Kinetics of two-species ballistic annihilation

Yu Jiang and F. Leyvraz
Instituto de Fisica, Laboratorio de Cuernavaca, Universidad Nacional Autónoma de México, Apartado Postal 139-B, Codigo Postal 62191, Cuernavaca, Morelos, Mexico
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We study the kinetics of two-species annihilation $A+B\to 0$, with dichotomic and continuous initial velocity distributions in one dimension. For a discrete model, the concentration and the domain size are found to change as $c_A(t)\sim t^{-0.497}$ and $v_{AB}(t)\sim t^{0.088}$, respectively; the decay of concentration is accounted for by a simple analysis. For a continuous model, a scaling relation for the exponents, which describe the decay kinetics and spatial structure of the system, is found to hold in one dimension.

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The dependence of chemical kinetics on the motion of reacting particles has been studied in great detail in the last ten years, with the discussion of geometrical and dimensional effects on diffusion-limited [1–4] as well as on ballistic reactions [5–7]. For irreversible diffusion-limited reactions, it is found that the density decays more slowly than the predictions of mean-field theory in spaces whose dimensions are below the critical dimension. In

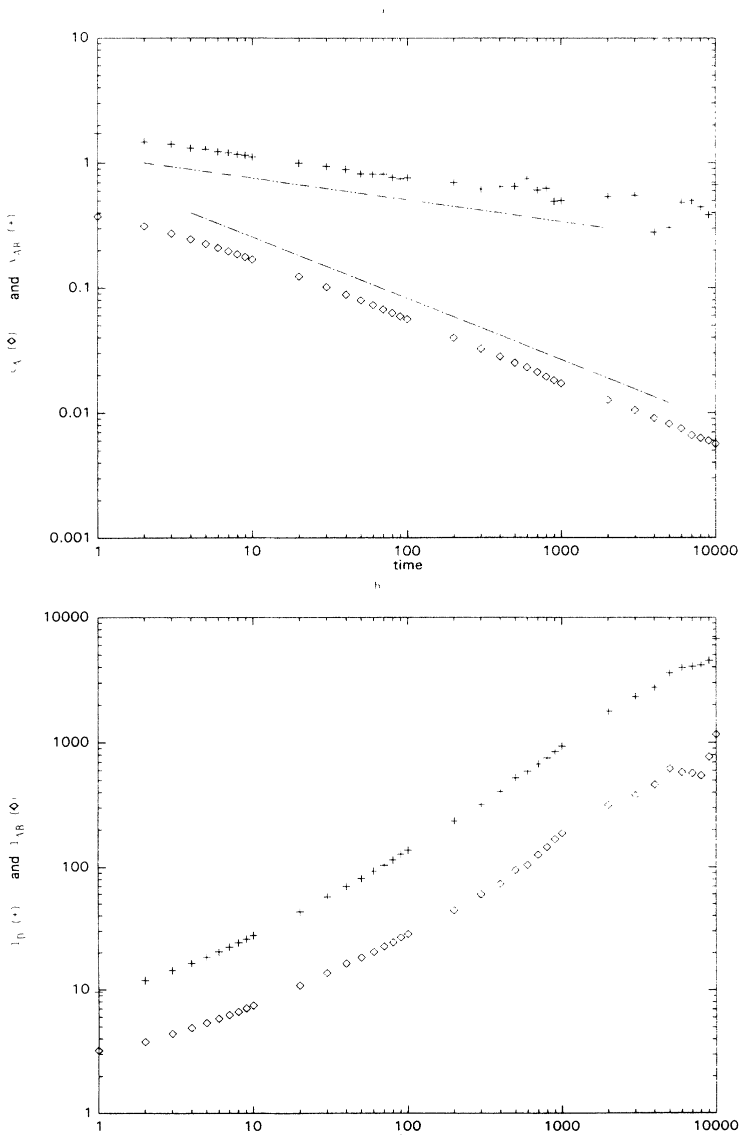

FIG. 1. Monte Carlo simulation results for the discrete model with ten realizations on a 100 000-site ring. (a) The concentration c_A (◇) and the typical velocity v_{AB} (+) vs time, (b) the interdomain spacing l_{AB} (◇) and the domain size l_D (+) vs time.

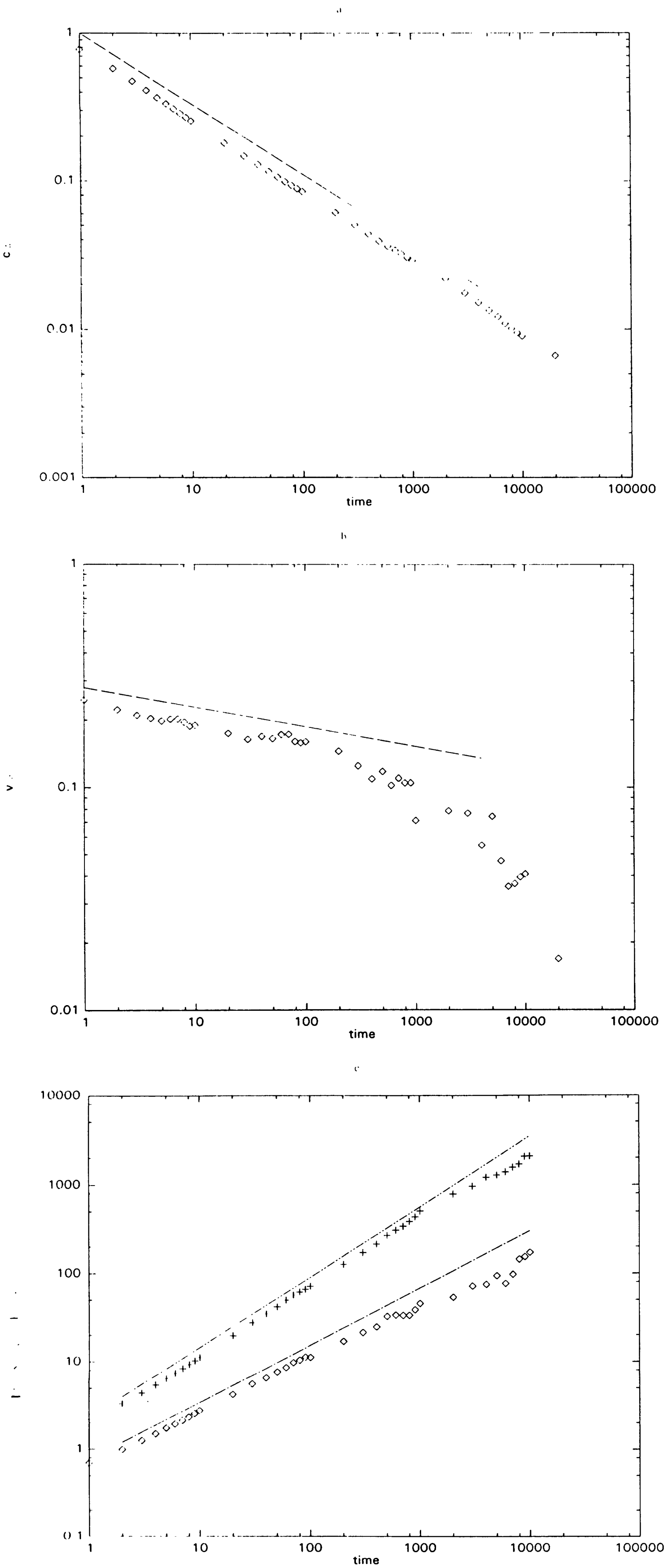

FIG. 2. Monte Carlo simulation results for the continuous model with ten realizations on a 100 000-site ring. (a) The concentration c_A against time, (b) the typical velocity v_{AB} vs time, (c) the interdomain spacing l_{AB} (◇) and the domain size l_D (+) vs time.

two-species annihilation, the dynamic formation of large-scale spatial heterogeneities is found in an initially homogeneous system. For ballistic annihilation reaction, $A+A\to 0$, it is found that the concentration decays as $c(t)\to t^{-1/2}$ for dichotomic initial velocity distribution [5], while the concentration and the rms velocity decay as $c(t)\to t^{-\alpha}$ and $v_{\rm rms}(t)\to t^{-\beta}$, respectively, with $\alpha+\beta=1$, for continuous initial velocity distribution [7].

In this presentation, we study the decay kinetics and the domain motion of the two-species annihilation process $A+B\to 0$, for both discrete and continuous initial velocity distributions. We consider an idealized model in which two species, A and B, are initially distributed on a real line. Their velocities are distributed according to an initial distribution $P(v,t=0)$ with zero mean. We focus on two special cases: the discrete model, in which the velocity of the particle will assume $+1$ or -1 while its position will take on the integers only, and the continuous model, in which a continuous initial velocity distribution is considered. Particles move according to their initial velocity until a collision between two unlike particles occurs, which results in the removal of both colliding particles. We are interested in determining the time dependence of the concentration c_A and the spatial structure characterized by the domain size l_D and interdomain spacing l_{AB} [4]. Assume that the concentration c_A, the velocity difference between two neighboring unlike particles v_{AB}, the interdomain spacing l_{AB}, and the domain size l_D behave asymptotically as

$$c_A\sim t^{-\alpha}\ , \tag{1}$$

$$v_{AB}\sim t^{-\beta}\ , \tag{2}$$

$$l_{AB}\sim t^{\gamma}\ , \tag{3}$$

$$l_D\sim t^{\delta}\ , \tag{4}$$

respectively. First, let us consider the discrete model. In this model, A's and B's are initially distributed uniformly on a periodic one-dimensional lattice chain. Their velocities take on either $+1$ or -1. The system may be divided into two groups: one consisting of A^+'s (particles of species A with velocity $v_A=+1$) and B^-'s, the other of B^+'s and A^-'s. Notice that there is no interaction between those two groups, due to the dichotomic initial velocity distribution considered in this model. It is easily seen that the subsystem is equivalent to the ballistic one-species annihilation, $A+A\to 0$, with discrete bimodal velocity distribution,

$$P(v,t=0)\propto p\delta(v-1)+(1-p)\delta(v+1)\ . \tag{5}$$

For $p=\frac{1}{2}$, one has [5]

$$c_A(t)\sim t^{-1/2}\ . \tag{6}$$

This result has been confirmed by the Monte Carlo simulations. In Figs. 1(a) and 1(b), we see that the concentration and the velocity difference decay according to some power laws. However, the discrete model has pathologies since the multiple pair reactions (at the same time) take place with a finite probability. So we found numerically that an initially homogeneous system does "coarsen" into alterating A-rich and B-rich domains, but the scaling is not obvious for the domain and interdomain sizes [see Fig. 1(c)].

For the continuous model, there will be typically a reaction in each gap in a time interval $\Delta t\sim l_{AB}/v_{AB}$. This leads to a change in concentration, which is proportional to the inverse domain size, hence,

$$\frac{\Delta c_A}{\Delta t}\simeq\frac{dc_A}{dt}\propto\frac{1/l_D}{l_{AB}/v_{AB}}\ . \tag{7}$$

Substituting Eqs. (1)–(4) into Eq. (7), one obtains a relation for the scaling exponents,

$$1+\alpha=\beta+\gamma+\delta\ . \tag{8}$$

We found numerically that $\alpha=0.4753$, $\beta=0.046$, $\gamma=0.7986$, and $\delta=0.5995$, showing that the scaling relation (8) is valid, at least in one dimension (see Fig. 2). It should be noticed that the scaling property for the mean-square value of velocity difference of unlike particles, i.e., $v_{AB}^2\sim t^{2\beta}$, is not obvious. This implies that the v_{AB} (defined as the velocity difference of two neighboring unlike particles) might not be the proper measure of two approaching adjacent domains. However, further investigation is required to clarify the situation.

In summary, the ballistic two-species annihilation with general particle initial velocity distribution exhibits a rich variety of decay kinetics and domain structure. Numerical results indicate nonuniversality in the exponents that describe the decay of the concentration and the typical velocity, as well as the domain motion. A simple analysis accounted for the decay of the concentration for the discrete model. Obviously, a general theory to account for the kinetical behavior of the two-species ballistic annihilation reaction is highly desirable.

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