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Trapping reaction with mobile traps

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We present the Monte Carlo results for the two-species trapping reaction $A+B\to B$ with diffusing A and B on lattices in one, two, and three dimensions. We use an algorithm that permits one to simulate the survival probabilities of A particles down to $<10^{-30}$ with high accuracy. The results for the survival probability agree much better with the exact asymptotic predictions of Bramson and Lebowitz [Phys. Rev. Lett. **61**, 2397 (1988)] than with the heuristics of Kang and Redner [J. Phys. A **17**, L451 (1984)]. But there are very large deviations from either, which show that even these simulations are far from asymptotia. This is supported by the rms displacement of A particles, which clearly shows that the asymptotic regime has not been reached, at least for $d=2$ and $d=3$.

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Even the simplest reaction diffusion systems with only two-body reactions and without particle production show very rich and not yet fully understood phenomena. One prototype is the absorption of diffusing particles on randomly located static sinks. This model, studied first by Smoluchowski nearly a hundred years ago [1], shows an exponential decrease of the particle density in mean field theory, but the exact asymptotic behavior found by Donsker and Varadhan [2] is a stretched exponential in any finite dimension d. Another classic example, the recombination $A+A\to A$, was studied by Feller [3]. It leads to $n_A\sim t^{-1/2}$ in $d=1$, as compared to the mean field solution $n_A\sim t^{-1}$ which holds for $d>2$.

Particle annihilation with two mobile species A and B, either of the type $A+B\to B$ or $A+B\to 0$, were studied by Ovchinikov and Zeldovich [4] and Toussaint and Wilczek [5]. The motivation of Ref. [5] stemmed from the fate of magnetic monopoles in the early universe, but applications to condensed matter physics and chemical kinetics are of course more numerous.

If one starts out with equal densities for A and B, $n_A(0)=n_B(0)$, then the reaction $A+B\to 0$ leads to $n\sim t^{-d/4}$ [5]. This is different from the cases $n_A(0)<n_B(0)$ and $A+B\to B$. Notice that the latter is simply related to the limit $n_A(0)\to 0$ of the reaction $A+B\to 0$. If we denote by $n_A(t)|_{n_A(0)}$ the density in the $A+B\to 0$ reaction, the one in the $A+B\to B$ reaction is $\lim_{\alpha\to 0}\alpha^{-1}n_A(t)|_{\alpha n_A(0)}$. In both these cases $n_A\ll n_B$ for late times, and one expects identical asymptotics. This was indeed proven rigorously by Bramson and Lebowitz [6,7] who obtained [8]

$$n_A(t)\sim\begin{cases}\exp(-\lambda_1\sqrt{t}), & d=1,\\ \exp(-\lambda_2 t/\ln t), & d=2,\\ \exp(-\lambda_d t), & d\geq 3,\end{cases}\qquad(1)$$

with unknown constants λ_d. In contrast to this, different asymptotics had been predicted for $A+B\to B$ and for $A+B\to 0$ with $n_A(0)<n_B(0)$ by Kang and Redner [9,10] by heuristic arguments.

Verifying Eq. (1) numerically has turned out to be about as difficult as verifying the Donsker-Varadhan stretched exponential. The first simulations of $A+B\to B$ with mobile B were done by Redner and Kang [10]. These agreed with their own heuristic asymptotics [which differ from the exact Eq. (1) by the absence of the logarithm for $d=2$]. Subsequent simulations [11,12] were judged even by the authors as inconclusive. The main problem seems to be that there are large finite time corrections to the asymptotic behavior. Thus one would like to simulate up to very long times. But with the straightforward approaches used so far it is practically impossible to estimate the survival probabilities smaller than $\approx 10^{-8}$, even with the most powerful present day computers.

It is the purpose of this work to present simulations for the reaction $A+B\to B$, which go far beyond this. We shall not give any results for $A+B\to 0$ since our special numerical methods cannot be applied to that case. More specifically, we consider regular lattices $\boldsymbol{Z}^d$ on which the B particles perform independent discrete time random walks: at each time step, each particle hops with equal chance to one of its two-dimensional (2D) nearest neighbors. A particles perform the same kind of random walks until they hit upon a B particle in which case they are instantaneously absorbed. Initial conditions are such that all Bs are uncorrelated with homogeneous concentration c. Since A particles do not interact with each other, their concentration is irrelevant. In the actual simulations we shall use either one or two A's in the initial configuration. Notice that in this model the B particles act as catalyzers, and their distribution is Poissonian at any time, if they start out independently at $t=0$.

Our algorithm is related to an algorithm used recently [13] for the trapping (Donsker-Varadhan) problem. There we were able to clarify the crossover from the mean field type to the stretched exponential behavior. In the present case we shall see that—despite going to much longer times than in the earlier simulations—we still do not yet fully understand the crossover to the Bramson-Lebowitz asymptotics.

The algorithm has several essential ingredients. The first is that we use cloning (''enrichment'') of configurations with surviving A particles and a bias [14] for the diffusion of A such that less of them are absorbed. This bias is compensated by suitably chosen weights, i.e., we always deal with non-

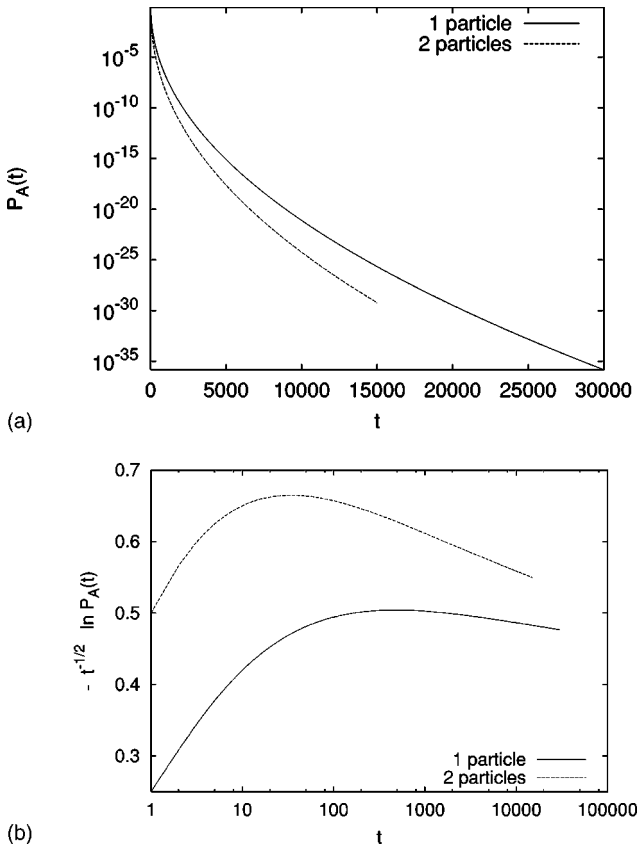

FIG. 1. (a) Semilogarithmic plot of the survival probability in $d=1$ for $c=0.5$. The upper curve is for a single A particle, while the lower one is the probability that *both* particles of a pair of A's survive, both of which had started at the same site. (b) $-t^{-1/2}\ln P_A(t)$ from the same data as in panel (a), plotted on a logarithmic horizontal scale.

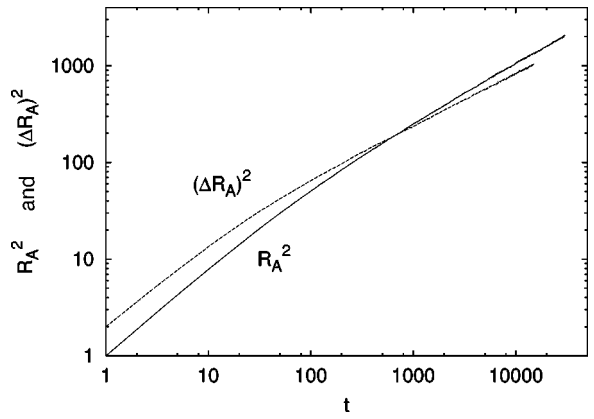

FIG. 2. The full line represents the mean squared displacement of the A particle in $d=1$, for $c=0.5$. The broken line represents the mean squared distance between two A particles, when conditioned on the the survival of both.

trivially weighted ensembles. On the other hand, the simulation is stopped as soon as one of the A's is absorbed, or if the weight of the configuration is too small. Thus all our results are based on *conditional probability distributions*, conditioned on the survival of all A's. These features are implemented by the pruning-cloning-Rosenbluth method (PERM) [15] that is a general growth method (using ''sequential importance sampling with resampling'' in the sense of Ref. [16]) and has been very successful in a large number of problems [13,17].

Assume that we have a single A (the case for k A particles with $k>1$ is straightforward) that has arrived at site i at time t. The fact that we condition on those events where A is not absorbed means that there cannot be a B at this site. Thus the homogeneity of the unconditioned distribution is broken, and an effective *hole* in the B distribution is introduced. For times $>t$ this hole makes a random walk. If it meets a hole produced at a time $\neq t$, the two recombine.

In principle, one could simulate these holes explicitly, i.e., one could simulate the A's in a background of B where a B [sic] particle is removed each time it hits an A. We indeed did perform such simulations. They agreed with the straightforward simulations not using the PERM or any conditioning and were more accurate, but the accuracy of both types of simulations was rather poor in comparison with our final algorithm.

Our final ingredient is that we do an exact summation over the B paths. This depends crucially on the fact that the B distribution is Poissonian. The latter is still true for the conditioned distribution (it would not be true in the reaction $A+B\rightarrow 0$, therefore our method cannot be used for it). A Poisson distribution is uniquely characterized by its mean. The evolution of this mean is described by a modified diffusion equation. More precisely, we describe the B density by a homogeneous background c minus a density $\rho(i,t)$ of holes. The latter is at every time step set equal to c at the actual A position, but otherwise evolves according to the simple diffusion equation $\rho(i,t+1)=(2d)^{-1}\Sigma_{\langle j,i\rangle}\rho(j,t)$. Its initial condition is $\rho(i,0)=0$. At each time step the A (which is assumed to be at site i) has a chance $\exp[\rho(i,t)-c]$ to be absorbed, i.e., the weight of the event in the conditioned ensemble decreases by a factor $\exp[c-\rho(i,t)]$. The algorithm used in Ref. [13] for the trapping problem is just a simplification where we omit the diffusion of the holes.

All our simulations were done on workstations, with a total of a few hundred hours of CPU time. All results were carefully checked for small t against straightforward brute force simulations with the most simple algorithm. In addition, we also made simulations with algorithms of intermediate complexity and efficiency. For $d=1$ and 1 A particle per configuration, we made, e.g., $\approx 54\,000$ configurations, out of which ca. 5000 independent ones survived up to the maximal time $t=30\,000$. In contrast, for brute force and Rosenbluth-Rosenbluth [14] methods we made runs that started altogether with $\approx 2\times 10^9$ A particles each. But all these particles were gone after a few thousand time steps, making these runs much less efficient. For higher dimensions the statistics were comparable.

We first discuss the results for $d=1$. Here we can use lattices so large that none of the holes ever reaches the boundary, thus we have no finite size effects at all. In Fig. 1(a) we show the survival chances $P_A(t)$ of a single A particle and of a pair of particles that started at the same site. For the latter, $P_A(t)$ is the probability that *both* particles of the pair survive. Although these probabilities become as small as 10^{-35}, the statistical errors are much smaller than

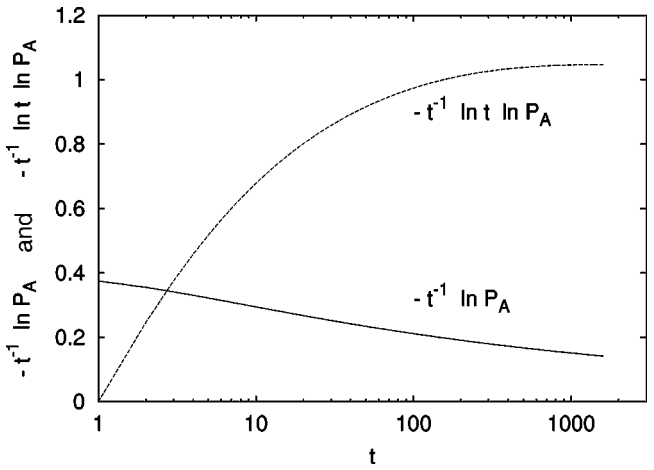

FIG. 3. The full line represents $-t^{-1}\ln P_A(t)$ for $d=2$ and $c=0.5$; the broken line represents the $-t^{-1}\ln t \ln P_A(t)$ from the same data. The horizontal scale is logarithmic, the vertical is linear.

the thickness of the lines. The fact that P_A for a pair is larger that the square of P_A for a single particle is easily understood. If already one A particle has survived in some region, there are less than average B particles in this region, and the second A particle has a bigger survival chance. Theoretically [6,7] we expect $P_A(t)\sim\exp(-\text{const}\sqrt{t})$, at least for a single particle. In Fig. 1(b) we thus show $t^{-1/2}\ln P_A(t)$ on a semilogarithmic scale. Error bars are here <0.001. Thus the decline for $t>1000$ is statistically highly significant for both curves. Unless we accept that there is an error in Refs. [6,7], we have to conclude that at least this decline of $-t^{-1/2}\ln P_A(t)$ for a single A particle is a finite t effect, and that the true asymptotic behavior sets in at $t\gg 10^4$. We also compared our data with the prediction $-\ln P_A(t)\sim t^{-1/4}$ of Ref. [9], with even worse agreement. Although that latter prediction was for $A+B\to 0$, $n_A(0)<n_B(0)$, we pointed out already that both models should show the same asymptotics. We thus conclude that the data are in rough agreement with Refs. [6,7], but the very big deviations are surprising (in particular since they are not monotonic) and not understood.

The mean squared displacement $\langle R_A^2\rangle$ of the (surviving) A particle is shown in Fig. 2. In this figure we also show the

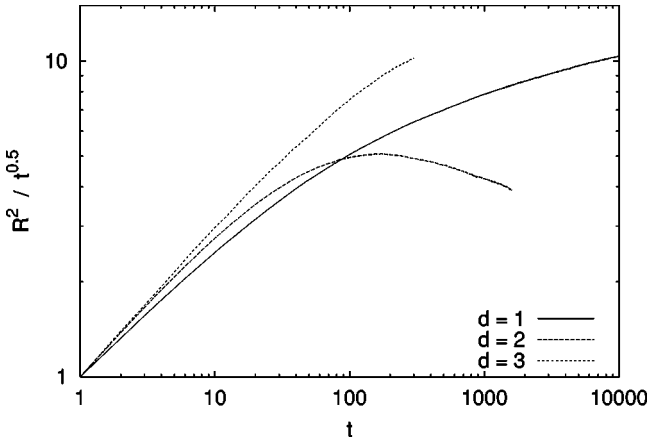

FIG. 4. Log-log plot of mean squared displacements in one, two, and three dimensions, divided by $\sqrt{t}$.

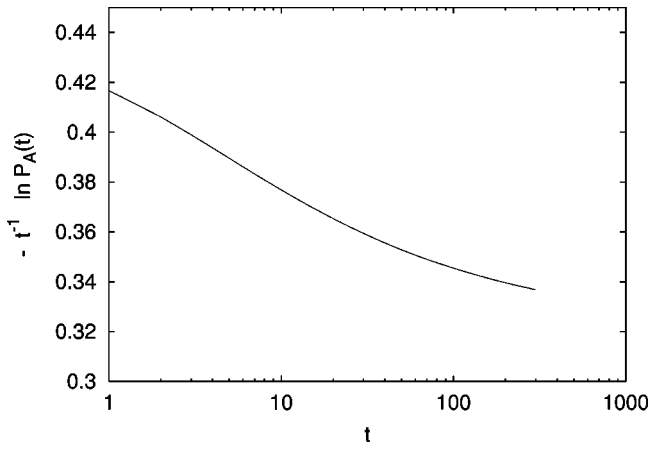

FIG. 5. Log-linear plot of $-t^{-1}P_A(t)$ for $d=3$, $c=0.5$.

squared distance between two A particles that started off simultaneously at the same site. We see that ΔR increases less fast than R, indicating an effective attraction mediated by the B particles. If already one A particle has survived in some region, there are less than average B particles in this region, and the second A particle will not only survive longer, but it will also survive preferentially in a region close to the first one. But this appears to be a weak effect. The most economic conclusion from Fig. 2 is that both curves converge to the same scaling behavior, $R^2\sim(\Delta R)^2\sim t^\nu$ with $\nu=0.5$ to 0.6. But any determination of a critical index should be taken with great caution in view of Fig. 1, we should not take any behavior seen for $t<10^5$ as reflecting the asymptotic behavior.

With increasing d, updating $\rho(i,t)$ becomes more and more time consuming. Thus we can simulate only for much shorter times, if we want to avoid excessive CPU times or large finite size corrections. For $d=2$, results for $t^{-1}\ln P_A(t)$ with $c=0.5$ are shown in Fig. 3, together with $-t^{-1}\ln t\ln P_A(t)$. For large values of t the data agree much better with Eq. (1) than with the alternative prediction $-\ln P_A(t)\sim at-bt^{1/2}$ of Ref. [10]. The factor $1/\ln t$ in Eq. (1) seems to be correct asymptotically, although it makes agreement worse for small t. Anyhow, deviations from Eq. (1) are substantial, and even for the largest t where the curve appears to be horizontal in the figure [and where, by the way, $P_A(t)\approx 10^{-98}$] it still shows a definite curvature.

The fact that the asymptotia could not have been reached by these 2D data is most clearly seen from $\langle R_A^2\rangle$. It is shown in Fig. 4, together with the analogous data from $d=1$ and $d=3$. To make the point particularly clear we show there $\langle R_A^2\rangle/\sqrt{t}$ against t. If $d=2$ is the upper critical dimension for $A+B\to B$ as suggested by Eq. (1), then we should expect $\langle R_A^2\rangle\sim t$ up to logarithmic corrections in $d=2$. We also should expect that the data for $d=2$ should fall between those for $d=3$ (where we expect $\langle R_A^2\rangle\sim t$) and $d=1$ (where $\langle R_A^2\rangle\sim t^\nu$ with $\nu<1$). Figure 4 shows a completely different behavior. On the one hand, $\langle R_A^2\rangle$ is *very far* from being $\sim t$, on the other hand the data are not monotonic with d.

One might expect that the asymptotic behavior is observed earlier for higher values of the concentration c. We

performed therefore also 2D simulations with $c=0.7$ and $c=1.0$. As expected, P_A and $\langle R_A^2 \rangle$ both decrease with an increase in c, but the strange time dependence of $\langle R_A^2 \rangle$ persisted.

Finally, we show in Fig. 5 the survival probability in $d=3$, again for $c=0.5$. More precisely, we show $-\ln P_A(t)/t$. It depends quite strongly on t, but its curvature is consistent with convergence to Eq. (1) without further surprises.

In conclusion, we have performed simulations of a trapping model in which both traps and trapped particles are mobile with equal mobilities. The simulations, undertaken with the hope of understanding the precise crossover to the exactly known asymptotic behavior, are much more extensive than the previous simulations of this model, in the sense of reaching much longer times and much lower survival probabilities. This was possible due to an algorithm used here. In spite of the vastly improved numerics we have not been able to understand all details of the model. Some of our results are indeed quite puzzling. On the other hand, our methods can be possibly applied also to other models where absorbers are free particles undisturbed by the particles that they absorb. One class of such models are, e.g., gated reaction-diffusion systems of the type $A+B\rightarrow 0$ with stochastically changing reaction rates [18].

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