Dynamic scaling behavior of an interacting monomer-dimer model

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We study the dynamic scaling behavior of a monomer-dimer model with repulsive interactions between the same species in one dimension. With infinitely strong interactions the model exhibits a continuous transition from a reactive phase to an inactive phase with two equivalent absorbing states. This transition does not belong to the conventional directed percolation universality class. The values of dynamic scaling exponents are estimated by Monte Carlo simulations for two distinct initial configurations, one near an absorbing state and the other with an interface between two different absorbing states. We confirm that the critical behavior is consistent with that of the models with the mass conservation of modulo 2.

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In recent years, nonequilibrium phase transitions occurring in surface reaction models [1–22] have attracted great interest, since they exhibit continuous transitions from a reactive phase into an absorbing phase. Many investigations of models for absorbing phase transitions have established a generally accepted belief that continuous transitions into a single absorbing state generically belong to one universality class, the directed percolation (DP) class [23–25]. This conjecture becomes extended to the multiple component models by the argument of Grinstein *et al.* [26].

Recently, a few models have appeared in the literature that are known to be in a different universality class from DP. Those are the models A and B of probabilistic cellular automa (PCA) introduced by Grassberger and co-workers [27,28], branching annihilating random walks with an even number of offspring (BAW) [29–32], nonequilibrium kinetic Ising (NKI) models with two different dynamics [33,34], and an interacting monomer-dimer (IMD) model [35]. Critical behaviors of these models are different from DP but seem to belong to the same universality class. The PCA, BAW, and NKI models are basically single component models (there are only two choices at a given site: vacant-occupied or spin-up–spin-down), while the IMD model is a multicomponent model (three choices: vacant-monomer-dimer). The common feature of these models is that the total number of particles (walkers in BAW, domain walls or kinks in PCA, NKI, IMD) is conserved of modulo 2. But there exist many types of kinks in the IMD model due to the multicomponent nature and each type of kink has no conservation law. So one needs to investigate the IMD model in more detail.

In our previous study of the IMD model [35], the steady-state exponents were numerically determined to be $\beta = 0.88(3)$, $\nu_\perp = 1.83(3)$, and $\nu_\parallel = 3.17(5)$, which agree well with the values of those exponents for the single component models [28,32,33]. In this study, we report the values of the dynamic exponents for the IMD model and show that these values are in excellent agreement with those of the BAW model with four offsprings recently studied in detail by Jensen [32].

The interacting monomer-dimer model is a generalization of the simple monomer-dimer model [5] on a catalytic surface, in which particles of the same species have nearest-neighbor repulsive interactions. This is parametrized by specifying that a monomer (A) can adsorb at a nearest-neighbor site of an already adsorbed monomer (restricted vacancy) at a rate $r_A k_A$ with $0 \leq r_A \leq 1$, where k_A is an adsorption rate of a monomer at a free vacant site with no adjacent monomer-occupied sites. Similarly, a dimer (B_2) can adsorb at a pair of restricted vacancies (B in nearest-neighbor sites) at a rate $r_B k_B$ with $0 \leq r_B \leq 1$, where k_B is an adsorption rate of a dimer at a pair of free vacancies. There are no nearest-neighbor restrictions in adsorbing particles of different species. Here we will consider only the adsorption-limited reactions. A nearest neighbor of the adsorbed A and B particles reacts immediately, forms the AB product, and desorbs the catalytic surface. Whenever there is an A adsorption attempt at a vacant site between an adsorbed A and an adsorbed B, we allow the A to adsorb and react immediately with the neighboring B, thus forming an AB product and desorbing the surface [36]. The case $r_A = r_B = 1$ corresponds to the ordinary noninteracting monomer-dimer model which exhibits a first-order phase transition between two saturated phases in one dimension. In the other limiting case $r_A = r_B = 0$, the system has no fully saturated phases of monomers or dimers, but instead two equivalent half-filled absorbing states. These states are comprised of only the monomers at the odd- or even-numbered lattice sites. A dimer needs a pair of adjacent vacancies to adsorb, so a state with alternating sites occupied by monomers can be identified with an absorbing state.

In this paper, we consider the one-dimensional IMD with $r_A = r_B = 0$ for simplicity. Then the system can be characterized by one parameter $p = k_A/(k_A + k_B)$ of the monomer adsorption-attempt probability. The dimer adsorption-attempt probability is given by $q = 1-p$. The order parameter of the system is the concentration of dimers in the steady state, which vanishes algebraically as p approaches the critical probability p_c from below. Finite-size-scaling analysis of the static Monte Carlo data reveals that this model behaves differently from the DP, but belongs to the same universality class as the models

in which the number of particles (or kinks) are conserved of modulo 2 [35].

We perform dynamic Monte Carlo simulations for the IMD model. We start with two distinct initial configurations, one near an absorbing state and the other with an interface between two different absorbing states. Dynamic simulations with the former initial configurations (conventional one) describe the evolution of a defect spreading on a nearly absorbing space. We call this "defect dynamics." The other dynamics with the latter initial configurations describe the evolution of interface spreading between two different absorbing states. In contrast to the defect dynamics, the system can never enter an absorbing state. We call this "interface dynamics."

In simulations for the defect dynamics, we start with a lattice occupied by monomers at alternating sites except at the central vacant site. Then the system evolves along the dynamic rules of the model. After one adsorption attempt on the average per lattice site (one Monte Carlo step), the time is incremented by one unit. A number of independent runs, typically 2.5×10^5, are made up to 8000 time steps for various values of p near the critical probabiility p_c. Most runs, however, stop earlier because the system gets into an absorbing state. We measure the survival probability $P(t)$ (the probability that the system is still active at time t), the number of dimers $N(t)$ averaged over all runs, and the mean-square distance of spreading $R^2(t)$ averaged over the surviving runs. At criticality, the values of these quantities scale algebraically in the long time limit [4],

$$P(t) \sim t^{-\delta}, \tag{1}$$

$$N(t) \sim t^{\eta}, \tag{2}$$

$$R^2(t) \sim t^{z}, \tag{3}$$

and double-logarithmic plots of these values against time show straight lines. Off criticality, these plots show some curvature. More precise estimates for the scaling exponents can be obtained by examining the local slopes of the curves. The effective exponent $\delta(t)$ is defined as

$$-\delta(t) = \frac{\ln [P(t)/P(t/b)]}{\ln\ b} \tag{4}$$

and similarly for $\eta(t)$ and $z(t)$. In Fig. 1, we plot the effective exponents against $1/t$ with $b = 10$. Off criticality these plots show upward or downward curvatures. From Fig. 1, we estimate $p_c \simeq 0.5325(5)$, which is fully consistent with the result of static Monte Carlo simulations [37]. The scaling exponent is given by the intercept of the critical curve with the vertical axis. Our estimates for the dynamic scaling exponents are

$$\delta = 0.29(2), \quad \eta = 0.00(2), \quad z = 1.34(20). \tag{5}$$

These values agree well with those of the BAW with four offspring [$\delta = 0.285(2), \eta = 0.000(1), z = 1.141(2)$] [32], although the exponent z shows very slow convergence. In fact, the value of z can be deduced from the values of the steady-state exponents by the scaling relation $z = 2\nu_\perp/\ \nu_\parallel$. Using the previous steady-state results, we find $z \simeq 1.15$, which is consistent with the above result

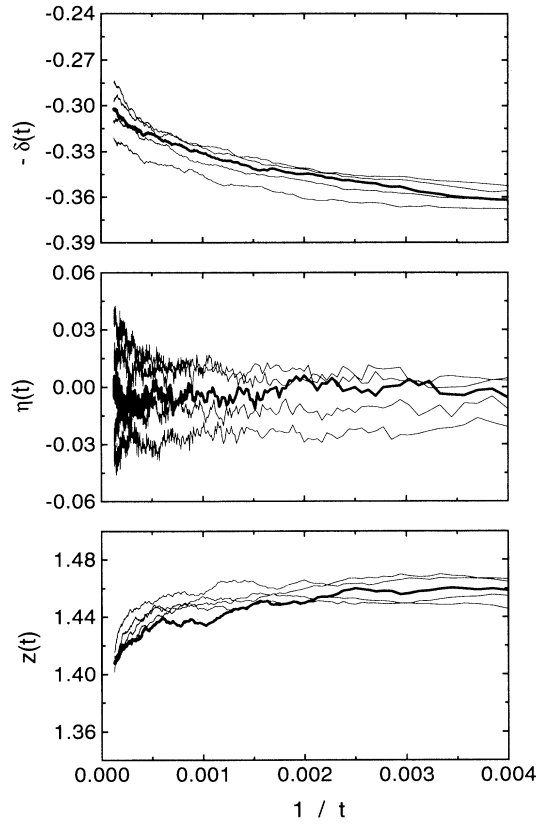

FIG. 1. Plots of the effective exponents against $1/t$ for the defect dynamics. Five curves from top to bottom in each panel correspond to $p = 0.5305$, 0.5315, 0.5325, 0.5335, and 0.5345. Thick lines are critical lines ($p = 0.5325$).

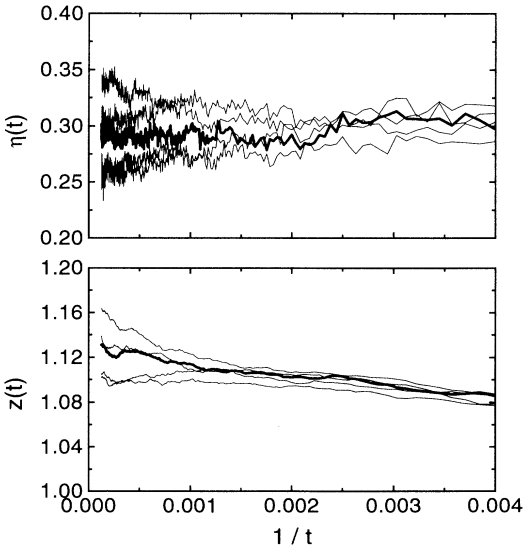

FIG. 2. Plots of the effective exponents against $1/t$ for the interface dynamics. Five curves from top to bottom in each panel correspond to $p = 0.5285$, 0.5305, 0.5325, 0.5345, and 0.5365. Thick lines are critical lines ($p = 0.5325$).

within errors. These values also satisfy the conventional hyperscaling relation $4\delta + 2\eta = dz$, where d is the spatial dimension [4].

For the interface dynamics, we start with a pair of vacancies placed at the central sites of a lattice and with monomers occupied at alternating sites. In this case, the system never enters an absorbing state, so that the survival probability exponent δ must be zero. 5000 independent runs are made during 8000 time steps and we measure $N(t)$ and $R^2(t)$. In Fig. 2, we plot the effective exponents $\eta(t)$ and $z(t)$ against $1/t$ with $b = 10$. The value of p_c obtained from these plots is consistent with the result from the defect dynamics. Our estimates for the dynamic scaling exponents are

$$\eta = 0.285(20), \qquad z = 1.14(2). \tag{6}$$

These values also agree well with those of the BAW with four offspring [$\delta = 0.282(4), z = 1.141(2)$] [32] and satisfy the generalized hyperscaling relation $2\delta + 2\beta/\nu_{\|} + 2\eta = dz$ recently proposed by Mendes *et al.* [38]. Even though the defect dynamics and the interface dynamics yield different values of dynamic exponents δ and η, their sum $\delta + \eta$ which is responsible for the growth of the number of kinks only in surviving samples seems to be the same. This property has been also observed in the models with infinitely many absorbing states [38]. In the IMD model, the boundaries of the active region contact one absorbing state (defect dynamics) or two different absorbing states (interface dynamics). But in the long time limit the active region becomes much bigger in the surviving samples and local dynamics near boundaries cannot distinguish which absorbing state is nearby. Therefore the defect dynamics and the interface dynamics should give the same result if only surviving samples are considered.

In summary, we have measured dynamic scaling exponents of the interacting monomer-dimer model with infinitely strong interactions by Monte Carlo simulations. This model exhibits a continuous transition from a reactive phase to an inactive phase with two equivalent absorbing states. Our results for the dynamic exponents are fully consistent with those of the branching annihilating walks with four offspring which conserve the number of particles of modulo 2. Thus now we firmly believe that these models belong to the same universality class [39].

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[36] If this process is not allowed, the IMD model possesses infinitely many absorbing states, which is currently under study.
[37] We found a minor mistake in applying a local dynamic rule of the IMD model in our previous paper [35]. Static Monte Carlo simulations were reperformed with the correct dynamic rule. We found that the critical probability is shifted downward to 0.5325(5) but there was essentially no change in the values of the steady-state exponents.
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