Anomalous segregation at a single trap in disordered chains

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(Received 11 March 1994)

We study the repulsion of Brownian particles induced by a single trap on disordered chains. Two different types of disorder are considered: random local bias fields (the Sinai model) and random transition rates. We discuss two possible measures of segregation for each system, and show that they can have either similar or different universal behavior, depending on the properties of diffusion subject to the hard-core potential in each system. We also report on anomalous scaling properties for the average trapping rate and the average density profile of the diffusing particles. It is surprisingly shown that the latter is not spatially linear in the vicinity of the trap, but rather has a flat tail in the case of random fields, and a nonuniversal power law in the case of random transition rates.

PACS number(s): 02.50.−r, 05.40.+j, 05.60.+w, 82.20.−w

A number of recent studies [1–15] analyze the problem of segregation at a single trap, which corresponds to the original Smoluchowski model of coagulation [16], a process which involves the trapping of diffusing particles, initially uniformly distributed throughout the space. By segregation we mean the depletion of the particles in the neighborhood of the trap induced by the trapping events. The depletion zone can be characterized either by the distance from the trap to a point at which the concentration profile of the diffusing particles, $P(x,t)$, reaches an arbitrary fraction θ ($0 < \theta < 1$) of its bulk value (which will be referred to as the *θ distance*) or by the distance between the trap and the nearest unreacted particle (*nearest-neighbor distance*). In low dimensions, these properties have been found to differ significantly from the classical three-dimensional results. In particular, in one dimension, the nearest-neighbor distance $\langle L(t)\rangle$ has been shown to increase asymptotically as $t^{1/4}$ [1], while the θ distance scales as $t^{1/2}$. A related quantity of practical importance, the trapping rate, has been found to decrease as $t^{-1/2}$ in the long-time limit. Physical examples of such systems are provided by exciton trapping, quenching or fusion, electron-hole and soliton-antisoliton recombination, phonon upconversion, and free-radical scavenging. Examples of reactions in confined geometries include quasi-one-dimensional crystals grown inside pores and microcapillaries, polymer chains in dilute blends, catalytic surface reactions, and heterofusion in ultrathin molecular wires, filaments, and pores [17–19].

All of these results pertain to diffusion of noninteracting particles in a translationally invariant space. It is therefore of interest to investigate the behavior of the two measures of segregation in *disordered* media, in which diffusive properties are generally anomalous [20–23]. Very few systems have been analyzed that are characterized by different forms of disorder. These include diffusion in a fractal medium [13], and a long-tailed continuous-time random walk [14,15] which mimics motion in disordered media.

In this Brief Report, we study the segregation at the single trap on two different types of disordered chains. The first is a chain with random local bias fields (the so-called Sinai model), and the second is the case of random transition rates which represents a weaker type of disorder. These are simplified models that mimic effects of external potentials or internal interactions on the kinetics of the depletion zone. Our study is based on extensive numerical simulations and scaling arguments. We shall discuss the similarities and the differences between the two systems, which shed light on some general properties of the segregation in disordered media.

We start with the case of random local bias fields, which is an example of the so-called Sinai model [24–29]. In this model, each site i along the linear chain has an associated transition probability of moving to the right, $P_i = \frac{1}{2}(1+E_i)$, where each E_i is assigned a value of $\pm E$ ($0 < E < 1$) with equal probability 1/2. Sinai proved [25] that the rms displacement of a particle diffusing in this system increases asymptotically as $\ln^2 t$, which represents a remarkable slowing down as compared to the standard diffusion process. This is due to the difficulty in moving against local fields induced by stretches of bias with the same sign. The Sinai model has been suggested as being relevant to various physical phenomena, such as $1/f$ noise, dynamics of dislocations in doped crystals, and slow dynamics of random-field magnets [24,29].

We have studied the segregation on the Sinai chain by extensive numerical simulations. These require a considerable amount of computing time, due to the extremely slow convergence to an asymptotic regime [26]. In order to obtain the average asymptotic profile near the trap at $x=0$, we used the exact enumeration method [21] to account for the diffusion process, with quenched local bias fields randomly imposed on the lattice. We have studied chains of 10^3 sites in length (to avoid finite-size effects), considered up to 10^6 time steps, and averaged the results over 10^4 configurations of Sinai chains. The results are shown in Fig. 1(a).

The main observation from this figure is that, unlike regular diffusion, the asymptotic spatial shape of the average density profile of the diffusion particles near the trap is not linear, but rather does flatten out in the vicinity of the trap as time evolves. This is similar to the result obtained for a system with constant bias which drives particles *away* from the trap [30]. The explanation of this result for the Sinai system is that in the asymptotic time limit, the dominant contribution to the average profile comes from configurations in which successive fields adjacent to the trap induce a net bias *away* from the trap. Other configurations are more likely to drive the particles towards the trap, but appear to have only a small effect on the long-time behavior. In Fig. 1(b) we show that the average profile $\langle P(x,t)\rangle$ is a scaling function of $x/\ln^2 t$. This implies that the θ distance scales as $\ln^2 t$, which follows from the Sinai type of diffusion of the bulk.

The average nearest-neighbor distance is defined as $\langle L(t)\rangle = \int_0^\infty Lf(L,t)dL$ where $f(L,t)$ is the probability density function for the distance L of the nearest particle to the trap at time t. The statistical properties of the average nearest-neighbor distance have been studied using an independent set of Monte Carlo simulations. In Fig. 2 we show a plot of $L\langle f(L,t)\rangle$ as a function of $L/\ln^2 t$, which suggests that the nearest-neighbor distance exhibits the same asymptotic dependence on time as does the θ distance, namely, both scale as $\ln^2 t$. This is surprising since, as we have noted, it differs from the result in regular diffusion where the two measures have different scaling behavior as a function of time.

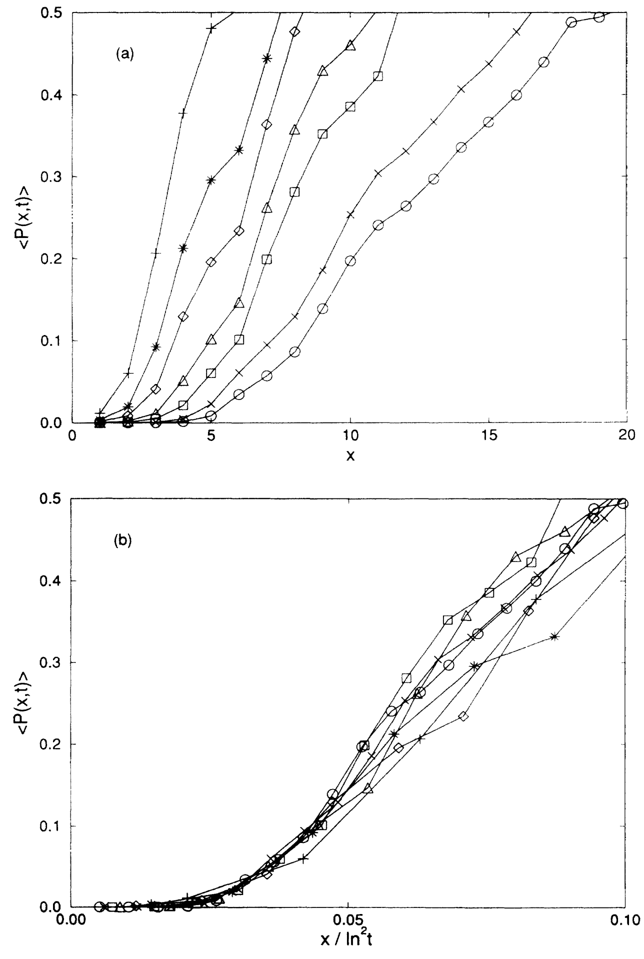

FIG. 1. (a) A plot of the spatial dependence of the average profile $\langle P(x,t)\rangle$ in the vicinity of the trap (at $x = 0$) on the Sinai chain. The curves summarize data obtained from exact-enumeration simulations with $E = 0.8$ for (from left to right) $t = (1,4,10,40,100,400,1000) \times 10^3$ time steps. The results represent an average over 10^4 configurations. (b) A scaling plot of $\langle P(x,t)\rangle$ as a function of $x/\ln^2 t$, for the results presented in (a).

We suggest that the explanation has to do with the relation between the nearest-neighbor distance measure and diffusive properties of tagged, hard-core particles. Keeping track of the *nearest* among *indistinguishable* particles is equivalent to following a tagged particle which cannot pass its successors along the chain. It is well known that the effect of the hard-core interaction in ordinary diffusion is to change the asymptotic rms displacement from a $t^{1/2}$ to a $t^{1/4}$ behavior [31,32], due to mutual interactions between the particles. Therefore, although the $t^{1/4}$ result for the nearest-neighbor distance in regular diffusion has been established for noninteracting particles, it basically reflects a measure which is related to diffusion with hard-core interaction [4]. In the Sinai model, one can argue that the localization induced by the random fields is so strong that hard-core effects are also negligible. Indeed, Koscielny-Bunde *et al.* [27] have recently examined in detail the effect of hard-core interaction on the diffusion properties of the Sinai model, and found that the leading asymptotic behavior of the rms displacement is the same as for noninteracting particles. Hence we expect that in those systems where hard-core interaction changes the asymptotic rms displacement of diffusion, the behavior of the nearest-neighbor distance and the θ distance should be different. In the second part of this work we test this prediction for the case of random transition rates chosen from a power-law distribution.

To complete our discussion of the Sinai chain, we consider the flux into the trap for this model. Since generally one cannot define the diffusion limit for a disordered system, we cannot use the definition for a one-dimensional

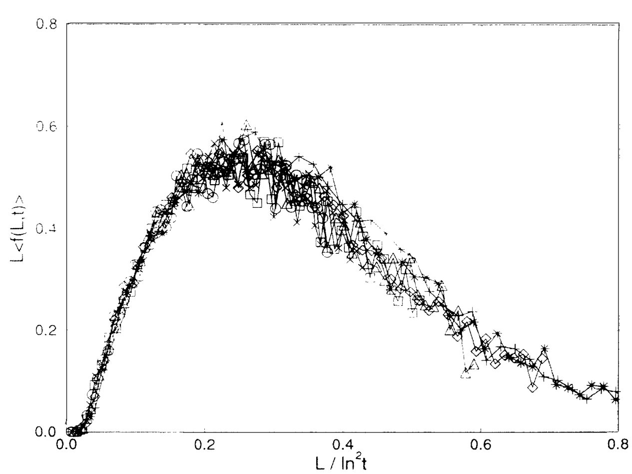

FIG. 2. A scaling plot of $L\langle f(L,t)\rangle$ as a function of $L/\ln^2 t$ for the Sinai model for $t = (1,2,5,10,20,50,100) \times 10^3$ time steps and $E = 0.8$. The results represent an average over 10^4 configurations.

flux, written in terms of a spatial derivative of the concentration. Instead we suggest a simple argument leading to a result supported by simulated data. The reaction rate at time t is proportional to the change in time of the cumulative number of particles reaching the trap up to time t. The latter is proportional to the typical distance of particles from the trap at time t, $\ln^2 t$, since it is unlikely that particles farther away from the trap can reach the trap by time t. Therefore we expect the flux to be proportional to the time derivative of the rms displacement, i.e., to $(\ln t)/t$ in the long-time limit. This anomalous result has been found to agree with our numerical simulations.

Next we study the segregation at the single static trap for a diffusion process with random transition rates W which are chosen from a slowly decaying distribution having the power-law form $P(W) \sim W^{-\alpha} (0 \le \alpha < 1)$. The asymptotic rms displacement of Brownian particles in this system is known to be proportional to t^{1/d_w}, with $d_w = (2-\alpha)/(1-\alpha)$ [21]. Using extensive numerical simulations in the exact-enumeration method, we found that the average profile near the trap at the origin scales asymptotically as $x/t^{1/d_w}$, with a corresponding θ-distance behavior of t^{1/d_w}. However, an interesting result is that the spatial behavior of this average profile is neither linear (as in regular diffusion), nor has an exponential tail (as in the case of fields). Rather, we found a surprising nonuniversal *algebraic* behavior which is shown in Fig. 3(a). Our numerical results for several values of α indicate that the average profile near the trap goes like $(x/t^{1/d_w})^{\beta}$, with β having the α-dependent value $(2-\alpha)/2(1+\alpha)$, which has been determined empirically. Note that $\alpha = 0$ corresponds to regular diffusion, without disorder. Typical scaling plots of the average profile are shown in Figs. 3(b) and 3(c).

The average nearest-neighbor distance for this case has been studied using Monte Carlo simulations. Following our discussion about the resemblance between this measure and the diffusive properties of particles which move subject to hard-core interaction, we refer again to Koscielny-Bunde *et al.* [27], who show that the effect of the hard-core interaction on diffusion in a system

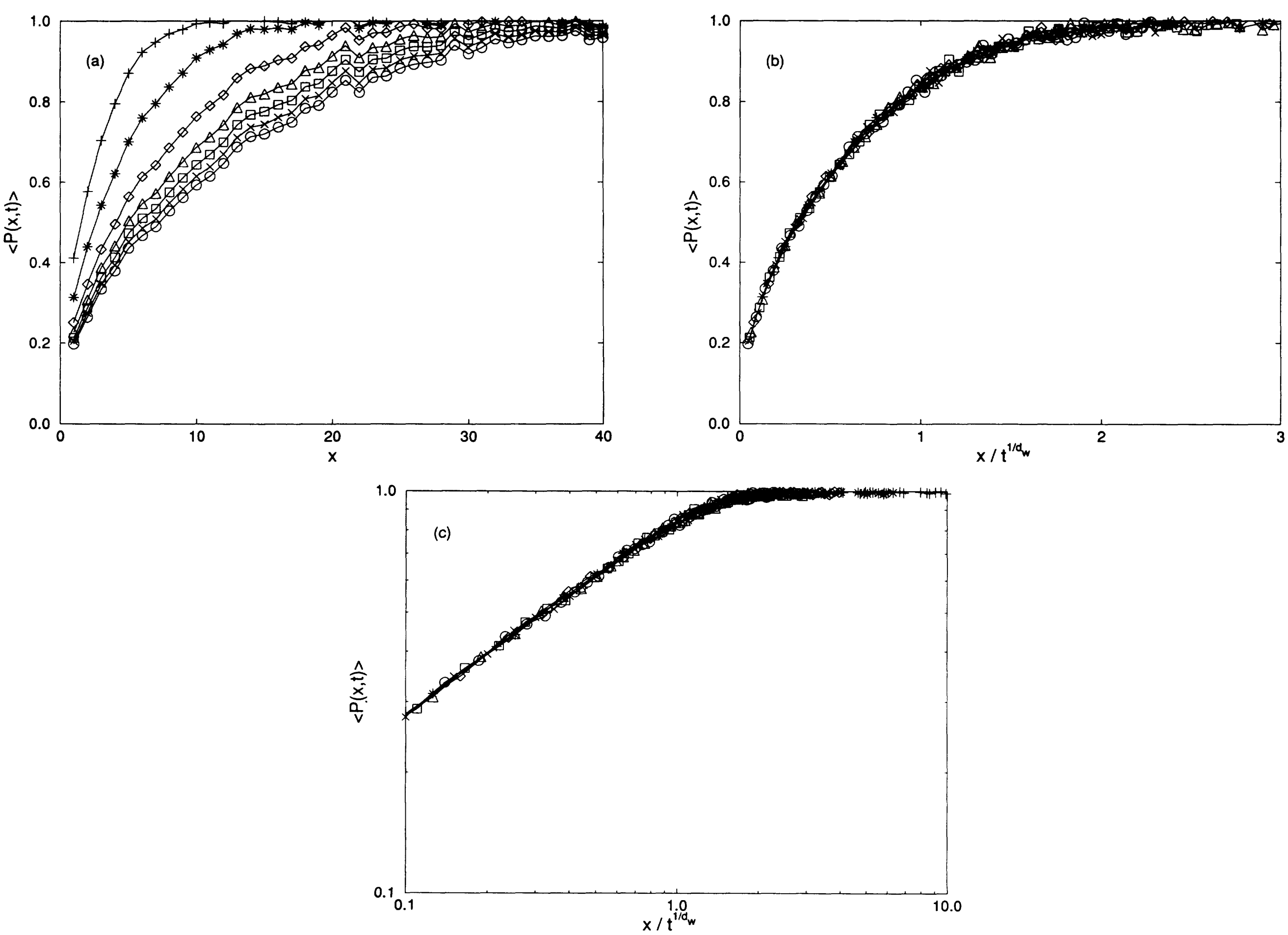

FIG. 3. (a) Numerical results for $\langle P(x,t)\rangle$ in the vicinity of the trap for a system with random transition rates. Results are shown for $\alpha = 0.5$, and, from left to right, $t = (1, 5, 20, 40, 60, 80, 100) \times 10^2$ time units, averaged over 10^5 configurations. (b) A scaling plot of $\langle P(x,t)\rangle$ as a function of $x/t^{1/d_w}$ for the results presented in (a). ($d_w = 3$). (c) A log-log plot of the scaling plot in (b). The value of the slope β in the vicinity of the trap is 0.5 for this value of α, in agreement with the empirical relation $\beta = (2-\alpha)/2(1+\alpha)$.

with such a long-tailed distribution of transition rates is to change the form of the asymptotic rms displacement from a proportionality to $t^{(1-\alpha)/(2-\alpha)}$ to a proportionality to $t^{(1-\alpha)/(4-3\alpha)}$. Hence we fit our results for the nearest-neighbor distance to this form. In Fig. 4 we plot $L\langle f(L,t)\rangle$ as a function of $L/t^{(1-\alpha)/(4-3\alpha)}$, and indeed, the data clearly agree with this prediction.

The flux into the trap in this disordered chain can be obtained using a similar argument to the one presented for random fields. Taking the time derivative of the asymptotic rms displacement in this system, t^{1/d_w}, with d_w as given above, one obtains t^{-1+1/d_w}, which was found to be in excellent agreement with our numerical data.

In summary, we have shown that the two measures of segregation studied here for disordered chains, the θ distance and the nearest-neighbor distance, can increase asymptotically either with the same or with different time dependence. This depends on the effect of hard-core interaction on diffusion in these systems. If such an interaction changes the leading asymptotic behavior of the rms displacement in that system, the nearest-neighbor distance measure also changes in a corresponding manner. The θ distance, however, always scales similarly to the rms displacement of regular diffusion in the system. In addition, we found anomalous trapping rates, and anomalous shapes for the average density profile near the trap. In the random bias (Sinai) model the average profile exhibits a tail similar to the case of global bias away from the trap, and for random transition rates it has a nonuniversal power-law behavior.

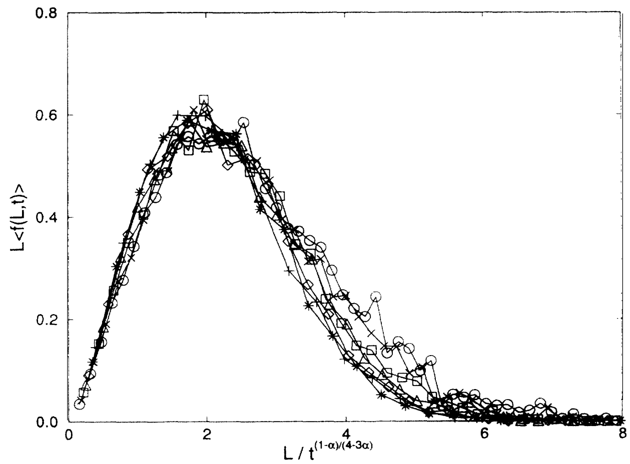

FIG. 4. A scaling plot of $L\langle f(L,t)\rangle$ as a function of $L/t^{(1-\alpha)/(4-3\alpha)}$ for $\alpha = 0.5$ $[(1-\alpha)/(4-3\alpha) = 0.2]$, and $t = (1,2,5,10,20,50,100) \times 10^2$ time steps. The results represent an average over 10^4 configurations.

We wish to thank Shlomo Havlin for fruitful discussions and useful suggestions, and the Bi-National U.S.-Israel Science Foundation (BSF) for partial support.

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