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Asymptotic behavior of $A+B \to$ inert for particles with a drift

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We consider the asymptotic behavior of the (one dimensional) two-species annihilation reaction $A + B \to 0$, where both species have a uniform drift in the same direction and like species have a hard core exclusion. Extensive numerical simulations show that starting with an initially random distribution of A's and B's at equal concentration the density decays like $t^{-1/3}$ for long times. This process is thus in a different universality class from the cases without drift or with drift in different directions for the different species.

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The irreversible two-species annihilation reaction $A+B \to 0$ has been studied for quite some time as an example of a reaction diffusion process where fluctuations are important, so that the density may decay more slowly than one would predict from the mean field rate equations (at least in low dimension) [1–7]. If the initial concentrations of the two species differ, then the density of the "lesser" species decays exponentially, as is expected from mean field theory. The more interesting case occurs when the concentrations are the same: the standard picture [1] is that in a region of size L it takes a time on the order of L^2 for all the particles to react, since they must diffuse around the region in order to annihilate. The remaining density will be proportional to the initial excess of either type A or type B particles in this region, which is proportional to the square root of the volume. Thus at time t one expects that the concentration $c(t)$ will behave as

$$\begin{aligned} c(t) &\sim [c(0)L^d]^{1/2}/L^d \sim [c(0)t^{d/2}]^{1/2}/t^{d/2} \\ &= c(0)^{1/2}t^{-d/4}, \end{aligned} \tag{1}$$

for dimension $d \leq 4$, i.e., $c(0)^{1/2}t^{-1/4}$ in dimension one, which has been verified rigorously [4,7]. In comparison the mean field result is $c(t) = [t + 1/c(0)]^{-1}$.

In order for this picture to be valid, it is necessary that the distribution of particles be actually determined by diffusion. The addition of a drift field can invalidate this assumption.

That this happens when the two species drift in opposite directions is not unexpected. If the dynamics are such that the two species have a relative velocity v, there will be two relevant length scales, with $L_{\parallel} \sim vt$ and $L_{\perp} \sim t^{1/2}$. Then using the same reasoning as above, one determines the concentration to be [8,9]

$$\begin{aligned} c(t) &\sim [c(0)vt^{(d+1)/2}]^{1/2}/[vt^{(d+1)/2}] \\ &= [c(0)v]^{1/2}t^{-(d+1)/4} \end{aligned} \tag{2}$$

for dimension $d \leq 3$, or $[c(0)v]^{1/2}t^{-1/2}$ in one dimension.

What is perhaps unexpected is that if the two species have a drift in the *same* direction, even if their relative velocity is zero, the result may still be different from the expected $t^{-d/4}$. This is because even after subtracting off the average motion, one does not necessarily recover diffusive behavior.

In order to proceed, we must specify the model further. To keep matters simple we consider a strong drift—particles move either to the right or not at all. We consider two types of particles moving on the one dimensional lattice (with periodic boundary conditions). At each (micro) time step, we randomly pick a site. If that site is occupied, we attempt to move the particle to the right. If the site on the right is unoccupied, the jump succeeds. If the site is occupied by a particle of the same species, the jump fails. If the site is occupied by a particle of the opposite species, both particles annihilate.

We now see why the diffusive picture might be invalid. If we just considered one species of particles, the model described above is the asymmetric simple exclusion process (ASEP), and the long time behavior is not governed by a linear diffusion equation. Instead one must consider a nonlinear stochastic equation such as the noisy Burgers equation [10],

$$\frac{\partial \rho}{\partial t} + \rho\frac{\partial \rho}{\partial x} = \nu\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial \xi}{\partial x}, \tag{3}$$

where ρ is a rescaled density, ν is the viscosity (representing the lattice spacing), and ξ is a random noise term, e.g., white noise where the covariance is

$$\langle \xi(x,t)\xi(x',t')\rangle = 2\nu\delta(x-x')\delta(t-t'). \tag{4}$$

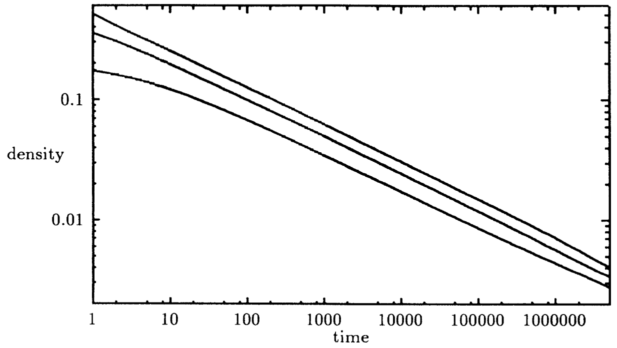

FIG. 1. Log-log plot of density vs time for system of size 4×10^6. Initial densities are 0.9, 0.5, and 0.2.

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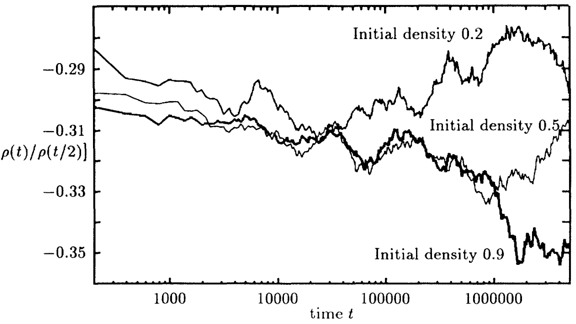

FIG. 2. Semilog plot of $\log_2[\rho(t)/\rho(t/2)]$ vs time for system of size 4×10^6. Initial densities are 0.9, 0.5, and 0.2.

Thus the exclusion rule, even for very low densities, can play a crucial role in the dynamics of the annihilation process, contrary to the popular view. The importance of the exclusion rule can also be seen by comparing this model with studies of the reaction $A+A\rightarrow 0$ [11], where there is no hard core exclusion and where the introduction of a drift does not change the asymptotic behavior of the decay of the density.

We studied the time evolution of the density for a variety of system sizes and initial densities (always taking equal concentration of A and B particles). We considered systems up to size 4×10^6 for up to 5×10^6 time steps. Some example runs are shown in Fig. 1. We see that qualitatively the asymptotic behavior seems to be independent of the initial density, and that there appears to be a power law decay of the density with exponent approximately equal to $-1/3$.

To get a better view of the slope of these curves we examined the behavior of $\rho(t)/\rho(t/2)$ as a function of time. Specifically, $\log_2[\rho(t)/\rho(t/2)]$ should give the slope of the line (i.e., the exponent of the power law behavior). Data for the same three runs as in Fig. 1 are plotted in Fig. 2. This confirms that the decay behaves similarly for the different initial densities, although the noise is now much more apparent. To reduce the effect of this, we averaged the slopes illustrated in Fig. 2 over 11 different initial densities. The resulting data are reproduced in Fig. 3. The error bars represent the standard deviation of the different slopes.

The error bars at early times are primarily systematic in origin. They represent the fact that the decay rates are initially different for different initial densities—the particle motion is diffusive in nature until the particles have had a chance to interact with each other, so that we see $t^{-1/4}$ behavior at early times for low density. On the other hand, the errors at large time are primarily random errors; fluctuations in the initial density are significantly amplified when the density gets small.

Extrapolating the data of Fig. 3 to infinite time is problematic. It is not clear whether the effective exponent will continue to decrease; all one can say with confidence is that it is less than -0.31. There are arguments, however, for believing that the answer should be $-1/3$, and in particular, not $-1/4$.

The exponent $-1/4$ for the diffusive case arises because the relevant diffusive length scale at time t is $t^{1/2}$. On the other hand, in the noisy Burgers equation (3) and thus in the one dimensional ASEP, there is superdiffusive behavior, so that fluctuations spread more quickly and the length scale is larger. Thus the relevant length scale is $t^{2/3}$ [12,13]. Thus one might expect the concentration to go as

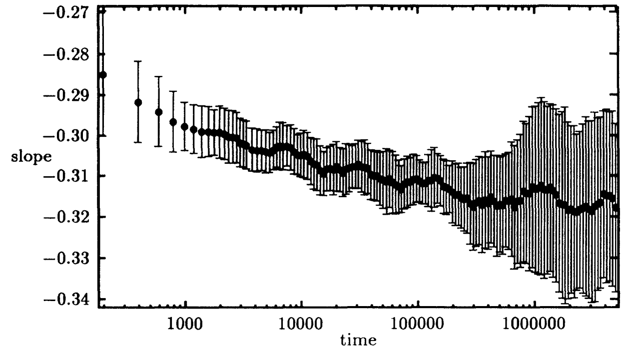

FIG. 3. Semilog plot of average slope vs time for system of size 4×10^6.

$$c(t)\sim L^{1/2}/L\sim[t^{2/3}]^{1/2}/t^{2/3}=t^{-1/3}, \tag{5}$$

certainly consistent with what is observed. Of course, this argument neglects the fact that only isolated clusters of one species undergo asymmetric simple exclusion dynamics, but one expects that clusters of each species do spend most of their time reasonably isolated from each other [5,6], so that this analysis should be applicable. Presumably a more detailed investigation of the correlations of the clusters, along the lines of [5,6], would shed light on this matter.

Additional evidence for this process being in a different universality class comes from work by Ben-Naim and Zhuo [14], which uses an exact enumeration of states to obtain the particle density via a power series in time. The best-fit exponent for the decay of this model, fitting the series using Padé approximants, is -0.305 [15], and appears to be decreasing (moving away from -0.25) as one computes more terms in the series.

One expects that the observed behavior should be universal for any system for which the dynamics are governed by the noisy Burgers equation (3). If instead of totally asymmetric dynamics one chose a lesser bias the exponent would be the same, although it would take longer for this to be apparent. For small bias one would expect initially to see diffusive behavior, followed by a crossover to the nonlinear regime. Unfortunately, given that one is just barely able to access the asymptotic regime in the totally asymmetric case, it does not seem likely that one will be able to directly observe this crossover. Truly different behavior would be expected only if the dynamics of the model were governed by a model with a different (nonquadratic) nonlinearity.

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