RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 32, NUMBER 5 1 SEPTEMBER 1985

Anomalous trapping: Effect of interaction between diffusing particles

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(Received 4 June 1985)

We present the first study of the effect of interactions on phenomena associated with trapping of diffusing particles. Specifically, we consider a single trap and a two-component mixture of T and F particles where only the T particles can be trapped. We show that the trapping rate $\dot{Q}$ is controlled by the ratio $R=c_F/c_T$ of the T and F concentrations, and satisfies the scaling law $\dot{Q}\sim R^2 f(tR^4)$. For t below a crossover value $t^\times$ (which scales as R^{-4}), we recover the conventional result $\dot{Q}\sim t^{-1/2}$. Above $t^\times$, we find new and anomalous behavior $\dot{Q}\sim(1/R)t^{-3/4}$.

What are the laws[1,2] that govern the behavior of diffusing particles in the presence of random trapping centers? This question has been the subject of great current interest, in part because of the large number of applications to real systems.[1] Moreover, several novel physical phenomena have been directly mapped onto trapping models; these include the Williams-Watt form of dielectric relaxation,[3] the self-attracting polymer chain,[4] and excitation decays in crystals.[5] Essentially all these studies are for systems where the diffusing particles are *noninteracting*: they are assumed to execute a random walk that is completely unconstrained. This assumption is not justified if one considers real particles with "excluded volume," especially for one dimension $(d=1)$: not only can particles not occupy the same point in space, but they cannot even pass by each other. For this reason Fick's law for noninteracting particles $\langle x^2\rangle\sim t$, is substantially changed to $\langle x^2\rangle\sim t^{1/2}$ on introducing simple "hard-core" interactions.[5-9] Although, by analogy, we expect substantial modifications in the conventional result for the number of noninteracting particles trapped per unit time by a single trap,

$$\dot{Q}\sim t^{-1/2}\ , \tag{1}$$

this important problem has not yet been addressed. Our purpose here is to provide the first investigation of how physical laws governing trapping are modified by the effect of hard-core interactions between the diffusing particles.

The model. To display the full richness of this problem, consider two types of particles, T and F ("thin" and "fat"), with initial concentrations c_T and c_F, which are diffusing on a linear chain with N sites (see Fig. 1, which also shows schematically the overall picture developed below). On the chain we have a single trap which traps only the T particles, thereby selecting one species over the other. In order to account for the finite volume of the particles we exclude double occupancy of the sites.

We have focused on how the trapping rate depends on c_T and c_F. First, sites are picked at random and occupied with T and F particles, avoiding double occupancy, until the desired initial concentrations c_T and c_F have been reached. To simulate the diffusive trapping process, particles are selected at random and moved to a randomly selected nearest-neighbor site. If this site is already occupied, the move is rejected. When a T particle reaches the trap, it is removed. After each trial the time is incremented by $1/N_{\rm surv}$, where $N_{\rm surv}$ is the number of surviving particles in the system. The simulations have been carried out for fixed total initial concentration $c=c_T+c_F=0.8$ and we have varied the ratio $R=c_F/c_T$. We have studied lattices with 100, 200, 400, and 800 sites with periodic boundary conditions. For time steps up to 6000 our results were the same

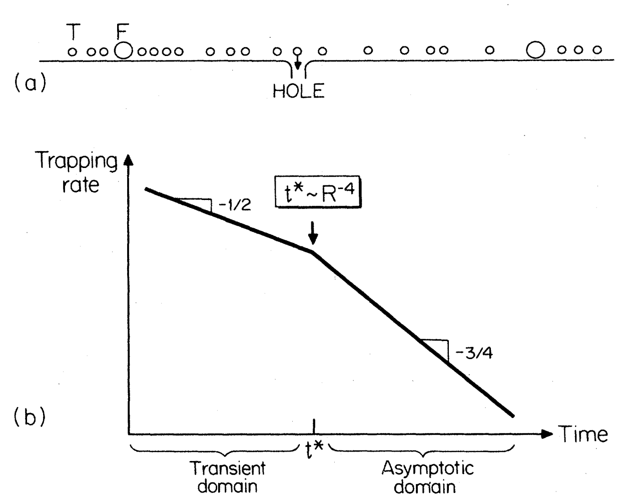

FIG. 1. Schematic illustration of (a) the model and (b) the overall physical picture developed in this Rapid Communication for $R=c_F/c_T<<1$. For $t<t^\times$ (the crossover time), the system behaves as if $R=0$ so $\dot{Q}\sim t^{-1/2}$. As R increases, $t^\times$ increases; in fact, $t^\times\sim R^{-4}$.

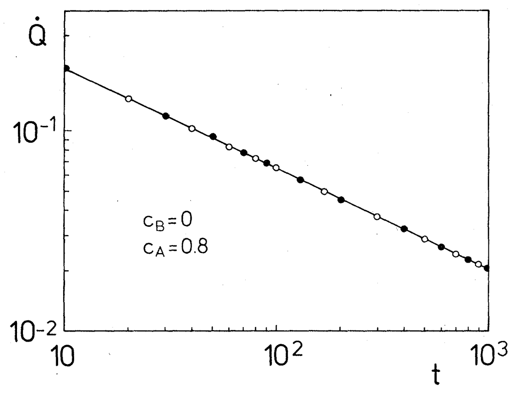

FIG. 2. The trapping rate $\dot{Q}$ vs time t of noninteracting particles (○) compared with the trapping rate of identical hard-core particles (●) for a linear chain with 800 sites. The initial particle concentration is $c = 0.8$.

for lattice sizes 400 and 800. To improve the statistics, we binned the results in bins of ten time steps.

Consider first the extreme case $R = 0$, where all particles can be trapped. Figure 2 shows the trapping rate as a function of time averaged over 6000 initial configurations compared with the trapping rate of noninteracting particles. Both rates are identical and are described by the conventional power law (1). This somewhat surprising result can be understood as follows: since for $R = 0$ the trap does not distinguish between the particles, the trapping rate is governed by the density fluctuations of *all* particles, rather than the density fluctuations of a *tagged* particle. The evolution equation for the occupation $n_l(t)$ of site l at time t that determines the concentration of surviving particles in the chain is the same for noninteracting particles and identical hard-core particles. Therefore, we expect identical trapping rates $\dot{Q}$ for noninteracting and hard-core particles. Now Q, the number of particles that have been trapped up to time t, is proportional[1,2] to $\langle s \rangle$, the mean number of distinct sites visited by a random walk. Since $\langle s \rangle \sim t^{1/2}$ in one dimension, we recover Eq. (1).

Now consider the opposite limit $R \to \infty$, where we have only one T particle that can be trapped. Now the trapping rate is governed by the number of distinct sites $\langle s \rangle_T$ visited up to time t by the "tagged" T particle in the presence of hard-core interactions. The time dependence of $\langle s \rangle_T$ can be deduced by simple scaling arguments. In one dimension we have $\langle s \rangle_T \sim (\langle x^2 \rangle)^{1/2}$ and therefore we expect

$$Q \sim \langle s \rangle_T \sim t^{1/4} \ . \tag{2a}$$

The probability P_0 that a marked particle will return to the origin at time t is proportional to $1/\langle s \rangle_T$. We have con-

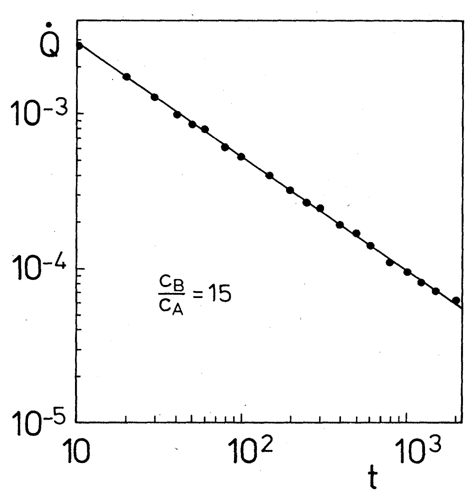

FIG. 3. Selective trapping rate $\dot{Q}$ of T particles coupled via hard-core interaction to T and F particles with initial concentrations $c_T = 0.05$ and $c_F = 0.75$ for a linear chain containing 400 sites.

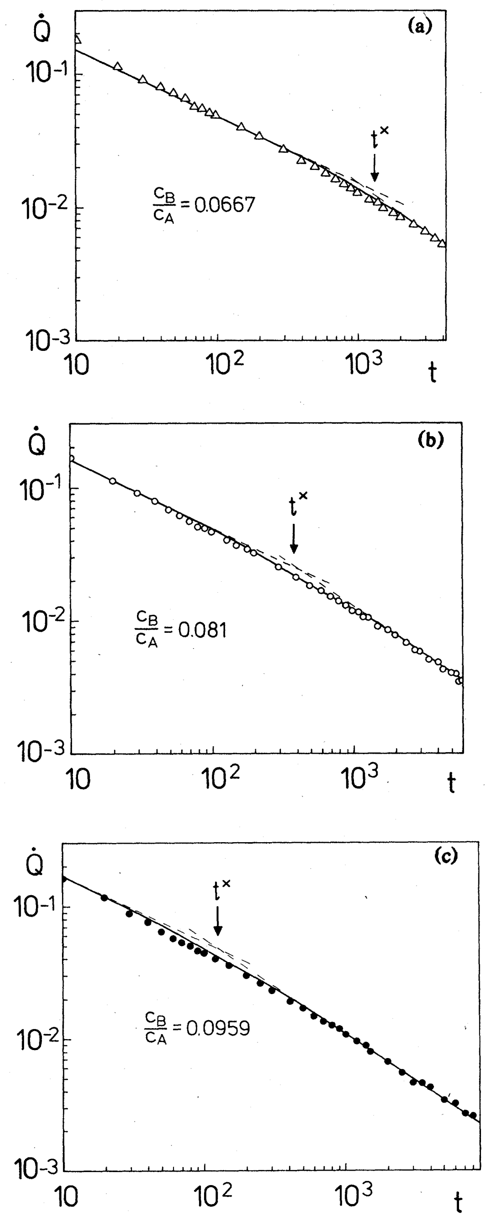

FIG. 4. Selective trapping rates $\dot{Q}$ of T particles coupled with hard-core interaction to T and F particles for a linear chain containing 400 sites and the particle concentrations (a) $c_T = 0.75$, $c_F = 0.05$; (b) $c_T = 0.74$, $c_F = 0.06$; and (c) $c_T = 0.73$, $c_F = 0.07$.

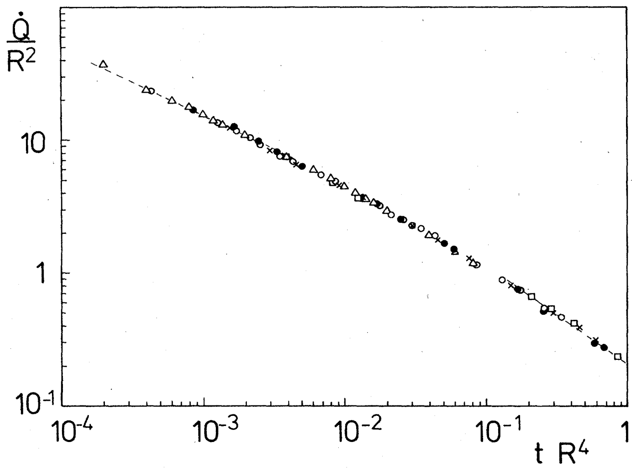

FIG. 5. The trapping rate $\dot{Q}$ divided by $R^2=(c_F/c_T)^2$ vs tR^4 for $c_T+c_F=0.8$ and $c_T=0.05$ (Δ), $c_T=0.06$ (○), $c_T=0.07$ (●), $c_T=0.08$ (×), and $c_T=0.10$ (□).

firmed (2a) by carrying out simulations of P_0. From (2a), we find

$$\dot{Q} \sim t^{-3/4} \quad . \tag{2b}$$

Figure 3 shows the trapping rate for $R=15$, averaged over 10 000 runs. The result confirms the power law (2b) for all times longer than 10.

Now let us consider the most interesting regime of small but finite concentrations of F particles. We have performed simulations covering a wide range of R values, $R << 1$ (for fixed total initial concentration $c_T+c_F=0.8$). Representative results are shown in Figs. 4(a)–4(c). For small times the trapping rate is not affected by the hard-core interaction, so those T particles that do not have an F particle between them and the trap are trapped easily, thereby obeying the $t^{-1/2}$ behavior of (1). For large times the trapping is determined by those F particles that hinder the T particles, so we recover the $t^{-3/4}$ behavior of (2b). The crossover time $t^\times$ between the two power laws, defined roughly as the intersection point between both curves in a log-log plot, depends crucially on R. Clearly, the average distance l any F particle must diffuse scales as R^{-1}. Since $l \sim t^{1/4}$, the time scales as R^{-4}. For $t << t^\times$, $\dot{Q}$ is independent of R, and for $R=0$, $\dot{Q} \sim t^{-1/2}$. Hence,

$$\dot{Q} \sim R^\alpha f(tR^4) \sim R^\alpha (tR^4)^{-1/2} \quad ,$$

which is independent of R only if $\alpha=2$. Thus, we conclude that $\dot{Q}$ should satisfy the scaling form

$$\dot{Q} \sim R^2 f(tR^4) \quad . \tag{3}$$

Here $f(x) \sim x^{-1/2}$ for $x << 1$ and $f(x) \sim x^{-3/4}$ for $x >> 1$. For $t > t^\times$, Eq. (3) predicts the new result $\dot{Q} \sim R^{-1} t^{-3/4}$. We have tested the scaling result (3) by plotting $\dot{Q}/R^2$ vs tR^4 for five different R values (see Fig. 5). The striking data collapse confirms Eq. (3). Note that these results have been obtained for a fixed total initial concentration. The scaling function itself depends on the total initial concentration.

In summary, we have elucidated the influence of particle interactions on the trapping rate of diffusing particles using a model with two kinds of particles, F and T, and one single trap which selects the T from the F particles. In the particular case of $c_F=0$, the hard-core interaction does not affect the trapping rate. In the general case of nonzero c_F, we found a new trapping law, the rate showing scaling behavior reminiscent of critical phenomena. In the more general case of a nonzero trap concentration, we expect for $c_F=0$ the same exponential decay of the trapping rate as has been found by Donsker and Varadhan[10] for noninteracting random walkers. However, for finite c_F we expect also this exponential form to change dramatically.[11]

We thank G. H. Weiss for helpful discussions. The Center for Polymer Studies, Boston University, is supported by grants from U.S. Office of Naval Research (ONR) and National Science Foundation (NSF). A.B. gratefully acknowledges the financial support from Deutsche Forschungsgemeinschaft (Bonn, Germany).

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[11]For noninteracting particles, the exponential decay of the survival probability (as well as the trapping rate) is of the form $s \sim \exp(-at^{1/3})$ in $d=1$, where a depends on the trap concentration for noninteracting walkers and t scales as x^2. Therefore, we expect s to scale as $s \sim \exp(ax^{2/3})$. For our system, consisting of F and T particles with hard-core interaction, t scales as x^4 and therefore we might expect the exponential part of the trapping to be of the form $\exp(-at^{1/6})$. Our expectation is confirmed by recent unpublished work of L. L. Mosely *et al.*