Self-Avoiding Walks on Diluted Networks

Yigal Meir[a]

Raymond and Beverly Sackler Faculty of Exact Sciences, School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel and Department of Nuclear Physics, Weizmann Institute, Rehovot 76100, Israel

A. Brooks Harris

Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104

(Received 29 June 1989)

It is shown that, contrary to recent suggestions, the exponent ν characterizing self-avoiding walks in a diluted lattice at the percolation threshold is determined by a fixed point different from the pure-lattice one. The full phase diagram of this system is obtained by a real-space renormalization-group treatment and five nontrivial fixed points are identified. A field-theoretical treatment yields $\nu=\frac{1}{2}+\epsilon/42$, with $\epsilon=6-d$. All these results are supported by exact enumeration analysis.

PACS numbers: 64.60.Ak, 05.40.+j, 05.70.Jk, 64.60.Kw

The problem of self-avoiding walks (SAW's) on diluted lattices, simulating linear polymers in quenched random disorder,[1] has been the subject of extensive research for more than a decade.[2-11] However, the main outstanding question in this topic is still unresolved; namely, does the disorder at the percolation threshold[12] induce a change in the asymptotic statistics of long SAW's? In this paper we answer this question affirmatively using several analytic and numerical approaches.

The statistics of SAW's are conveniently discussed in terms of the generating function $G(i,j;K)$, defined by $G(i,j;K)\equiv\sum_N C_N(i,j)K^N$, where $C_N(i,j)$ is the number of N-step SAW's between sites i and j and K is the fugacity of each step. It is easy to show[6,7] that in the presence of dilution, $[G(i,j;K)]_p$, where $[\,]_p$ denotes average over configurations in which each bond is occupied with probability p, is trivially given by $G(i,j;pK)$, i.e., the pure-system function with a renormalized fugacity. This result led to the claims[7] (for a review see Ref. 2) that disorder has only trivial effects. However, it is not clear how disorder affects the average end-to-end distance of N-step SAW's, $\langle R_N^2\rangle$, defined by[6]

$$\langle R_N^2\rangle=\left[\sum_j C_N(i,j)r_{ij}^2\Big/\sum_j C_N(i,j)\right]_p'\sim N^{2\nu},\qquad(1)$$

where r_{ij} is the geometrical distance between sites i and j and the prime indicates that the average is over all configurations which support at least one N-step SAW starting from site i. Equation (1) defines the SAW exponent ν. $\langle R_N^2\rangle$ is the quantity that has been studied by numerical simulations.[3,4,10,11] Early studies[3,5] concluded that for $p>p_c$, where p_c is the percolation threshold,[12] $\nu(p)=\nu(p=1)$, the pure-system value, which is equal to $\frac{3}{4}$ for $d=2$ dimensions and $\simeq 0.588$ for $d=3$. At $p=p_c$ those works indicated a larger exponent, $\nu(p=p_c)\simeq 0.77$ in 2D and $\simeq 0.65$ in 3D. Recently, Lee and Nakanishi[10] pointed out an error in Kremer's analysis,[3] which would have changed the original estimate to $\nu(p=p_c)\simeq 0.62$ in 3D, much closer to the pure-system value. Moreover, their extensive numerical simulation[10,11] suggested $\nu(p_c)=\nu(p=1)$, at least within the errors of their calculation.

In this Letter we use the renormalization group (RG) (both real space and momentum space) in conjunction with exact enumeration data to show that the exponent $\nu(p_c)$ is determined by a fixed point different from the pure-system one, leading to the conclusion that $\nu(p_c)\neq\nu(p=1)$. For $p>p_c$ our formulation gives $\nu(p_c)=\nu(p=1)$ as found previously.[3] In the following we denote $\nu(p=p_c)$ by ν. A detailed presentation of the results summarized below will be published separately.

In Fig. 1 we show the phase diagram obtained by a real-space RG calculation described below. Five nontrivial fixed points are identified. Points A (at $p=1$), B (at $p=p_c$), and C (at $p=0$) describe SAW's, respectively, on a pure lattice, at the percolation threshold, and on lattice animals,[12] i.e., clusters larger than the percolation correlation length, ξ_p. Interestingly, two other fixed points are found at $p=p_c$, D and E, corresponding to the maximal and minimal walks at the percolation threshold, respectively.

We construct a field theory describing SAW's at the percolation threshold. Using an ϵ expansion, with $\epsilon=6-d$, we find a fixed point at a critical value of K,

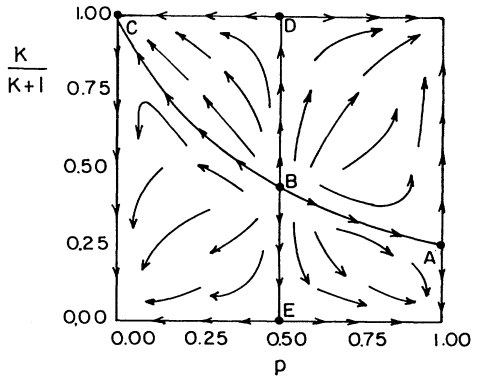

FIG. 1. Fixed points and RG flows for SAW's on a dilute lattice. The flows are defined by the recursion relations of Eq. (8) for p and for $\ln K$. The interpretation of the various fixed points is discussed in the text.

which is unstable with respect to both p and K, in agreement with Fig. 1. This treatment gives $\nu=\frac{1}{2}+\epsilon/42$. As discussed below, this value obeys the obvious bound $\nu_{\min}\geq\nu\geq\nu_{\max}$, where $\nu_{\min}$ and $\nu_{\max}$ describe the scaling of the minimal and maximal SAW's, respectively, at the percolation threshold.

Since $\langle R_N^2\rangle$ of Eq. (1) is not a convenient one to study within the framework of the field theory, we instead study N as a function of R, viz.,

$$[\bar{N}_{ij}(K)]_p\equiv\left[\frac{v_{ij}\sum_N NK^N C_N(i,j)}{\sum_N K^N C_N(i,j)}\right]_p\Big/[v_{ij}]_p$$
$$=\frac{\partial}{\partial(\ln K)}[v_{ij}\ln G(i,j;K)]_p/[v_{ij}]_p\,, \tag{2}$$

where v_{ij} is unity if i and j are connected in a given configuration and zero otherwise. $[\bar{N}_{ij}(K)]_p$ is the number of steps averaged over all SAW's between sites i and j restricted to be in the same cluster. As we shall see below, there is a critical value of K, denoted K_0, such that

$$[\bar{N}_{ij}(K_0)]_p\sim r_{ij}^{1/\nu}\equiv r_{ij}^{\phi/\nu_p}\,, \tag{3}$$

with ν_p the percolation correlation exponent. Hence, calculation of ϕ yields the required information on ν.

The main complexity of this model stems from the fact that, unlike the randomly diluted Ising Model,[13] the dilute x-y model,[14] or the random resistor network,[14,15] the first average in Eq. (2) cannot be decoupled. The decoupling in the cited models can be performed since in these models there exists a multicritical fixed point at $p=p_c$, where the correlation functions

$$G^{(k)}(p,T)\equiv\sum_j[\langle S_1(r_i)S_1(r_j)\rangle_T^k]_p \tag{4}$$

become critical simultaneously for all k. Here $S_1(r_i)$ is the first component of the spin at site i and $\langle\ \rangle_T$ denotes a temperature average with respect to the relevant Hamiltonian. Although the statistics of SAW's can be obtained[16] from the $n\to 0$ limit of the n-component Heisenberg-like Hamiltonian, the behavior of this model in the high-temperature regime, when diluted, is unique. Using the $1/\sigma$ expansion[17] to calculate the critical fugacity, $K_k(p)$, of the above correlation functions (here K plays the role of temperature), we find that for this model there is no such multicritical point in the p-K plane for all $G^{(k)}$. Thus, as pointed out by Derrida,[9] as either K or p changes, a series of transitions occur whenever a phase boundary for each $G^{(k)}$ is crossed. This is due to the exponential dependence of $C_N(i,j)$ on r_{ij}. Accordingly, we are led by Eq. (2) to study the correlation function

$$F(p,K)\equiv\sum_j[v_{ij}\ln G(i,j;K)]_p\,. \tag{5}$$

(A similar suggestion was made by Derrida.[9]) Expanding in powers of $\ln(K/K_0)$, one can write

$$F(p,K)=F(p,K_0)+\ln(K/K_0)\chi_p[\bar{N}(K_0)]_p$$
$$+O(\ln^2(K/K_0))\,, \tag{6}$$

where χ_p, the percolation susceptibility, is $\chi_p\equiv\sum_j[v_{ij}]_p$ and

$$\bar{N}(K_0)\equiv\sum_j[\bar{N}_{ij}(K_0)]_p[v_{ij}]_p/\chi_p$$

is essentially $\bar{N}_{ij}$ for $r_{ij}\sim\xi_p$. Here K_0 is chosen such that the first term on the right-hand side of Eq. (6) will be given asymptotically by $C_0\chi_p$, where C_0 is at most of order unity. In view of Eq. (3) we have to order $\ln(K/K_0)$,

$$F(p,K)\simeq C_0(p_c-p)^{-\gamma_p}[1+A\ln(K/K_0)(p_c-p)^{-\phi}]\,, \tag{7}$$

with γ_p the percolation susceptibility exponent and A a constant. Thus ϕ may be obtained as the crossover exponent associated with "turning on" the variable $\ln(K/K_0)$ near the fixed point $(p=p_c,\ K=K_0)$, in the same way as the crossover exponent for the dilute Ising model is obtained by turning on the variable $\exp(-J/kT)$ near the fixed point $(p=p_c,\ T=0)$. The physical meaning of K_0 (<1) is that it is determined such that it will exactly balance the exponential growth of $C_N(i,j)$ in typical configurations.

To illustrate the above idea, we have performed a cumulant real-space RG[18] (CRSRG) calculation on a Wheatstone bridge for the two variables p and $\ln K$ (which is equal to $\ln G$ for the renormalized bond), and obtained the recursion relations

$$p'=2p^2+2p^3-5p^4+2p^5\,, \tag{8a}$$
$$p'\ln(K')=4\ln(K)p^2+6\ln(K)p^3$$
$$+[\ln(2)-14\ln(K)+4\ln(K+1)]p^4$$
$$+[6\ln(K)-3\ln(K+1)]p^5\,. \tag{8b}$$

These recursion relations lead to the phase diagram displayed in Fig. 1. Points A $(p^*=1;\ K^*=0.366)$, B $(p^*=\frac{1}{2},\ K^*=0.788)$, and C $(p^*=0,\ K^*=\infty)$ correspond to SAW's on the pure lattice, SAW's at the percolation threshold, and SAW's on lattice animals, respectively. At the percolation threshold one has $\phi=\ln(\lambda_K)/\ln(\lambda_p)$, where $\lambda_K=\partial K'/\partial K$ and $\lambda_p=\partial p'/\partial p$ at the fixed point. We find $\lambda_p=\frac{13}{8}$ and $16\lambda_K=(34+39K^*)/(1+K^*)$. For point B, $\phi\sim 1.682$, leading to $\nu=\nu_p/\phi\sim 0.793$ (using[19] $\nu_p=\frac{4}{3}$). It should be noted that the corresponding recursion relation for $G^{(1)}$ $(=K)$, $p'K'=2p^2K^2+2p^3K^3$, can be totally decoupled, in terms of the variable pK, from the one for p (8a). This means that p_c plays no particular role in the scaling of $[G(i,j;K)]_p$ $(=G(i,j;pK))$, as discussed above and in Ref. 7.

An interesting (and desirable) consequence of the

CRSRG is the appearance of two other fixed points at the percolation threshold, corresponding to the minimal and maximal SAW's. Using the values $K^*=0$ and $K^*=\infty$, we find $\phi_{\min}\simeq 1.55$ and $\phi_{\max}\simeq 1.835$ in exact agreement with the direct evaluation of these exponents on the same structure.[18] The meaning of these fixed points is easy to understand. For large enough K ($K>K_0$), $G(i,j;K)$ is dominated by the contribution of the longest SAW, of $N_{\max}(i,j)$ ($\sim r^{\phi_{\max}/\nu_p}$) steps. Hence $[\ln G(i,j;K)]_p \sim r^{\phi_{\max}/\nu_p}$. This argument agrees with the results of Ref. 4, which obtained, for $K=1>K_0$, $\phi\simeq 2.09$ (compared to $\phi_{\max}=2.0+0.2$ from series analysis[20]), though we believe they misinterpreted their results. Similar arguments involving $\phi_{\min}$ may be used for $K<K_0$, where the minimal walk will dominate the sum. It should be noted that our approach is different from previous RSRG calculations.[5] Those concerned the renormalization of $G^{(1)}$, which has nothing to do[6] with $\langle R_N^2\rangle$.

The structure of the phase diagram was confirmed by exact enumeration studies. Series in general spatial dimension for $F(p,K)$ were constructed to eleventh order in p and analyzed by the nonhomogeneous differential Padé approximants[21] for their exponents. These exponents exhibit a crossover from $\gamma_p+\phi_{\min}$ for small K to $\gamma_p+\phi_{\max}$ at large K in all dimensions, as expected from Eq. (6), with $\phi_{\min}$ and $\phi_{\max}$ agreeing with previous estimates.[20] Similar crossover phenomena occur for the exponents obtained by the analysis of the series generated for $[\bar{N}(K)]_p$. Other results from the series analysis will be mentioned below.

Having established the above phase diagram, we now construct a field theory to describe the scaling of $[\ln G]_p$ near the fixed point B. To do this we study the recursion relations for $G^{(k)}$ for $k\to 0$, because

$$G^{(k)}(p,K)\equiv\sum_j [v_{ij}G(i,j,K)^k]_p = \chi_p + kF(p,K)+O(k^2)\,. \tag{9}$$

To treat dilution we start from the m-replicated version of the n-component Heisenberg-like model Hamiltonian for which

$$\exp(-\beta H^{(n,m)})=\left[\exp\left\{-\tfrac{1}{2}K\sum_{ij}\epsilon_{ij}\sum_{\alpha=1}^{n}\sum_{\beta=1}^{m}S_\alpha^\beta(r_i)S_\alpha^\beta(r_j)\right\}\right]_p, \tag{10}$$

where $\epsilon_{ij}=1$ if the nearest-neighbor bond i-j is occupied and is zero otherwise. Introducing fields $\Psi_k(\alpha_1,\alpha_2,\ldots,\alpha_k;\beta_1<\beta_2<\cdots<\beta_k;\mathbf{r})$ conjugate to $\prod_{j=1}^k S_{\alpha_j}^{\beta_j}(\mathbf{r})$ by a Stratonovich transformation and passing to the continuum limit, we obtain the effective Hamiltonian in terms of the Ψ fields up to order Ψ^3 as

$$-\beta H_{\rm eff}=\tfrac{1}{2}\int d^dq\sum_k[r_k^{(0)}+q^2]\Psi_k(q):\Psi_k(-q)+\tfrac{1}{6}w\int d^dr\,\Psi^3(r)\,, \tag{11}$$

where $\Psi_k(q)$ is the Fourier transform of $\Psi_k(r)$ and $\Psi_k(q):\Psi_k(-q)$ denotes an inner product,

$$\Psi_k(q):\Psi_k(-q)=\sum_{\alpha_1,\alpha_2,\ldots,\alpha_k}\ \sum_{\beta_1<\beta_2<\cdots<\beta_k}|\Psi(\alpha_1,\ldots,\alpha_k;\beta_1,\ldots,\beta_k;q)|^2\,. \tag{12}$$

The meaning of $\Psi^3(r)$ is similar to that for the dilute Ising model, namely the only cubic terms allowed are those for which all pairs (α,β) of replica labels appear either twice or not at all. However, there is a sum from 1 to n over each α index, which means that in a diagrammatic perturbation theory, if a replica label (α,β) only appears on internal propagators, the sum over the associated α will be zero and thus such a diagram need not be kept. The recursion relations are obtained following the scheme of Ref. 22, in close parallel with the dilute Ising model[13] and the dilute xy model.[14] We find

$$\frac{dr_k}{dl}=(2-\eta)r_k+\frac{2\epsilon}{7}G_kG_0-\frac{\epsilon}{7}\sum_{s=0}^{\infty}\frac{k!}{K-s!s!}G_sG_{k-s}\,, \tag{13}$$

where G_k is the propagator associated with $\langle\Psi_k(q)\times\Psi_k(-q)\rangle$ and $\eta=-\epsilon/21$. To get Eq. (13) we added and subtracted the terms with $s=0$ and $s=k$ which are not allowed (if there are no replicas, there is no propagator) and we set w equal to its fixed point value, $w=2\epsilon/7$. Also in Eq. (13) the sum over s was extended from 0 to ∞ since the summand vanishes for $s>k$, the original upper limit of the sum. As usual[22] we set $G_k=(1+r_k)^{-1}$ and we only need to keep track of terms up to linear order in the small parameter r_k. For $k=0$, Eq. (13) reduces to that for percolation and gives[23] $1/\nu_p=2-5\epsilon/21$. We now set $r_k=r_0+ku$, for small k, and obtain the recursion relation for u by taking the $k\to 0$ limit of Eq. (13). We obtain

$$\frac{du}{dl}=\left(2-\eta-\frac{\epsilon}{7}\right)u+\frac{\epsilon}{7}\sum_{s=1}^{\infty}\frac{1}{s}(-1)^sG_sG_{-s}\,, \tag{14}$$

which is of the form $d(u-u_c)/dl=(u-u_c)/\nu$, where u_c, which should be identified with $\ln(K_0)$, has fluctuation corrections at order ϵ and $\nu=\frac{1}{2}+\epsilon/42$. This value lies midway between the bounds for the exponents for the shortest and longest walks, which are given by[24,25] $\nu_{\min}=\frac{1}{2}+7\epsilon/168$ and $\nu_{\max}=\frac{1}{2}+\epsilon/168$. Moreover, independently of our result, the assumption that $\nu(p=p_c)=\nu(p=1)$ violates this bound in first order in ϵ, since $\nu(p=1)=\frac{1}{2}$ for $d>4$.

Furthermore, we have used exact enumeration to study $[\overline{N}(K)]_p$ from which we obtain the following values of ν: 0.76 ± 0.08, 0.67 ± 0.04, 0.63 ± 0.02, and 0.54 ± 0.02 for $d = 2$, 3, 4, and 5, respectively, which exclude the pure-lattice values for $d > 2$. The 2D value agrees well with the CRSRG result, $\phi \simeq 0.793$. The series estimates are well controlled by the fact that they are in the crossover regime between the known values[20] of $\nu_{\min}$ and $\nu_{\max}$.

In view of Eqs. (6) and (7) and the above discussion, one obtains the scaling representation, valid near the critical point at $(p = p_c, K = K_0)$:

$$F(p,K) = C_0(p_c - p)^{-\gamma_p} f\left[\frac{\ln(K/K_0)}{(p_c - p)^{\psi}}\right]. \quad (15)$$

Consequently, all cumulants of $[\overline{N}(K)]_p$ (e.g., $[\overline{N^2} - \overline{N}^2]_p$) scale with a constant gap exponent. This was verified by our series analysis, substantiating further our detailed picture of this critical point. Interestingly, a constant gap was found in Ref. 4 for the positive moments for $K = 1$, well above the critical point.

To conclude, we have shown that, unlike recent suggestions, SAW's at the percolation threshold are described by an exponent different from the pure-system value. We have constructed real-space and momentum-space renormalization-group treatments which elucidate for the first time the nature of the scaling of SAW's on percolating clusters. Accordingly, we feel that we have provided a satisfactory resolution of this long-standing problem.

We acknowledge helpful discussions with A. Aharony. This work was supported by grants from the U.S.-Binational Science Foundation and from the Israel Academy of Sciences and Humanities. The work done at the University of Pennsylvania was supported in part by the National Science Foundation under Grants No. DMR 85-19509 and No. DMR 88-15469. A.B.H. acknowledges the hospitality of Tel Aviv University and the Sackler Institute of Solid State Physics.

[a]Present address: Department of Physics, MIT, Cambridge, MA 02139.

[1]P. G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell Univ. Press, Ithaca, 1979); P. J. Flory, *Principles of Polymer Chemistry* (Cornell Univ. Press, Ithaca, 1969).

[2]A. K. Roy and B. K. Chakrabarti, J. Phys. A **20**, 215 (1987), and references therein.

[3]K. Kremer, Z. Phys. B **45**, 149 (1981).

[4]L. Furuburg, A. Aharony, J. Feder, and T. Jossang, in *Time-Dependent Effects in Disordered Materials,* edited by R. Pynn and T. Riste (Plenum, New York, 1987).

[5]A. K. Roy and B. K. Chakrabarti, Phys. Lett. **91A**, 393 (1982); P. M. Lam and Z. Q. Zhang, Z. Phys. B **56**, 155 (1984); M. Sahimi, J. Phys. A **17**, L379 (1984).

[6]J. Lyklema and K. Z. Kremer, Z. Phys. B **55**, 41 (1984).

[7]A. B. Harris, Z. Phys. B **49**, 347 (1983).

[8]Y. Kum, J. Phys. C **16**, 1345 (1983).

[9]B. Derrida, Phys. Rep. **103**, 29 (1984).

[10]S. B. Lee and H. Nakanishi, Phys. Rev. Lett. **61**, 2022 (1988).

[11]S. B. Lee, H. Nakanishi, and Y. Kim, Phys. Rev. B **39**, 9561 (1989).

[12]D. Stauffer, Phys. Rep. **54**, 1 (1979).

[13]M. J. Stephen and G. S. Grest, Phys. Rev. Lett. **38**, 567 (1977).

[14]A. B. Harris and T. C. Lubensky, Phys. Rev. B **35**, 6964 (1987).

[15]A. B. Harris and A. Aharony, Phys. Rev. B **40**, 7230 (1989).

[16]P. G. de Gennes, Phys. Lett. **38A**, 339 (1972).

[17]M. E. Fisher and D. S. Gaunt, Phys. Rev. **133**, A224 (1964); A. B. Harris, J. Phys. A **20**, L1011 (1987).

[18]D. C. Hong and H. E. Stanley, J. Phys. A **16**, 2525 (1983); Y. Meir and A. Aharony, Phys. Rev. A **37**, 596 (1987).

[19]M. P. M. de Nijs, J. Phys. A **12**, 1857 (1979).

[20]For estimates of $\phi_{\min}$ see Y. Meir, R. Blumenfeld, A. Aharony, and A. B. Harris, Phys. Rev. B **34**, 3424 (1986), and references therein; for estimates of $\phi_{\max}$ see Y. Meir, R. Blumenfeld, A. B. Harris, and A. Aharony, Phys. Rev. B **36**, 3950 (1987).

[21]J. L. Gammel, in *Padé Approximants and Their Applications,* edited by B. R. Graves-Morris (Academic, New York, 1973).

[22]J. Rudnick and D. R. Nelson, Phys. Rev. B **13**, 2208 (1976).

[23]A. B. Harris, T. C. Lubensky, W. K. Holcomb, and C. Dasgupta, Phys. Rev. Lett. **35**, 327 (1975); **35**, 1397(E) (1975).

[24]J. Cardy and P. Grassberger, J. Phys. A **18**, L267 (1985); K. H. Janssen, Z. Phys. B **58**, 311 (1985).

[25]A. B. Harris, Phys. Rev. B **35**, 5056 (1987), gives the crossover exponent ϕ (α) to order ϵ for the nonlinear random resistor network with $V = rI^{\alpha}$. For $\alpha \to 0^+$ (0^-), ϕ (α) is identical to $\phi_{\min}$ ($\phi_{\max}$) as discussed in R. Blumenfeld, Y. Meir, A. Aharony, and A. B. Harris, J. Phys. A **19**, L791 (1986).