk (TSAW [13]) without self-intersections because, apart from the trapping problem, it is essentially the same as the latter in the limit $g \to \infty$. This is quite analogous to the situation where a SAW is viewed as a random walk without self intersections. Therefore, we adapt Pietronero's survival probability approach [12] to this problem, and consider an N-step kinetic walk (KW)— *either* a random walk or a TSAW—on an infinite percolating cluster.

Let $P(r;N)$ denote the probability that an N-step KW has an end-to-end distance r. Then the probability distribution $Q(r;N)$ for the end-to-end distances of N-step SAW's or KGW's can be written as the product

$$Q(r;N) \equiv P_S(r;N)P(r;N) , \tag{1}$$

where $P_S(r;N)$ represent the probability that a KW will survive up to N steps without self-intersections. We may write

$$P_S(r;N) \approx \exp(-Np) , \tag{2}$$

with p denoting the probability per step that the walk will be trapped into a self-intersecting situation. How to estimate p?

As we move on the walk from one end to the other, at every step we may find some (or all) of the nearest neighbors occupied by the walk. So, naturally, we may define the encounter probability p_E as the probability that a nearest neighbor site will be an occupied one. Assuming that the monomers fill a volume $V \approx r^D$ (D is the fractal dimension of the space in which the walks are realized) uniformly with an average density $\rho \approx N/V$, we may identify p_E with ρ^α, where α is the number of occupied nearest neighbors encountered, and is referred to as the order of encounter. The functional dependence $p_E(\rho) \approx \rho^\alpha$ satisfies the expectation that $p_E \to 0(1)$ as $\rho \to 0(1)$.

Pietronero has argued [12] that this definition of α is wrong in view of the topological connectedness of the walk. For a Gaussian random walk in a regular Euclidean space, he has defined it as the number of *walk segments* encountered whose contour lengths far exceed the correlation length pertaining to the directions of successive steps. This definition of α is also applicable to the TSAW in a space of dimension of $d \geq 2$, because it has the same asymptotic behavior as the Gaussian random walk. He has further demonstrated that encountering the walk is necessary but not sufficient to trap a KGW. Hence he has proposed the following expression for p:

$$p = \sum_\alpha \rho^\alpha p_T^{(\alpha)} , \tag{3}$$

where the summation is due to the fact that α is arbitrary and $p_T^{(\alpha)}$ denotes the probability that an encounter of order α also traps the walk. In the case of a SAW, we may write $p \approx \sum_\alpha \rho^\alpha$.

A random walk on an infinite percolating cluster, however, is non-Gaussian with the end-to-end distance exponent ν_P^{RW} having a value $\nu_P^{\mathrm{RW}} \approx 0.3484$ in two dimensions [14]. Even though Pietronero's definition of α is not applicable directly in the present case, we refer to α *formally* as the order of encounter, and assume that Eq. (3) is still valid. The survival probability for the walk can then be written formally as

$$P_S(r;N) \approx \exp\left\{-N\sum_\alpha \rho^\alpha p_T^{(\alpha)}\right\}, \tag{4}$$

where $\alpha = 1,2,3,\ldots$.

The probability distribution $P(r;N)$ for the end-to-end distances of N-step KW's on an infinite percolating cluster has the form [14]

$$P(r;N) \approx \exp\left\{-N\left[\frac{(r)^{d_{\min}}}{N}\right]^{\tilde{\delta}_{\mathrm{KW}}}\right\},$$
$$\tilde{\delta}_{\mathrm{KW}} \equiv (1-\nu_P^{\mathrm{KW}}/\tilde{\nu})^{-1}, \tag{5}$$

where $d_{\min}$ is the chemical dimension, and $\tilde{\nu} \approx 1/d_{\min}$ ($\approx 0.883 \pm 0.003$ in two dimensions [14]). ν_P^{KW} is the corresponding end-to-end distance exponent. The required probability distribution $Q(r;N)$ can now be obtained by substituting the above forms of $P_S(r;N)$ and $P(r;N)$ in Eq. (1); the exponent ν_P^{KSW} for kinetic walks *without* self-intersections (KSW) can be obtained by minimizing the saddle-point function

$$F(r;N) = N\left[\frac{(r)^{d_{\min}}}{N}\right]^{\tilde{\delta}_{\mathrm{KW}}} + N\sum_\alpha \rho^\alpha p_T^{(\alpha)} . \tag{6}$$

It may be noted here that Lhuillier's form [15] for F is a special case of Eq. (6). Since the maximum contribution comes from the lowest value of α with nonzero $p_T^{(\alpha)}$, we have the general formula

$$\nu_P^{\mathrm{KSW}} = \frac{\alpha + \tilde{\delta}_{\mathrm{KW}}}{D\alpha + \tilde{\delta}_{\mathrm{KW}} d_{\min}} , \tag{7}$$

which is a more generalized version of the Chang-Aharony formula [16] for ν^{SAW} on a fractal. Pietronero [12] has argued that a first order encounter ($\alpha = 1$) is sufficient to trap the walk in two or three dimensional space. This argument should also be valid for a percolating cluster because it provides less escape routes for a walk than its embedding Euclidean space. The exponent ν_P^{KSW} will correspond to that of either SAW or KGW depending on whether the kinetic walk considered is a random walk or a TSAW.

In order to calculate ν_P^{KGW}, we need to have the value of ν_P^{TSAW} at the percolation threshold. It is possible to obtain some theoretical estimate of ν_P^{TSAW} by considering a TSAW as a random walk with a tendency to move towards regions not yet visited. The probability distribution $P_a(r;N)$ for such an asymmetric walk can be expressed in terms of $P(r;N)$, Eq. (5):

$$P_a(r;N) = P(r;N)\exp\{-g\bar{n}(r)\} , \tag{8}$$

where $\bar{n}(r)$ represents the average number of times an N-step random walk has been found at a distance r. The factor $\exp(-g\bar{n})$ in the above expressions ensures that a walk which revisits a site is given lesser weight; g is known as the self-avoidance parameter. If we assume that the walk is equally likely to be anywhere in the region of volume, $V \approx (r)^{d_f}$, then we have $\bar{n}(r) = \rho$. Here d_f is the fractal dimension of the percolation cluster ($= \frac{91}{48}$ in two dimensions [14]). The exponent ν_P^{TSAW} is then obtained by minimizing the saddle-point function appearing in Eq. (8):

$$\nu_P^{\mathrm{TSAW}} = \frac{\tilde{\delta}_{\mathrm{RW}}}{d_f + \tilde{\delta}_{\mathrm{RW}} d_{\min}}, \quad \tilde{\delta}_{\mathrm{RW}} \equiv (1-\nu_P^{\mathrm{RW}}/\tilde{\nu})^{-1} . \tag{9}$$

Substituting the appropriate two dimensional values in Eq. (9), we obtain $\nu_P^{\mathrm{TSAW}} \approx 0.438$. Numerically, this compares well with that (≈ 0.48) estimated by Bouchard and Georges [17]. Equation (9) may be written in the equivalent form

$$\tilde{\delta}_{\mathrm{TSAW}} \equiv \left[1 - \frac{\nu_P^{\mathrm{TSAW}}}{\tilde{\nu}}\right]^{-1} = 1 + \left[\frac{d_{\min}}{d_f}\right]\tilde{\delta}_{\mathrm{RW}} . \tag{10}$$

Since $d_{\mathrm{RW}} > d_f$ and $d_{\mathrm{RW}} > d_{\min}$ in all dimensions [14], we have the result $\tilde{\delta}_{\mathrm{TSAW}} > \tilde{\delta}_{\mathrm{RW}}$ with the following implications for the SAW and KGW on percolating clusters.

Since asymptotically long SAW's are supported by the percolation backbone, we also need to consider the KGW's on the percolation backbone in order that they can be compared. Substituting $D = d_B$ in Eq. (7), we have the ratio

$$\frac{\nu_B^{\mathrm{KGW}}}{\nu_B^{\mathrm{SAW}}} = 1 + \frac{\alpha(\tilde{\delta}_{\mathrm{TSAW}} - \tilde{\delta}_{\mathrm{RW}})(d_B - d_{\min})}{(d_B\alpha + \tilde{\delta}_{\mathrm{TSAW}} d_{\min})(\alpha + \tilde{\delta}_{\mathrm{RW}})} . \tag{11}$$

In view of the fact that $d_B > d_{\min}$ for percolating clusters in less than six dimensions [14], the inequality $\tilde{\delta}_{\mathrm{TSAW}} > \tilde{\delta}_{\mathrm{RW}}$ leads to the result

$$\nu_B^{\mathrm{KGW}} > \nu_B^{\mathrm{SAW}} \quad \text{for } d < 6,$$
$$\nu_B^{\mathrm{KGW}} = \nu_B^{\mathrm{SAW}} \quad \text{for } d = 6 . \tag{12}$$

Substituting appropriate values of Eq. (7), we have $\nu_B^{\mathrm{KGW}} \approx 0.768$, which is only slightly greater than $\nu_B^{\mathrm{SAW}} \approx 0.758$. Since the value of ν_B^{SAW} is bounded below by the Flory value ν_F, the bounding interval for ν_B^{SAW} shrinks to the classical value $\frac{1}{2}$ as $d \to 6$.

In order to find numerical support for Eq. (7), we have generated KGW's on a square lattice at the percolation threshold using the ROLL algorithm of Honeycutt and Thirumalai [18]. The size of the lattice has been chosen such that the longest walk generated does not suffer from boundary effects. Every site is assumed to exist in one of the three states, blank (B) (yet to be decided), available (A) (neither occupied nor forbidden), or unavailable (U)

(not A), respectively. Initially, all the sites are in the B state. We start generating a KGW by first occupying the center of the lattice. At every stage in the growth process, we first decide the state of the nearest neighbor B sites, if there are any, by comparing a random number p $(0<p<1)$ with the (site-) percolation probability p_c $(=0.592\,745$ for the square lattice [19]). If $p>p_c$, then it becomes a U site; otherwise it becomes an A site. The growth of the walk proceeds by choosing one of the A sites at random. If no A site is available for further growth, then the lattice is cleared and a fresh walk begins from the center. The number of statistically independent cluster configurations sampled is clearly the same as the number of KGW's generated. Therefore, disorder averaging is automatically performed while we compute the mean square end-to-end distance $\langle R_N^2(N)\rangle$ or the radius of gyration $\langle S_N^2(N)\rangle$.

We have generated KGW's of lengths N ranging from 19 to 96 steps, and then calculated $\langle S_N^2(N)\rangle$, which has smaller statistical fluctuations than $\langle R_N^2(N)\rangle$. Out of the hundred million attempts made to generate them, only about two hundred walks survived up to 96 steps. For each value of N, we have not only computed $\langle S_N^2(N)\rangle$ and $\langle S_N^4(N)\rangle$, but also the fraction $f(N)$ of surviving KGW's. We have repeated this process ten times with different random seeds, and obtained the mean values.

We have calculated $\nu_P(N)$ values using Lam's recipe [4], and plotted them against $1/N$ in Fig. 1. We have used $\langle S^4(N)\rangle$ data and the standard error analysis techniques to estimate the error on $\nu_P(N)$. The exponent increases linearly in the region, $0.0315\geq 1/N\geq 0.0165$. A simple extrapolation would lead to a value $\nu_P^{\mathrm{KGW}}\approx 0.725\pm 0.007$. This compares well with the value (≈ 0.721) obtained by setting $D=d_f$, and substituting the value $\nu_P^{\mathrm{RW}}\approx 0.3484$ [14] in Eq. (7).

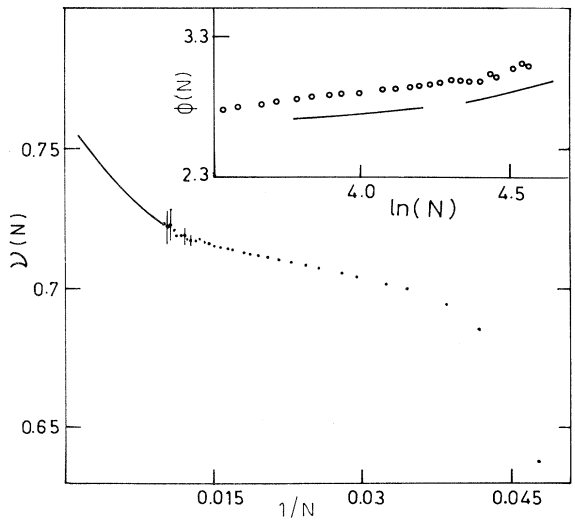

FIG. 1. $\nu(N)$ as a function of $1/N$. The curve drawn represents an attempt to extrapolate the data to the value, $\nu_B^{\mathrm{KGW}}\approx 0.768$. The inset represents a plot of $\Phi(N)\equiv -\ln[\nu_B^{\mathrm{KGW}}-\nu(N)]$ against $\ln(N)$. Solid lines with slopes 0.2 and 0.5, respectively, have been drawn to guide the eye.

However, the data show a definite trend to curve up in the region $1/N<0.0165$. This behavior is suggestive of a crossover to a higher value of ν. As mentioned earlier, the fraction of walks which survived up to 96 steps is of the order of two thousand in one billion. Hence it is difficult to obtain more accurate data in this crossover region without resorting to some sample enrichment scheme. We have already seen that setting D equal to the backbone dimension d_B in Eq. (7) yields the value $\nu_B^{\mathrm{KGW}}\approx 0.768$ in two dimensions. Even though our data in the region $1/N<0.0165$ show a definite tendency to curve up, they are not accurate enough for reliable extrapolation. Nevertheless, we have plotted $-\ln[\nu_B^{\mathrm{KGW}}-\nu(N)]$ against $\ln(N)$ in the inset of Fig. 1. Solid lines with slopes 0.2 and 0.5 have been drawn to guide the eye. We have attempted an extrapolation of the data using the formula [20], $\nu(N)\approx\nu_B^{\mathrm{KGW}}-(\Delta/2)BN^{-\Delta}$ with $\Delta\approx 0.6$ and $B\approx 3$, and indicated the same by an extrapolating curve. It may be noted that the attempted extrapolation, though not reliable, is quite compatible with the trend of the data.

This therefore represents the signature of a crossover in the asymptotic behaviour of KGW, with a crossover length $N_c\approx 60$. It will be extremely difficult to make a similar observation in three dimensions, because N_c could be of the order of thousands. Nevertheless, on the basis of this small scale simulation, we can say that there exists a crossover length beyond which the backbone influences the asymptotic behavior of KGW.

It may be noted that the formulas for ν_P^{KSW} and ν_P^{TSAW} [Eqs. (7) and (9)] are valid whatever the type of disorder—quenched or annealed. This follows from the general validity of the asymptotic scaling form of the probability distribution $P(r;N)$, given by Eq. (5). Therefore, the results obtained from these formulas will be valid for the kind of disorder to which corresponds the value of ν_P^{RW} used.

The ROLL algorithm, used in our simulations, may be said to generate different configurations of a *finite* walk at different locations of the *infinite* random medium. If we juxtapose one end of all the configurations, we see that they sample different random environments. With this mental picture, we expect that the effect of the annealed disorder might be washed out on the average. Recent

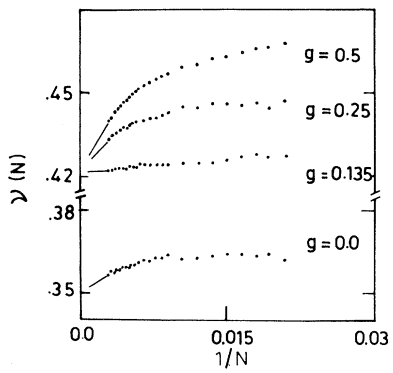

FIG. 2. $\nu(N)$ as a function of $1/N$ for TSAW.

studies [21,22], however, have indicated that constrained annealed disorder may have nontrivial effects on the behaviour of random walks with weak self-avoidance.

Using the ROLL algorithm, we have also generated one million TSAW configurations of length N ranging from 50 to 300 steps on a square lattice at the percolation threshold for $g=0.0$, 0.135, 0.25 and 0.5. We have calculated the values of $\nu(N)$ using Lam's procedure [4], and plotted them against $1/N$ in Fig. 2. A simple extrapolation of the data yields $\nu_P^{\mathrm{RW}} \approx 0.35$ for $g=0$, thus agreeing well with the quenched value (≈ 0.3484) reported in the literature [14]. The data for $g>0$ can all be extrapolated to the value $\nu_P^{\mathrm{TSAW}} \approx 0.422 \pm 0.005$, which compares fairly well with the value $\nu_P^{\mathrm{TSAW}} \approx 0.438$, obtained from Eq. (9) by substituting $\nu_P^{\mathrm{RW}} \approx 0.3484$. Accurate simulations with much longer walks may be necessary for making conclusive statements. However, for all practical purposes, our simulation data may be taken to correspond to quenched disorder.

To sum up, we have presented survival probability arguments that lead to generalized formulas for the end-to-end distance exponents of the SAW, KGW, and TSAW on a percolating cluster. In particular, ν_B^{SAW} has been shown to be bounded above by ν_B^{KGW} for $d<6$. Simulation data for KGW's on a two dimensional percolation cluster have been presented as numerical support for these formulas. The observation of a crossover in the asymptotic behavior of the KGW at a crossover length $N_c \approx 60$ has been interpreted as a numerical evidence of the fact that the KGW latches onto the backbone as it grows longer.

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[1] K. Kremer, Z. Phys. B **45**, 149 (1981).
[2] J. Lyklema and K. Kremer, Z. Phys. B **55**, 41 (1984).
[3] K. Barat and B. K. Chakrabarti, Phys. Rep. **258**, 377 (1995).
[4] P. M. Lam, J. Phys. A **23**, L831 (1990).
[5] P. Grassberger, J. Phys. A **26**, 1023 (1993).
[6] M. D. Rintoul, J. Moon, and H. Nakanishi, Phys. Rev. E **49**, 2790 (1994).
[7] S. B. Lee and H. Nakanishi, Phys. Rev. Lett. **61**, 2022 (1988); S. B. Lee, H. Nakanishi, and Y. Kim, Phys. Rev. B **39**, 9561 (1989).
[8] H. Nakanishi and S. B. Lee, J. Phys. A **24**, 1355 (1991).
[9] I. Majid, N. Jan, A. Coniglio, and H. E. Stanley, Phys. Rev. Lett. **52**, 1257 (1984).
[10] A. Coniglio, N. Jan, I. Majid, and H. E. Stanley, Phys. Rev. B **35**, 3617 (1987).
[11] K. Kremer and J. Lyklema, Phys. Rev. Lett. **55**, 2091 (1985).
[12] L. Pietronero, Phys. Rev. Lett. **55**, 2025 (1985).
[13] D. J. Amit, G. Parisi, and L. Peliti, Phys. Rev. B **27**, 1635 (1983); L. Pietronero, *ibid.* **27**, 5887 (1983); J. Bernasconi and L. Pietronero, *ibid.* **29**, 5196 (1984).
[14] S. Havlin and D. Ben Avraham, Adv. Phys. **36**, 695 (1987).
[15] D. Lhuillier, J. Phys. (Paris) **49**, 705 (1988).
[16] I. Chang and A. Aharony, J. Phys. (France) I **1**, 313 (1991).
[17] J. P. Bouchaud and A. Georges, Phys. Rev. B **39**, 2846 (1989).
[18] J. D. Honeycutt and D. Thirumalai, J. Chem. Phys. **93**, 6851 (1990).
[19] R. M. Ziff and B. Sapoval, J. Phys. A **19**, L1169 (1990).
[20] Z. V. Djordjevic, I. Majid, H. E. Stanley, and R. J. dos Santos, J. Phys. A **16**, L519 (1983).
[21] A. Baumgartner and B. K. Chakrabarti, J. Phys. (Paris) **51**, 1679 (1990).
[22] S. M. Bhattacharjee and B. K. Chakrabarti, Europhys. Lett. **15**, 259 (1991).