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Two-species annihilation with drift: A model with continuous concentration-decay exponents

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We propose a model for diffusion-limited annihilation of two species, $A+B\rightarrow A$ or B, where the motion of the particles is subject to a drift. For equal initial concentrations of the two species, the density follows a power-law decay for large times. However, the decay exponent varies *continuously* as a function of the probability of which particle, the hopping one or the target, survives in the reaction. These results suggest that diffusion-limited reactions subject to drift do not fall into a limited number of universality classes.

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Diffusion-limited reactions (DLR's) in low dimensions have been extensively studied because of their anomalous kinetics, and because they serve as simple prototypes of complex, nonequilibrium dynamical systems [1–10]. Recently, attention has focused on anisotropic DLR's: the particles move preferentially in one spatial direction, giving rise to an effective drift [11–16].

For the one-species DLR of coalescence, $A+A\rightarrow A$, and annihilation, $kA\rightarrow 0$, it has been shown that the spatial anisotropy introduces no appreciable changes [11,15,16]. However, the two-species annihilation process, $A+B\rightarrow 0$, exhibits markedly different behavior with or without drift [12–14]. In one dimension, when the initial concentrations of A and B particles are equal, the total concentration decays as $t^{-1/4}$ in the isotropic case, and as $t^{-1/3}$ in the presence of drift. This interesting behavior is attributed largely to the hard core repulsion between particles of like species. A heuristic explanation, based on the Burgers equation, for the $t^{-1/3}$ decay has been presented along these lines [13,14]. A recent exact analysis of a two-species annihilation model with no hard core interactions confirms their essential role: in their absence, the concentration decays as $t^{-1/4}$, with or without the drift [16].

In this work, we introduce an anisotropic two-species annihilation model, with hard core interactions between like species. A distinct characteristic of our model is that it contains an adjustable parameter. We find that the concentration power-law decay exponent depends *continuously* on this parameter. Nonuniversal exponents are a surprising feature. Our finding is based on extensive numerical Monte Carlo simulations to be detailed below.

Our model is defined on a one-dimensional lattice. Each lattice site can be in one of the three states: empty (0), occupied by a single A particle, or occupied by a single B particle. Numerical results were obtained for the case of maximum anisotropy [12–14], where particles may hop only to the nearest site to their right:

$$\ldots A0\ldots \rightarrow \ldots 0A\ldots,\quad \ldots B0\ldots \rightarrow \ldots 0B\ldots, \tag{1}$$

with equal rates for A and B. Hopping is disallowed if the target site is occupied by a particle of the same species; this models hard core interactions. If the target site is occupied by a particle of the opposite species, hopping is allowed and reaction takes place with outcome determined by the probabilistic rule

$$\ldots AB\ldots \rightarrow \begin{cases} \ldots 0A\ldots, & \text{prob. } p \\ \ldots 0B\ldots, & \text{prob. } 1-p, \end{cases}$$

and (2)

$$\ldots BA\ldots \rightarrow \begin{cases} \ldots 0B\ldots, & \text{prob. } p \\ \ldots 0A\ldots, & \text{prob. } 1-p. \end{cases}$$

The reaction may then be represented as

$$A+B\rightarrow A \text{ or } B\ , \tag{3}$$

where the product species is that of the hopping particle, with probability p, or that of the target particle, with probability $1-p$. Thus p may be thought of as a parameter which represents the "persistence" of the hopping particle. Stoichiometrically, however, the reaction rule is equivalent to the symmetric annihilation reaction

$$A+B\rightarrow \tfrac{1}{2}A+\tfrac{1}{2}B\ , \tag{4}$$

regardless of the value of p, because the number of AB nearest-neighbor pairs is equal to the number of BA nearest pairs (assuming homogeneous initial distributions), even for unequal concentrations of A and B particles.

We have performed concurrent simulations of the above model on a cluster of over 50 IBM RS6000 workstations, for lattices of 10^6 sites, with periodic boundary conditions. Simulations ran up to times $t=10^6$. Particle hopping was random and independent, with the rate defined so that in one time unit each of the surviving particles performs an average of one hopping attempt. The attempt could lead to motion, reaction, or be discarded, depending on the state of the target site.

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Data from about 50 such runs were collected for five different persistence values: $p=0$, 0.25, 0.5, 0.75, and 1. All runs began with an 80% full lattice, with equal concentrations of A and B particles, distributed randomly.

In Fig. 1, we show a log-log plot of the concentration decay as a function of time as obtained from simulations. The data exhibit an asymptotic power-law decay with a p-dependent exponent. In Fig. 2, we plot the local slopes of the decay curves as a function of time. The decay exponents are obtained through extrapolation to time $t \rightarrow \infty$. Our estimates for the decay exponent for different values of the persistence parameter are listed in Table I.

One of the recognized fluctuation effects in two-species reactions is the tendency of the system to develop large alternating domains of A and B particles [7,13,14,17,18]. We also collected data for some quantities of interest associated with this phenomenon. These include $\langle l_{AB}(t) \rangle$, the average distance between nearest particles of opposite species; $\langle l_{AA}(t) \rangle$, the average distance between nearest particles of the same species; $\langle L(t) \rangle$, the average length of a domain of like particles, measured between the first particles of adjacent domains; and $\langle n(t) \rangle$, the average number of particles per domain. In the large-time asymptotic limit, each of these quantities grows as a power of t. The relation $c \sim \langle n \rangle / \langle L \rangle$ was used to check for consistency. Simulation results (from about 600 runs on 10^5-site lattices) are summarized in Table I. The error margins in the table are meant only as rough estimates and may be overly optimistic. They merely represent the spread of values we have obtained by extrapolating the data with different powers of $1/t$.

The case of $p=1$ seems special in that the number of particles per domain remains bounded and of order unity, even after very long times. In addition, the concentration decays as $t^{-1/2}$, similar to isotropic one-species coalescence, $A+A \rightarrow A$. These results are particularly interesting in view of the following considerations.

Suppose that through fluctuations large domains of A and B particles were created, for general p. Left alone, each domain moves with the drift velocity, while the particle distribution in it is governed by the hard core constraint and is related to the Burgers-equation theory; see [13,14] and references therein. However, reactions at both ends modify the domain structure. Our results suggest that the interplay of the two processes is nontrivial for all $0 \leq p < 1$, and the domain size measures involve nontrivial, varying exponents; see Table I. Self-organization by formation of large domains has been viewed as an essential condition for non-mean-field behavior in low-dimensional reactions [6,7,17,18].

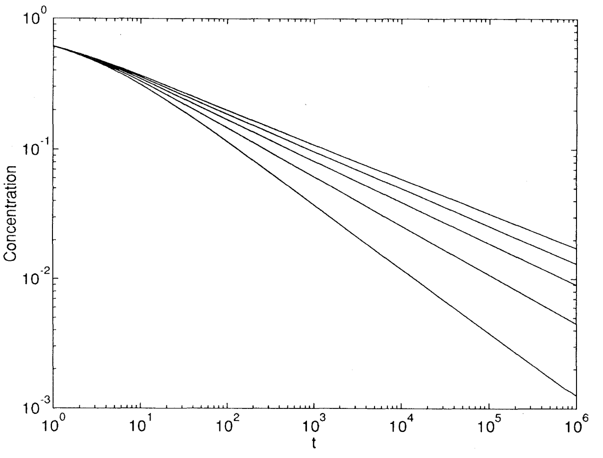

FIG. 1. Concentration decay for different values of the persistence parameter. The solid curves represent simulation data for $p=0$, 0.25, 0.5, 0.75, and 1 (top to bottom).

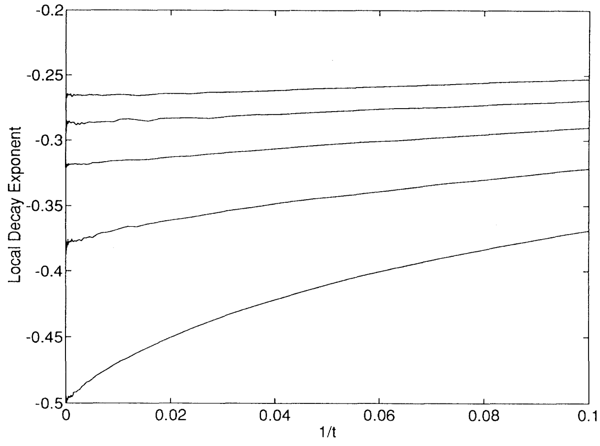

FIG. 2. Local power-law decay exponents for $p=0$, 0.25, 0.5, 0.75, and 1 (top to bottom) as a function of inverse time. The power-law decay exponents are obtained from the local slopes of the curves in Fig. 1.

However, for $p=1$, we find that there are no large domains. This indicates that, if a large domain of, for instance, A particles, were formed, it would be destroyed by B particles "catching up" from the left. Indeed, for $p=1$ the incoming, hopping particle determines the species of the reaction product with probability 1. Thus, regardless of the size of the A domain, its denser, left end will be destroyed by B particles faster than its dilute, right end could catch up with other A particles, while eliminating the B particles in between. The formation of the shocklike profile due to the interplay of *hard core* and *anisotropy* is essential for this phenomenon, i.e., we need the two domain ends to have different densities.

Once the $p=1$ system is mixed, one would naively anticipate the mean-field behavior, $\sim 1/t$. However, we

TABLE I. Characteristic exponents for various values of the persistence parameter p. The exponents are $c \sim t^{-\alpha}$, $\langle l_{AA} \rangle \sim t^{\beta}$, $\langle l_{AB} \rangle \sim t^{\gamma}$, $\langle L \rangle \sim t^{\delta}$, and $\langle n \rangle \sim t^{\eta}$. The error margins represent the spread of values obtained from extrapolations with various powers of $1/t$.

p	α	β	γ	δ	η
0	0.266(3)	0.292(3)	0.32(1)	0.662(6)	0.41(1)
0.25	0.289(3)	0.311(3)	0.34(1)	0.660(7)	0.39(1)
0.5	0.320(3)	0.345(3)	0.38(1)	0.619(5)	0.309(6)
0.75	0.380(2)	0.400(4)	0.44(1)	0.585(5)	0.215(7)
1	0.499(1)	0.504(6)	0.500(6)	0.499(6)	0.003(4)

know from reactions like $A+A\rightarrow 0$, or A, that non-mean-field fluctuations can also arise in "well-mixed" situations (no domains), in the form of non-mean-field interparticle distributions [19]. Detailed studies of the interparticle distribution for the $p=1$ model will be reported in the future. Since all known one-dimensional reaction-diffusion systems, with or without hopping isotropy, possess only one "diffusive" length scale, $\sim t^{1/2}$, the exponent values of $\frac{1}{2}$ for the $p=1$ model (see Table I) are probably exact.

The case of $p=\frac{1}{2}$ resembles the anisotropic two-species annihilation model, $A+B\rightarrow 0$, studied by Janowsky [12,13] and by Ispolatov, Krapivsky, and Redner [14]. Notice that the difference in the number of particles between the two species, N_A-N_B, is locally conserved (in every reaction event) in the Janowsky [12] model, but only *globally* conserved in the present model. This distinction is of no serious consequence in the isotropic case of no drift [20]. In the case of drift, we argue that the two models should be similar. In particular, the heuristic arguments of Ispolatov, Krapivsky, and Redner [14] could be repeated for our model with $p=\frac{1}{2}$, almost without change, obtaining the same conclusions and predictions. Indeed, our simulation results for $p=\frac{1}{2}$ are not inconsistent with those already published for $A+B\rightarrow 0$.

An interesting observation is that for $p=\frac{1}{2}$ the convergence to the long-time asymptotic behavior of our model seems faster than that of the Janowsky model. An example is shown in Fig. 3, where we plot the time-dependent exponent of the concentration decay [obtained from local slopes of $\log(c)$ vs $\log(t)$], for both cases. We have no explanation for this phenomenon. Perhaps it could be exploited to settle the slight discrepancies between the numerical findings of Janowsky [12,13] and the results of Ispolatov, Krapivsky, and Redner [14].

In summary, we have proposed a one-dimensional DLR model with continuously varying exponents. It is important to emphasize that our density-exponent values were determined largely by numerical studies, and furthermore, the actual estimates range from $\frac{1}{2}$ for $p=1$ down to near $\frac{1}{3}$ at $p=\frac{1}{2}$, and to about $\frac{1}{4}$ for $p=0$. Since all three values $\frac{1}{4}$, $\frac{1}{3}$, and $\frac{1}{2}$, and only these values, have been encountered for various universality classes of other one-dimensional reactions, one could suspect that our observation of continuous exponents is an artifact of finite-time numerics. However, our numerical simulations were really "large scale" by modern standards, and the data presented seem to suggest error limits which clearly favor continuous variation rather than a smooth crossover between three universal values.

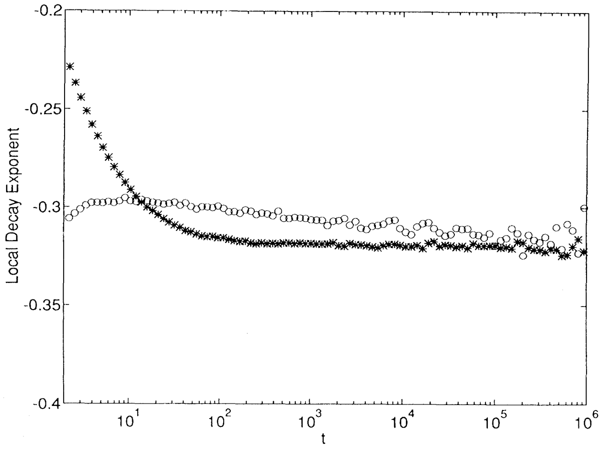

FIG. 3. Comparison of the local slopes of $\log(c)$ vs $\log(t)$ between our model with $p=\frac{1}{2}$ ($*$) and the anisotropic annihilation model, $A+B\rightarrow 0$ ($\circ$).

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