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Diffusion in random structures with a topological bias

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We study biased diffusion on a topological random comb with an exponential distribution of dangling ends which is relevant to the essential physics of biased diffusion in random structures such as percolation systems above criticality. By mapping the problem onto a linear chain with a power-law distribution of transition rates we find that above a bias threshold, diffusion is anomalous in two respects: d_w (the fractal dimension of a random walk) is above 1, and depends continuously upon the magnitude of the bias. Our analytic results are confirmed by extensive computer simulations.

How are the laws of transport changed when the system of interest is not uniform but random? This physics question of general interest has recently attracted researchers in various scientific disciplines; the spectrum ranges from intercalation fronts in solids and oil extraction from porous rocks to the physics of aggregates and amorphous materials.[1-4]

In this Brief Report, we study the effect of a constant bias field on the diffusion properties in random systems. We consider a topological variant of the random comb model that encompasses essential features of random structures, yet is simple enough to be treated rigorously and thus is able to display the richness of the problem. In this model, a "pressure" source at one point of the random medium gives rise to a "topological" bias rather than a "Pythagorean" bias (see Fig. 1). While much progress has occurred recently in understanding the physics of *non-biased* diffusion in random structures,[5-9] the physics of *biased* diffusion is not yet understood.[10-17] Here we study analytically and numerically the mean length $l(t)$ of the path (chemical distance) a random walker travels in time t on the random structure under the influence of a topological bias field. By *mapping* this problem to the problem of biased diffusion on a linear chain with a power-law distribution of transition rates we find that the results for the diffusion exponent d_w^l defined by

$$t \sim l^{d_w^l} \tag{1}$$

are significantly different from unbiased diffusion in random media, and also are different from biased diffusion in a Euclidean network.

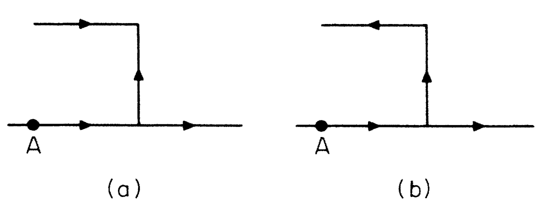

FIG. 1. Comparison between (a) Pythagorean bias and (b) "topological" bias for a simple structure. The pressure source is at A. In (b), every point in the flow experiences a field E to "move away" in chemical distance (or path length) from the origin. The arrows denote the direction of the local bias in each bond.

In contrast to biased diffusion on a uniform Euclidean network, where even the slightest field changes d_w^l from 2 to 1, there exists a critical bias field $E=E_c$. We find that below E_c, d_w^l has the constant value $d_w^l=1$, but for $E>E_c$, d_w^l increases *continuously* with E. Our results concern the following model, which is a topological variant of the random comb structure (Fig. 2). Choose two points A and B at random on this structure, one of which (A) shall be the source of a bias field. Consider now the minimum path between A and B, from which emanate many dangling ends of all possible sizes and shapes. The length L of each dangling end is a random variable chosen from the distribution function

$$P_0(L) \propto \lambda^L \equiv e^{-bL} , \tag{2}$$

where $0<\lambda<1$ is a tunable parameter. Our choice for

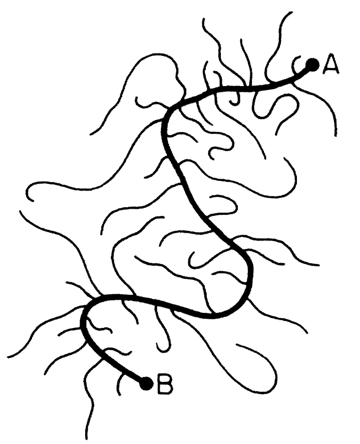

FIG. 2. Typical random structure considered in this work. Two points A and B are chosen at random and a pressure field is applied at one of them (A). The bonds on the minimum path between A and B are termed the backbone, while the remaining bonds constitute the dangling ends. In our model, the length L of each dangling end is chosen from the probability distribution (2).

the distribution (2) is motivated by the distribution of dead ends in percolation (for $p > p_c$) which is believed to have an exponential behavior on large length scales. Of course, the incipient infinite cluster in percolation—a standard model for porous media—has loops in the backbone and loops and branches in the dangling ends. However, we shall argue below that such features do not affect our results, and we believe our model reflects much of the essential physics of *biased* diffusion in random media.

The topological bias is introduced as follows: Every bond experiences the (constant) 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 path length 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), 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.

Our goal is to calculate transport along the backbone from A to B, which is an effective one-dimensional system. The physical effect of a set of dangling ends is to provide a set of random delays along the backbone, each with a characteristic time $\tau(L)$. To calculate $\tau(L)$, we consider a walker on a dangling end of length L at a chemical distance j from the backbone. Let T_j be the mean first time to reach the backbone and note that $T_1 \propto \tau$. It can be shown[18] that T_j satisfies the recursion relation

$$T_j - 1 = \tfrac{1}{2}(1-E)T_{j-1} + \tfrac{1}{2}(1+E)T_{j+1} , \tag{3a}$$

subject to the boundary conditions[19]

$$T_{j=0} = 0, \; T_L = T_{L-1} + 2/(1-E) , \tag{3b}$$

since $j=0$ and $j=L$ are "absorbing" and "reflecting" points, respectively. We solve for T_1 with the result

$$T_1 = \frac{1}{E}\left[\left(\frac{1+E}{1-E}\right)^L - 1\right] . \tag{4a}$$

The behavior is dominated by the long dangling ends, so we consider the asymptotic limit (see also Ref. 12)

$$\tau \sim T_1 \sim \left(\frac{1+E}{1-E}\right)^L , \; (L \gg 1) . \tag{4b}$$

The transition rate $W(L)$ to pass by this dangling end (on the backbone) is given by the reciprocal of the mean time $\tau(L)$ spent in a dangling end of length L. Hence from (4b),

$$W(L) \sim \left(\frac{1-E}{1+E}\right)^L \equiv e^{-cL} . \tag{5}$$

The rates $W(L)$ are random variables whose probability distribution $P(W)$ is directly related to the distribution $P_0(L)$ for finding a dangling end of length L. Since $P(W) = P_0(L)dL/dW$ we obtain from (2) and (5) that $P(W)$ follows a power law distribution

$$P(W) \sim W^{-\alpha} , \tag{6}$$

where

$$\alpha = 1 - b/c = 1 - \ln\lambda / \ln[(1-E)/(1+E)] .$$

By this, the problem of biased diffusion on the random comb structure is mapped rigorously to the problem of biased diffusion on a linear chain with a power-law distribution of transition rates, Eq. (6).

Now consider the effect of this transition rate distribution on biased diffusion. Hence we consider the time t_{AB} to walk from A to B under the influence of the bias field

$$t_{AB} \sim \sum_{i=1}^{N_{AB}} \tau_i \sim \sum_{i=1}^{N_{AB}} \frac{1}{W_i} . \tag{7}$$

Here the sum runs over all the N_{AB} dangling ends which emanate from the backbone between A and B. Note that in our model N_{AB} is proportional to the length l_{AB} of the path between both points. From (6) and (7) we obtain (see also Ref. 20)

$$t_{AB} \sim l_{AB} \int_{W_{\min}}^{1} \frac{dW}{W} P(W) \sim l_{AB} W_{\min}^{-\alpha} . \tag{8}$$

This result holds for $\alpha > 0$ when the integral is dominated by the lower integration limit. For $\alpha \le 0$, we recover the result for uniform Euclidean lattices $t_{AB} \sim l_{AB}$ with a logarithmic correction when $\alpha = 0$. Since $W_{\min}$ depends on l_{AB} via[21] $W_{\min} \sim l_{AB}^{-1/(1-\alpha)}$, we obtain $t_{AB} \sim l_{AB}^{d_w^l}$, with

$$d_w^l = \begin{cases} 1 + \dfrac{\alpha}{1-\alpha}, & 0 \le \alpha < 1 , \\ 1, & \alpha < 0 . \end{cases} \tag{9}$$

We have also considered a somewhat different model in which the topological bias is not operative along the backbone bonds. Following a similar approach, we have calculated the conductivity Σ between A and B. Using the Einstein relation $D \sim l_{AB}\Sigma$ between Σ and the diffusion constant $D \sim l_{AB}^2/t_{AB}$, we find

$$d_w^l = \begin{cases} 2+\dfrac{\alpha}{1-\alpha}, & 0 \le \alpha < 1 \ , \\ 2, & \alpha < 0 \ . \end{cases} \tag{10}$$

The results for both models can be summarized as follows:

$$d_w^l = \begin{cases} d_w^0, & E < E_c(\lambda), \\ d_w^0 + \dfrac{\ln[(1-E)/(1+E)]}{\ln\lambda} - 1, & E > E_c(\lambda), \end{cases} \tag{11a}$$

where d_w^0 is the diffusion exponent in the absence of dangling ends. The critical topological bias field, corresponding to $\alpha = 0$, is given by (see also, Refs. 10 and 12)

$$E_c(\lambda) = \frac{1-\lambda}{1+\lambda} \ . \tag{11b}$$

Equations (11a) and (11b) represent the main results of this Brief Report. To test them, we have performed extensive numerical studies of biased diffusion on a topologically random comb. We have used the exact enumeration method, which provides excellent statistics in other problems.[6,22] We calculated the diffusion exponent d_w^l for a range of bias fields E and for different distributions of the dangling ends [characterized by the parameter λ of Eq. (2)]. Results for three values of λ are shown in Fig. 3. The curves for $\lambda = \frac{1}{3}$ and $\frac{1}{2}$ are for the present model, while the curve for $\lambda = \frac{2}{3}$ is for the second model in which there is no topological bias along the backbone bonds. The agreement shown is striking, particularly in view of the fact that there are no adjustable parameters in the theoretical expression.

In summary, then, we have obtained an analytic expression for the diffusion exponent d_w^l for a system designed to mimic biased transport in random media, such as those modeled by percolation theory. The diffusion exponent d_w^l "sticks" at its uniform Euclidean value for all values of E up to a bias threshold $E = E_c$. Above E_c, d_w^l increases continuously with the bias field E, becoming infinite only as $E \rightarrow 1$. Thus a particle is completely "trapped" only in the limit of perfect bias ($E = 1$). A second trapping limit is when $\lambda \rightarrow 1$, which represents the case $\langle L \rangle \rightarrow \infty$. This result explains Stauffer's recent finding[15] that $d_w \rightarrow \infty$ for percolation at criticality, where dangling ends have $\langle L \rangle = \infty$. The dangling ends of our model (Fig. 2) have no loops or branches, in contrast to real random media. However, we can argue that *for a topological bias* loops and branchings can be taken into account by assigning an effective mean length L_{eff} for the dangling ends. In percolation, L_{eff} depends only on the concentration of the random material and decreases with increasing p. For each concentration p, we expect, therefore, that d_w^l increases with

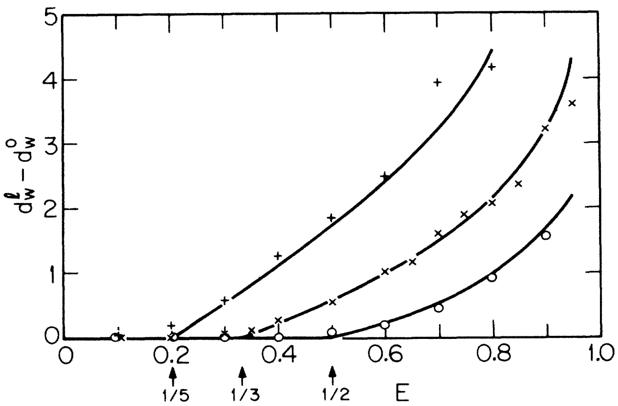

FIG. 3. Dependence on bias "topological" parameter E of the departure of d_w from its value for an unbiased system. The curve $\lambda = \frac{1}{3}$ and $\frac{1}{2}$ (○ and ×) for the present model, while the curve for $\lambda = \frac{2}{3}$(+) is for the second model in which there is no topological bias along the backbone bonds.

the bias field E in the predicted way, Eqs. (11), where $1/\ln\lambda$ has to be replaced by L_{eff} now. Accordingly, even though our rigorous results for the diffusion exponent are for an idealized model of random media, they also describe the physical situation in the more realistic percolation model, which so far could not be solved exactly.[23]

The interesting feature of our result is that a critical exponent (the diffusion exponent d_w^l) is independent of a system parameter (the bias field E) over a wide range of E values. Specifically, d_w^l sticks at its classical value $d_w^l = 1$ (a Euclidean lattice) for all E less than a critical bias E_c and then varies continuously with E for $E > E_c$. The analogy with exponents in critical phenomena is immensely intriguing: Critical exponents are independent of a system parameter (the lattice dimension d) for a wide range of d values. Specifically, they stick at the classical values (the mean field theory) for all d above a critical dimension d_c, and then vary continuously with d for $d < d_c$. This subtle parallel is the object of present study. A second analogy is with the dynamic phase transition[24] that occurs when the motion of random walkers in external potentials is studied where the height of the barrier has an exponential distribution. In this case, the system parameter is the temperature.

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