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Diffusion in the presence of random fields and transition rates: Effect of the hard-core interaction

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We study diffusion of hard-core particles in linear chains where disorder arises from two distinct sources, (i) random bias fields and (ii) random transition rates. In the case of random *bias fields*, the step probability to the left and right is randomly chosen to be $(1+E)/2$ and $(1-E)/2$ with equal probability. Using Monte Carlo simulations and scaling arguments we find that the mean-square displacement is given by $\langle x^2(t)\rangle \sim [A(c)(\ln t)]^4$, and the probability density $P(x,t)$ scales as $P(x,t)\sim\langle x^2(t)\rangle^{-1/2}G(x/\langle x^2(t)\rangle^{1/2})$. Here c is the concentration of particles; for $c\rightarrow 0$, $\langle x^2(t)\rangle$ reduces to the Sinai result for noninteracting particles. We find that the scaling function $G(u)$ has the form $G(u)\sim\exp(-u^{\alpha})$, with $\alpha=1.5$, a value distinctly different from the value for noninteracting particles ($\alpha=1.25$) and from the value for zero-bias field ($\alpha=2$). In contrast, in the case of random *transition rates* with a power-law distribution, we find that the asymptotic behavior of $\langle x^2(t)\rangle$ as well as $P(x,t)$ is changed by the hard-core interaction.

In recent years, the problem of diffusion in random media has received much interest (see, e.g., Refs. 1-3). In one-dimensional systems, due to the presence of disorder, diffusion in general is anomalously slow and depends on the type of disorder. If, for example, random bias fields are applied on each site where the bias is taken to be $+E$ or $-E$ with equal probability, then diffusion is logarithmically slow[4] and the mean-square displacement is proportional to $(\ln t)^4$. Similar behavior was found for diffusion in random structures such as random combs and percolation systems at criticality under the influence of a constant bias field.[5-9] If random transition rates with a power-law distribution instead of random fields are considered, then $\langle x^2(t)\rangle$ is characterized by a power law in time.[1]

Essentially, all these studies are for systems where the diffusing particles are *noninteracting*. This assumption is not justified if one considers real particles with "excluded volume," especially for one dimension. Here, particles not only cannot occupy the same site in the chain, but they cannot even pass by each other. For this reason, Fick's law is changed from $\langle x^2(t)\rangle\sim t$ to $\langle x^2(t)\rangle\sim t^{1/2}$ on introducing simple hard-core interactions.[10-13] It is known that this change in the diffusion properties of tagged particles can lead to strong effects in related problems, e.g., when considering trapping of diffusing particles by random sinks.[14,15]

In this communication we study the influence of hard-core interaction on the diffusion of particles in linear chains, in the presence of random bias fields. This bias is taken to be $+E$ or $-E$ on each site with same probability. Using Monte Carlo simulations and scaling arguments we find that, asymptotically, the form of the distribution function $P(x,t)$ is changed by the hard-core interaction, but the asymptotic behavior of $\langle x^2\rangle$ remains unchanged (except for a concentration-dependent amplitude). In contrast, if instead of random bias fields random transition rates with power-law distribution are taken, then also the asymptotic power-law behavior of $\langle x^2(t)\rangle$ is changed by the hard-core interaction.

First, we consider the case of random bias fields. Hard-core particles of concentration c are distributed along the chain. A particle at site i has the probability $p_+=(1+E_i)/2$ to step to the right (if the site to the right is empty) and the probability $p_-=(1-E_i)/2$ to step to the left (if the left site is empty). Here, E_i can accept the values $+E$ or $-E$ with equal probability. If a neighbor site is occupied by another particle, the particle cannot move to that site. To simulate the diffusive process of tagged particles, particles are selected at random and moved to a nearest-neighbor site according to the above probabilities. If this site is already occupied, the move is rejected. After each trial, the time t is incremented by $1/N$, where N is the number of hard-core particles in the chain. We have recorded the displacement of each particle as a function of t, and by averaging over all particles we obtain $\langle x^2\rangle$ and $P(x,t)$.

The simulations have been carried out for $E=0.8$ and several values of concentration c. We have studied chains of 20000 sites with periodic boundary conditions, averaged over up to 50 configurations, and considered up to 80000 time steps. Figure 1(a) shows the mean-square displacement of a tagged particle on the chain for several values of c. For large t, $\langle x^2(t)\rangle^{1/4}$ is proportional to $\ln t$, showing that the asymptotic time dependence is the same as for noninteracting particles, i.e.,

$$\langle x^2(t)\rangle\sim[A(c)\ln t]^4 \ . \tag{1}$$

The hard-core interaction does not change the power of $\ln t$, but rather changes the prefactor $A(c)$. Figure 1(b) shows the dependence of $A(c)$ on concentration c. For small concentrations ($c<0.2$) $A(c)$ is nearly constant, while $A(c)$ drops sharply for large c.

Next consider the distribution function $P(x,t)$, the probability to find the particle at time t at distance x from

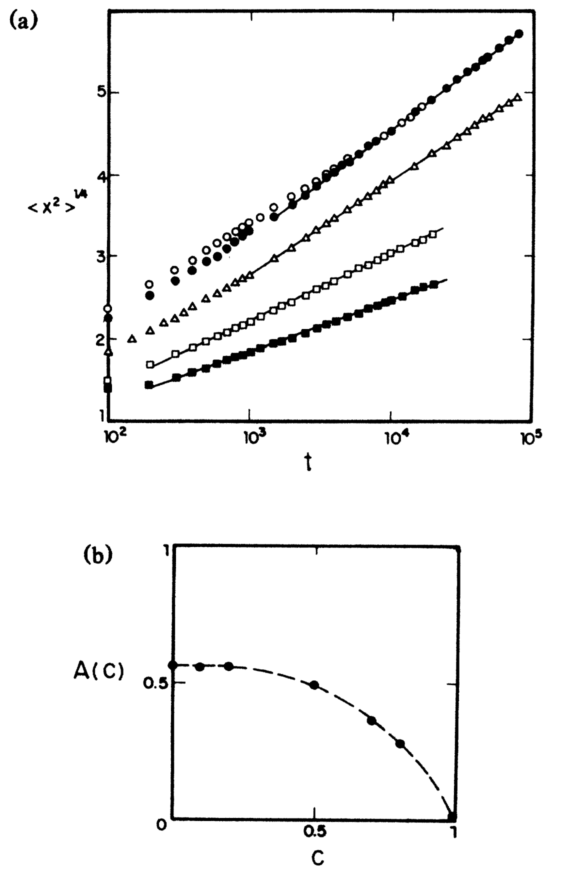

FIG. 1. (a) Plot of $\langle x^2 \rangle$ vs $\ln t$ for the concentrations $c=0.1$ (○), 0.2 (●), 0.5 (△), 0.7 (□), and 0.8 (■). (b) Plot of $A(c)$ vs c. $A(c)$ are the values of the slopes in Fig. 1(a). t is in units of $1/N$.

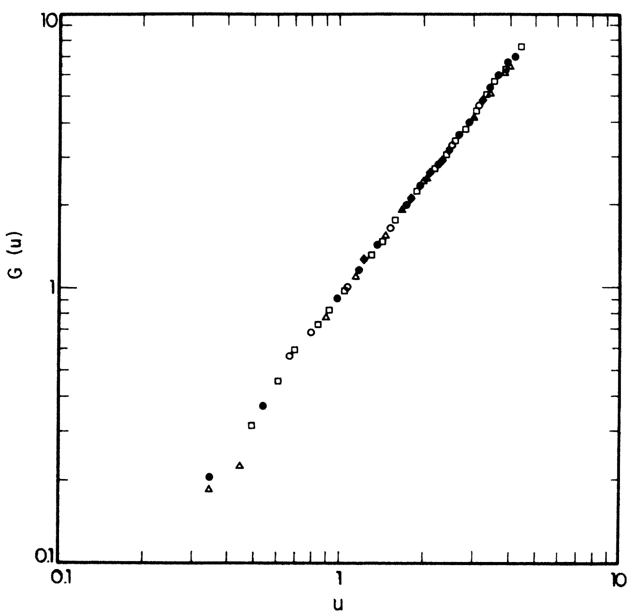

FIG. 2. Plot of the scaling function $G(u)$ from Eq. (2) vs $u=x/R$ for different values of c, x, and t; $c=0.2$, $t=20000$ (×); $c=0.2$, $t=40000$ (○); $c=0.5$, $t=5000$ (△); $c=0.5$, $t=10000$ (●); $c=0.5$, $t=20000$ (◇); $c=0.7$, $t=20000$ (△).

its starting point at $x=0$. A simple scaling form for $P(x,t)$ is

$$P(x,t)=P(0,t)G\left[\frac{x}{\langle x^2(t)\rangle^{1/2}}\right] , \tag{2}$$

where $G(u)=1$ at $u=0$. The probability of return to the origin $P(0,t)$ is proportional to $\langle x^2(t)\rangle^{-1/2}$ asymptotically. This scaling form has been found useful to describe the case of noninteracting particles, where asymptotically $G(u)\sim\exp(-u^{a})$ with $a=1.25$.[16] For zero-bias field, on the other hand, $P(x,t)$ is Gaussian in x (Refs. 10 and 11) and $a=2$. To test the scaling ansatz and to determine the asymptotic behavior of the scaling function we have plotted in Fig. 2, $-\ln[P(x,t)/P(0,t)]$ as a function of $x/\langle x^2(t)\rangle^{1/2}$, on a double logarithmic scale. The data collapse, obtained for several concentrations and x and t values, supports Eq. (2) and the slope determines the exponent a. For intermediate u values the slope is close to the value of noninteracting particles, $a=1.25$, while for larger u values the slope is $a=1.5$. We have also performed calculations of $\ln[P(x,t)/P(0,t)]$ as a function of $u=x/\langle x^2(t)\rangle^{1/2}$ for zero-bias fields and several concentrations and found an excellent data collapse. The slope of $-\ln G(u)$ approached $a=2$ already at small values of u.

To explain our result for the mean-square displacement we make use of the fact that the random field problem can be mapped[3] onto a diffusion problem with random transition rates W, which are chosen from the distribution

$$P(W)\sim\frac{1}{W(\ln W)^3} . \tag{3}$$

In order to find the asymptotic behavior of $\langle x^2(t)\rangle$ we follow scaling arguments similar to that used by Harder, Havlin, and Bunde[17] in the context of diffusion on fractals with a singular waiting-time distribution. Due to the hard-core interaction, the mean-squared range $R^2=\langle x^2(t)\rangle$ of a tagged particle scales with the number of steps N as

$$R^2\sim N^{1/2} . \tag{4}$$

The effect of the distribution (3) is to provide additional random delays. After N steps, the elapsed time t is

$$t=N\bar{t} , \tag{5}$$

where $\bar{t}$ is the average time the particle spends in one site. The average time is

$$\bar{t}=\frac{1}{R}\sum_{i=1}^{R}\frac{1}{W_i}=\int_{W_{\min}}^{1}dW\frac{1}{W}P(W) . \tag{6}$$

Here $W_{\min}$ is the minimum transition rate encountered by the particle when traveling the distance R. From (3) we obtain[3,7] $W_{\min}\sim\exp(-R^{1/2})$. From (3) and (5) we find that asymptotically $\bar{t}\sim\exp(R^{1/2})$ and hence $t=N\bar{t}\sim R^4\exp(R^{1/2})$. This yields asymptotically $R\sim(\ln t)^2$, in agreement with our numerical finding.

Next we consider the effect of hard-core interaction on the diffusion of a tagged particle when the transition rates follow a power-law distribution,

$$P(W) \sim \frac{1}{W^{\gamma}}, \ \gamma < 1 \ . \tag{7}$$

For noninteracting particles, $R^2 \sim t$ for $\gamma \leq 0$ and $R^2 \sim t^{2(1-\gamma)/(2-\gamma)}$ for $\gamma > 0$.[1] For deriving R for interacting particles we follow the procedure outlined above, Eqs. (4)–(6). For the power-law distribution, $W_{\min} \sim R^{-1/(1-\gamma)}$ and hence, from (6), $\bar{t} \sim R^{\gamma/(1-\gamma)}$ for $\gamma > 0$ and $\bar{t} = \text{const}$ for $\gamma \leq 0$. Using (4) and (5) we obtain $R^2 \sim t^{2/d_w}$, where

$$d_w = \begin{cases} (4-3\gamma)/(1-\gamma), & \gamma > 0 \ ; \\ 4, & \gamma \leq 0 \ . \end{cases} \tag{8}$$

To test the prediction of Eq. (8), we carried out extensive Monte Carlo simulations for two concentrations of hard-core particles, $c = 0.1$ and $c = 0.2$, for three different values of γ, $\gamma = 0$, $\frac{1}{2}$, and $\frac{2}{3}$. For obtaining R^2, we have studied chains of 10000 sites with periodic boundary conditions. We averaged up to 40 configurations for each case. Equation (8) predicts $2/d_w = \frac{1}{2}$, $\frac{2}{5}$, and $\frac{1}{3}$, respectively, for the choices $\gamma = 0$, $\frac{1}{2}$, and $\frac{2}{3}$, independent of the value of c. From the slopes of data such as those shown in Fig. 3, we find $2/d_w = 0.49 \pm 0.02 (\gamma = 0)$, 0.39 ± 0.03 $(\gamma = \frac{1}{2})$, and $0.31 \pm 0.03 (\gamma = \frac{2}{3})$, in substantial agreement with the prediction.

In summary, then, we have discussed the influence of hard-core interactions on the diffusion of tagged particles in linear chains with random fields and random transition rates. We have found that in the case of a power-law distribution of transition rates the asymptotic time behavior of the mean-square displacement changed as a result of the hard-core interaction, while it did not change for the case of random fields (which is equivalent to a logarithmic distribution of transition rates). In this case, only logarithmic corrections to the logarithmic time dependence of $\langle x^2(t) \rangle$ occur as a result of the hard-core interaction which do not affect the leading asymptotic behavior. The reason for this difference is that the time delays due to the hard-core interaction are negligible compared with the time delays due to the random fields, while for random transition rates both types of delays are of the same order of magnitude as long as γ is not too close to 1. For $\gamma \rightarrow 1$, the time delays due to the interactions are also negligible.

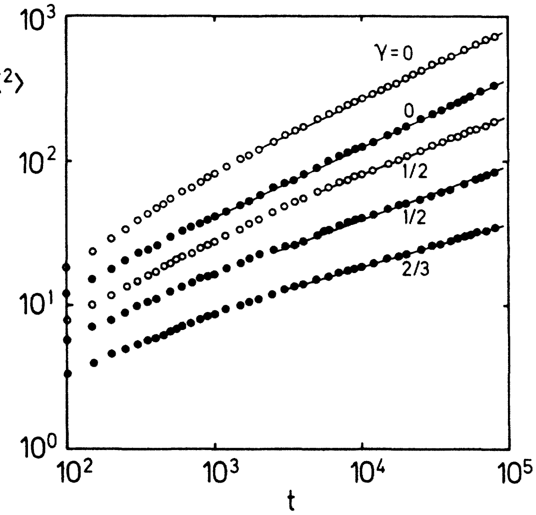

FIG. 3. Log-log plot of R^2 against t for several values of the parameter γ. Note that the slopes depend on γ but not on the concentrations c of hard-core particles, $c = 0.1$ (○) and $c = 0.2$ (●).

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[1]S. Alexander, J. Bernasconi, W. R. Schneider, and R. Orbach, Rev. Mod. Phys. **53**, 179 (1981).

[2]J. W. Haus and K. W. Kehr, Phys. Rep. **150**, 263 (1987).

[3]S. Havlin and D. Ben-Abraham, Adv. Phys. **36**, 695 (1987).

[4]Ya. Sinai, Theory Probab. Its Appl. **27**, 256 (1982).

[5]A. Bunde, S. Havlin, H. E. Stanley, B. L. Trus, and G. H. Weiss, Phys. Rev. B **34**, 8128 (1986).

[6]D. Stauffer, J. Phys. A **18**, 1827 (1985).

[7]S. Havlin, A. Bunde, Y. Glasser, and H. E. Stanley, Phys. Rev. B **34**, 3492 (1986).

[8]A. Bunde, H. Harder, S. Havlin, and H. E. Roman, J. Phys. A **20**, 1987.

[9]S. Havlin, A. Bunde, H. E. Stanley, and D. Movshovitz, J. Phys. A **19**, L693 (1986).

[10]T. E. Harris, J. Appl. Prob. **2**, 323 (1965).

[11]P. M. Richards, Phys. Rev. B **16**, 1363 (1977).

[12]P. A. Fedders, Phys. Rev. B **17**, 40 (1978).

[13]S. Alexander and P. Pincus, Phys. Rev. B **18**, 2011 (1978).

[14]A. Bunde, S. Havlin, R. Nossal, and H. E. Stanley, Phys. Rev. B **32**, 3367 (1985).

[15]A. Bunde, L. L. Moseley, H. E. Stanley, D. Ben-Avraham, and S. Havlin, Phys. Rev. A **34**, 2575 (1986).

[16]A. Bunde, S. Havlin, H. E. Roman, G. Schildt, and H. E. Stanley, J. Stat. Phys. (to be published).

[17]H. Harder, S. Havlin, and A. Bunde, Phys. Rev. B **36**, 3874 (1987).