Diffusion with a topological bias on random structures with a power-law distribution of dangling ends

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We study diffusion with a topological bias on random structures having dangling ends whose length L is chosen from a power-law distribution $P(L)\sim L^{-(\alpha+1)}$. We find that the mean-square displacement $\langle x^2\rangle$ of a random walker on the backbone varies asymptotically as $\langle x^2\rangle\sim(\log t)^{2\alpha}$, slower than any power of t, in contrast with $\langle x\rangle\sim t$, the conventional result for a nonrandom lattice. Our predictions are confirmed by numerical simulations for percolation and for the random comb.

How are the laws of physics for random materials different from those for ordered ones? This question has been the object of great current study. In general, laws of diffusion in random media have been characterized by power-law relations of the form[1–4]

$$\langle x^2\rangle\sim t^{2/d_w} . \tag{1}$$

Here d_w represents the fractal dimension of the walk. For diffusion on a nonrandom lattice structure, $d_w=2$ and (1) reduces to Fick's law of diffusion. For random structures, $d_w\neq 2$; rather d_w depends sensitively on the nature of the random structure. Accordingly, it is of considerable interest to find which features of the random structure determine d_w and which features are irrelevant.

In this Brief Report we study how the laws of diffusion are changed under the influence of a "topological" bias field E. We find that the distribution of dangling ends in the random structure is a relevant feature which characterized the diffusion. Specifically, we consider here a topological random comb with a power-law distribution

$$P(L)\sim L^{-(1+\alpha)},\ \ \alpha>0 , \tag{2}$$

of the length L of the teeth ("dangling ends"). We find that the (asymptotic) laws of diffusion are changed from the *power* law (1) to the *logarithmic* form

$$\langle x^2\rangle\sim\left[\frac{\log t}{A(E)}\right]^{2\alpha} , \tag{3}$$

where $\langle x^2\rangle$ is the mean-square displacement of the random walker along the backbone of the comb. We argue that the rigorous result may also be relevant for the incipient infinite cluster at the percolation threshold. Indeed a logarithmic form for $\langle x^2\rangle$ was suggested by Stauffer from numerical simulations results in this case.[5]

The topological bias is introduced as follows: every bond experiences the topological bias field E which drives the walker away from the source. Consequently the walker has an enhanced probability $p_+\propto(1+E)$ that the next step increases the topological pathlength to the source, and a decreased probability $p_-\propto(1-E)$ that the next step decreases the topological path length to the source (Fig. 1). Note that for a topological bias (in contrast to a Pythagorean bias[5–11]), the random comb is similar to a percolation cluster above p_c, since for both structures the topological bias drives a random walker toward the tips of the dangling ends. Such a situation might arise for diffusion inside a porous medium when a pressure source exists at one point.

To obtain (3), we note that the average time τ a random walker spends on a dangling end of length L scales as[7,12]

$$\tau\sim\left[\frac{1+E}{1-E}\right]^L\equiv e^{\lambda L} . \tag{4}$$

Correspondingly the transition probability W to pass by a dangling end on the backbone in the direction of the bias field scales as $W\sim\tau^{-1}\sim e^{-\lambda L}$. Combining (2) and (4), we find that the probability distribution $P(W)$ of

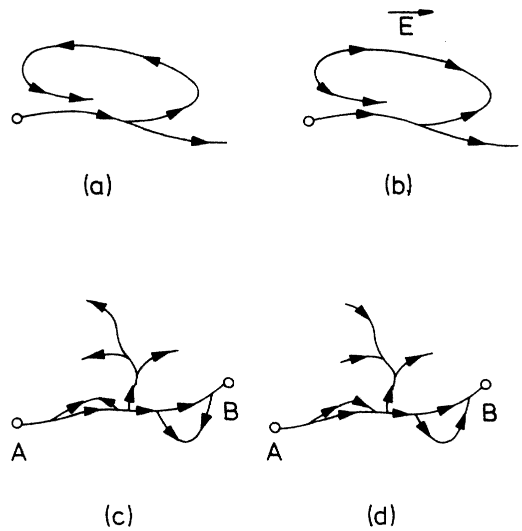

FIG. 1. Illustration of the differences between topological bias and Pythagorean bias. The arrows represent the direction of the bias field along the shortest path (a) for topological bias, (b) for Pythagorean bias. Figures (c) and (d) represent the same, respectively, for a part of the incipient infinite cluster. Note that every dead end and longer path along the shortest path between the two points A and B delays the topological bias diffusion, (a) and (c), similar to the random comb problem.

transition rates along the backbone is given by

$$P(W)\sim\frac{1}{W(\log W)^{1+\alpha}} . \tag{5}$$

Now consider the time t the walker needs to pass by l dangling ends on the backbone, under the influence of the topological bias. Since the dominant contribution is from the "random delays" arising from the dangling ends, we can neglect the time the walker spends on the backbone. Along the backbone in the direction of the field, the number of sites visited is proportional to the number of distinct visited sites (see also Ref. 13). Hence

$$t\sim\sum_{i=1}^{l}\tau_i\sim l\int_{W_{\min}}^{1}\frac{dW}{W^2(\log W)^{1+\alpha}} . \tag{6}$$

It can be shown[14] that for the distribution (5),

$$W_{\min}\sim\exp[-A(E)l^{1/\alpha}] , \tag{7a}$$

where

$$A(E)\sim\log[(1+E)/(1-E)] . \tag{7b}$$

Solving (6) with (7a), we obtain that asymptotically $t\sim\exp[A(E)l^{1/\alpha}]$. Hence

$$l^{1/\alpha}\sim\log t/A(E) , \tag{8}$$

from which (3) follows. For testing (8) we have carried out computer simulations of random walks on random combs with various α and E values using the exact enumeration method.[15] Our results are in striking agreement with (8). Figure 2 shows representative results for $\alpha=2$ for several values of E.

An interesting application of the above idea is to percolation, especially since it is widely believed that the dangling ends obey the distribution (2). As noted in Ref. 12, under the influence of a *topological* bias, a random comb and a percolation cluster should be similar. The effect of branching and loops in the dangling ends as well as longer paths on the backbone can be taken into account by introducing an effective dead-end length with replaces L in Eqs. (2) and (4). The analogy between the structure of a random comb and a percolation cluster is more plausible in higher dimensions, since the role of loops is less pronounced. Above $d=6$, loops are irrelevant, so we studied numerically the incipient infinite in percolation, *both* for $d=2$ and for the Cayley tree ($d\geq 6$).

For both cases we obtain best agreement with (8) for the choice $\alpha=1$ (Figs. 3 and 4). This finding can be understood for the Cayley tree: A random walker along the backbone of the incipient infinite cluster is trapped along

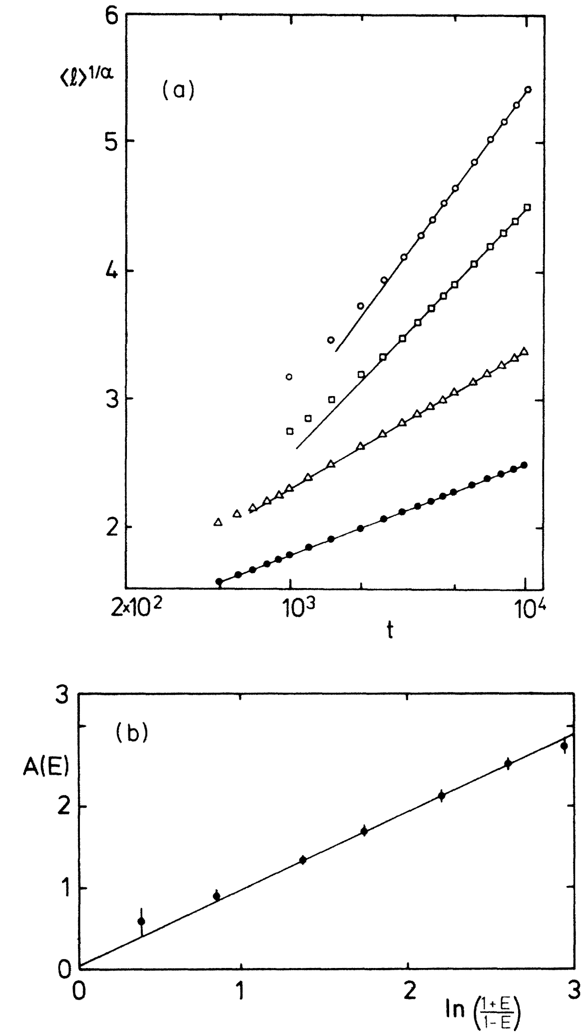

FIG. 2. (a) Plot of $l^{1/\alpha}$ vs $\ln t$ on the random comb with $\alpha=2$ for different values of bias fields: ● ($E=0.9$), △ ($E=0.7$),($E=0.4$), ○ ($E=0.2$). The lines represent the best asymptotic straight lines. (b) The points represent the inverse of the slopes presented in (a) and the line represent the theory [Eq. (7b)]. For our calculations we generated combs of size $l=300$ and averaged over 100 configurations each.

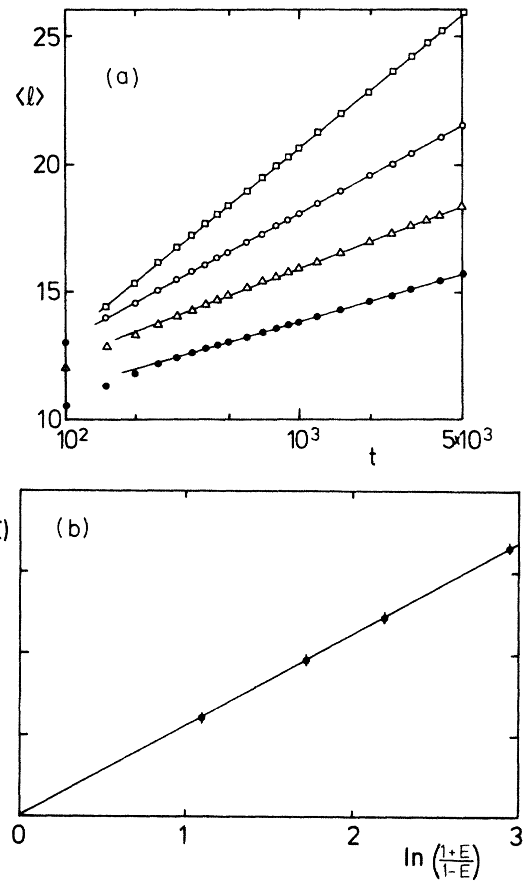

FIG. 3. (a) Plot of l vs $\ln t$ on percolation clusters generated on a Cayley tree at criticality, for different values of bias fields: ● $(E=0.9)$, △ $(E=0.8)$, ○ $(E=0.7)$,$(E=0.5)$. The solid lines are best straight lines. (b) The points represent the inverse of the slopes presented in (a) and the line represents the theory [Eq. (7b)]. For our calculations we generated clusters up to 200 shells and averages were made over 100 configurations.

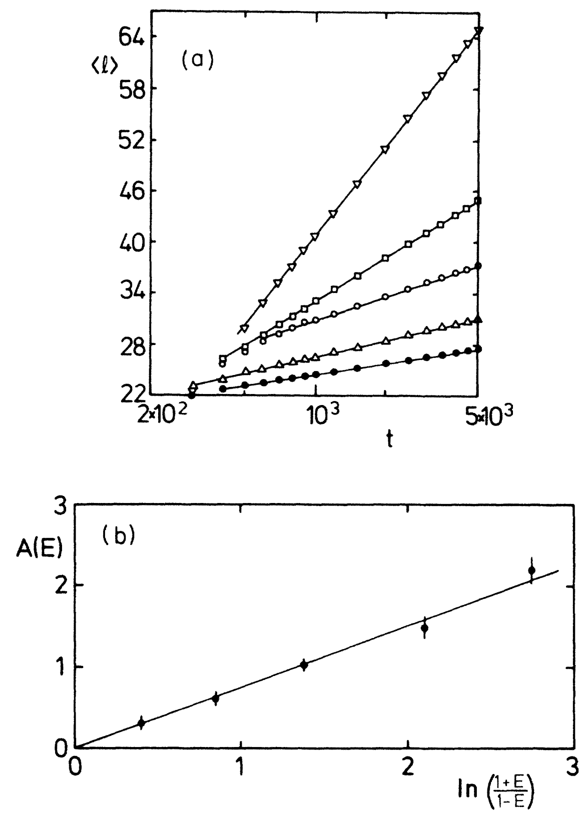

FIG. 4. (a) Plot of l vs $\ln t$ on percolation clusters generated in $d=2$ at criticality, for different values of bias fields: ● $(E=0.9)$, △ $(E=0.8)$, ○ $(E=0.7)$,$(E=0.5)$. The solid lines are best straight lines. (b) The points represent the inverse of the slopes presented in (a) and the line represents the theory [Eq. (7b)]. For our calculations we generated clusters up to 200 shells and averages were made over 100 configurations.

its way be dangling ends whose mass distribution is given by[16] $P_0(S) \sim S^{-\tau+1}$ with $\tau=\frac{5}{2}$. Now the pathlength L is related to the mass S by $S \sim L^2$. Hence

$$P(L)=P_0(S)(dS/dL) \sim L^{2(1-\tau)+1} \sim L^{-2} . \quad (9)$$

Comparing (2) and (9), we see that $\alpha=1$ for the Cayley tree. For $d=2$, loops are relevant, so the argument leading to (9) fails; indeed, if we were to use (9), we would predict $\alpha \simeq 0.1$, while we find $\alpha \simeq 1.0$.

We conclude with several remarks.

(i) It is interesting to compare our result with recent findings for *other* types of probability distribution for the dangling ends. In the case of an exponential distribution, $P(L) \sim \exp(-bL)$, it was found[12] that the diffusion was characterized by power-law relations and a dynamic phase transition. Below a critical field E_c, diffusion is classical and $d_w=1$. Above E_c, diffusion is anomalous and d_w increases continuously with E.

(ii) Our result (8) seems to be independent of the dimension of the backbone of the comb, since the argument leading to (8) also hold for higher dimensions of the backbone. However, in the case of a bias field only in the direction of the teeth, (8) *will* depend on the backbone dimension. Similar arguments as above lead to

$$l^{1/\alpha} \sim \frac{\log t}{A(E)}, \quad d=1 \quad (10a)$$

and

$$l^{2/\alpha} \sim \frac{\log t}{A(E)}, \quad d \geq 2 . \quad (10b)$$

(iii) The integral (6) leads to logarithmic corrections to the leading behavior of (8): to the left-hand side of (8) should be added a term proportion to $\log t$.

(iv) Sinai[17] has recently considered a random bias-field model in $d=1$: the bias field on each bond is a random variable chosen from a distribution with zero mean. Sinai obtains $\langle x^2 \rangle \sim (\log t)^4$, *just as we do for our model* in the case $\alpha=2$. The physical parallels between the two models are striking, since our random walkers spend a long time in the dangling ends, while Sinai's random walkers spend a long time in "compensated regions" where bonds of opposite bias point to the same lattice site. It would be interesting to attempt to relate the two models, and this is an object for present investigation.

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[14]In order to calculate $W_{\min}$ we estimte $L_{\max}$ which is the average "maximum length" of dangling ends for a system of size l. We choose x so that $p(L)dL \sim 1 \cdot dx$ from which follows $x \sim L^{-\alpha}$. Since x is an homogeneous random variable we expect $x_{\min} \sim 1/l$ and thus $L_{\max} \sim l^{1/\alpha}$. Substituting this result in (4) we obtain (7a).

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