

## Critical Behavior of an Interacting Monomer-Dimer Model

Mann Ho Kim and Hyunggyu Park

*Department of Physics, Inha University, Incheon, 402-751, Korea*

(Received 13 December 1993)

We study 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. Monte Carlo simulations show that the critical behavior is different from the conventional directed percolation universality class but seems to be consistent with that of the models with the mass conservation of modulo 2.

PACS numbers: 64.60.-i, 02.50.-r, 05.70.Ln, 82.65.Jv

A monomer-dimer model was introduced by Ziff, Gulari, and Barshad to describe the oxidation of carbon monoxide on a catalytic surface [1]. In this model, a monomer (CO) adsorbs onto a single vacant site, while a dimer ( $O_2$ ) adsorbs onto a pair of adjacent vacant sites and then immediately dissociates. A nearest neighbor of adsorbates, composed of a dissociated O atom and a CO atom, reacts and forms a  $CO_2$  molecule and desorbs from the metal surface. In two dimensions, as the CO gas pressure is lowered, the system undergoes a first-order transition from a CO-saturated inactive phase into a reactive steady state and then a continuous transition into an  $O_2$ -saturated inactive phase. This continuous transition is shown to be in the same universality class as the directed percolation (DP) and the Reggeon field theory (RFT).

Motivated by the monomer-dimer model, many related lattice models have been formed to study nonequilibrium phase transitions. One of the simplest models is the monomer-monomer model [2,3] in which particles of two different species can adsorb on a single vacant site. If two adsorbates of different species are nearest neighbors to each other, they react and form a product which desorbs immediately from the surface. The system exhibits a first-order transition from a phase saturated with one species to another. Allowing desorptions of one species leads to a continuous transition which belongs to the DP universality class [4,5].

In both the monomer-monomer and the monomer-dimer models, interactions between adsorbing particles are ignored except for the actual surface reaction which converts the reactants into the products. Recently, an interacting monomer-monomer model [6,7] has been introduced where particles of the same species have *variable* repulsive interactions. When the interaction strength is weak, the interaction model exhibits only a first-order phase transition between two saturated phases. At the critical value of the interaction strength, a first-order line terminates at a tricritical point beyond which two continuous-transition lines appear. The two saturated phases are separated from a reactive steady state by these two lines. These two continuous transitions are shown to be in the DP universality class again.

A common feature of these models is that they exhibit a phase transition from a reactive phase into an inactive phase of a *single* absorbing state. The resulting critical behaviors are classified into the category of the so-called "DP conjecture" [8-10] which depicts that models exhibiting a continuous transition to a single absorbing state generally belong to the universality class of the directed percolation.

The universality class for models with a single absorbing state is well established. But few studies have been made for models with more than one absorbing states. Very recently Jensen and Dickman [11,12] have extensively studied some nonequilibrium lattice models with infinitely many absorbing states, the pair contact process (PCP), and the reaction dimer (RD) model. Both models have a continuous transition from a reactive phase into an inactive phase with infinitely many absorbing states, which is shown, rather surprisingly, again in the DP universality class.

In contrast to the well-established DP universality class, only a few models have appeared in literature which are known to be in a different universality class from DP. Grassberger, Krause, and von der Twer [13,14] studied two models of probabilistic cellular automata (PCA), namely models *A* and *B*. Both models exhibit a continuous transition from an active phase into an absorbing phase, in which the system is trapped in one of two (translationally) symmetric states with particles and vacancies placed in the alternating sites. But these models behave differently in the absorbing phase. Once the system enters into one of the two absorbing states, it remains in that state forever in model *A* but oscillates from one state to the other in model *B*. In spite of the discriminating behavior in the absorbing phase, both models are shown to be in the same universality class but different from DP. The order-parameter exponent  $\beta$  was obtained by static Monte Carlo simulations  $\beta = 0.6 \pm 0.2$  [13], but later by dynamic Monte Carlo simulations  $\beta = 0.93 \pm 0.12$  utilizing the hyperscaling relation [14]. The DP value of  $\beta$  is 0.2769(2) in one dimension. The evolution rules for both models in common involve the processes  $X \rightarrow 3X$  and  $2X \rightarrow 0$  that the number

of particles is conserved modulo 2. Grassberger has addressed in [14] that this conservation law might be responsible for the non-DP behavior.

Another model which conserves the number of particles by modulo 2 can be found in branching annihilating random walks with an even number of offsprings (BAW). Even though the BAW has a single absorbing state, static Monte Carlo simulations [15] show clearly non-DP behavior with  $\beta = 0.7 \pm 0.1$  in one dimension. This value seems to be consistent with that of the PCA, even though heavy numerical errors obscure the fact. The critical behavior of BAW with an odd number of offsprings is compatible with DP [16].

All previous works [11–15] seem to imply as a whole that more important in determining the universality class of nonequilibrium phase transitions is not the number of absorbing states but the mass conservation law in dynamics. This shows a sharp contrast to the case of equilibrium phase transitions where the number of ground states is relevant to the universality class. The symmetry between absorbing states may be more important than the number of absorbing states in determining the universality class. In the PCP, the infinitely many absorbing states are *not equivalent* probabilistically. Some absorbing states can be reached more easily than other absorbing states by the PCP dynamics. Therefore, it is important to study a model with multiple *equivalent* absorbing states. The PCA models have two equivalent absorbing states but also another conserving quantity, the mass conservation of modulo 2, which is claimed to be responsible for the non-DP behavior. In this Letter, we address a question of whether a model with multiple equivalent absorbing states may have non-DP behavior without any mass conservation law. As one of the simplest such models, we introduce a monomer-dimer model with infinitely strong repulsive interactions between the same species [17].

The interacting monomer-dimer model (IMD) is a generalization of the simple monomer-dimer model, 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. 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  $r_A = r_B = 0$ , there exists no fully saturated phase of monomers or dimers. However, this does not mean that this model has no absorbing states.

In fact, there are two equivalent absorbing states in this model. These states comprise 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 Letter, we consider the IMD with  $r_A = r_B = 0$  only for simplicity. General phase diagram of the IMD will appear elsewhere [18]. 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  $\bar{p}$  in the steady state, which vanishes algebraically as  $p$  approaches the critical probability  $p_c$  from below:

$$\bar{p} \sim (p_c - p)^\beta, \quad (1)$$

where  $\beta$  is the order-parameter exponent. There is a characteristic length scale  $\xi$  and time scale  $\tau$  which diverge at criticality as

$$\xi \sim |p_c - p|^{-\nu_\perp}, \quad (2)$$

$$\tau \sim |p_c - p|^{-\nu_\parallel}, \quad (3)$$

where  $\nu_\perp$  ( $\nu_\parallel$ ) is a correlation length exponent in the space (time) direction. It is quite difficult to measure the order parameter accurately near criticality by static Monte Carlo simulations due to the critical slowing down. Moreover, there are strong finite-size effects near criticality because of the diverging correlation length. In this Letter, we utilize the finite-size scaling (FSS) idea developed for nonequilibrium phase transitions by Aukrust, Browne, and Webman [19].

Various ensemble-averaged quantities depend on system size through the ratio of the system size and correlation length  $L/\xi$ . Thus, we can take the concentration of dimers near criticality as the following form:

$$\bar{p}(p, L) \sim L^{-\beta/\nu_\perp} f[(p_c - p)L^{1/\nu_\perp}], \quad (4)$$

such that at  $p_c$

$$\bar{p}(p_c, L) \sim L^{-\beta/\nu_\perp} \quad (5)$$

and

$$f(x) \sim x^\beta \quad \text{as } x \rightarrow \infty. \quad (6)$$

In the supercritical region ( $p < p_c$ ), the concentration  $\bar{p}$  remains finite in the limit  $L \rightarrow \infty$ , but it should vanish exponentially in the subcritical region ( $p > p_c$ ).

For the time dependence of the order parameter at criticality, one may assume a scaling form

$$\bar{\rho}(L, t) \sim L^{-\beta/\nu_{\perp}} g(Lt^{-\nu_{\perp}/\nu_{\parallel}}), \quad (7)$$

so that for a short time (or  $L \rightarrow \infty$ )  $\bar{\rho}$  has a power-law dependence on  $t$  as

$$\bar{\rho} \sim t^{-\beta/\nu_{\parallel}}. \quad (8)$$

The characteristic time  $\tau$  for a finite system is defined as the elapsing time for a finite system to enter into the (quasi)steady state. An elementary FSS analysis finds  $\tau$  at  $p_c$

$$\tau(p_c, L) \sim L^{\nu_{\parallel}/\nu_{\perp}}. \quad (9)$$

We run static Monte Carlo simulations. The initial configuration is far from absorbing states with all sites vacated, and we use periodic boundary conditions. Then the system evolves along the dynamical rules of our model. After one adsorption attempt on the average per lattice site (one Monte Carlo step), the time is incremented by one unit. The system reaches a quasisteady state first and stays for a reasonably long time before finally entering into an absorbing state. We measure the concentration of dimers in the quasisteady state and average over some independent samples which have not yet entered the absorbing states. The number of independent samples varies from 50 000 for system size  $L = 32$  to 300 for  $L = 2048$ . The number of time steps ranges from 500 to  $2 \times 10^5$  and, at least, 200 samples survive until the end of simulations.

At  $p_c$ , we expect the ratio of the concentrations of dimers for two successive system sizes  $\bar{\rho}(L/2)/\bar{\rho}(L) = 2^{\beta/\nu_{\perp}}$ , ignoring corrections to scaling. This ratio converges to unity for  $p < p_c$  and diverges to infinity for  $p > p_c$  in the limit  $L \rightarrow \infty$ . We plot the logarithm of this ratio divided by  $\log_{10} 2$  as a function of  $p$  for  $L = 64, 128, 256, 512, 1024$ , and 2048 in Fig. 1. This plot shows strong corrections to scaling. The crossing points between lines for two successive sizes move to the right as the system size grows. In the limit  $L \rightarrow \infty$ , we estimate the crossing points converge to the point at  $p_c \approx 0.5815(5)$  and  $\beta/\nu_{\perp} \approx 0.48(2)$ . The critical probability  $p_c$  can be more accurately estimated from dynamic Monte Carlo simulations [20]. The value of the exponent ratio  $\beta/\nu_{\perp}$  is clearly different from the standard DP value of 0.2524(5) which is combined with  $\nu_{\perp} = 1.0972(6)$  and  $\beta = 0.2769(2)$ .

In Fig. 2, we have plotted  $\bar{\rho}L^{\beta/\nu_{\perp}}$  against  $x = (1 - p/p_c)L^{1/\nu_{\perp}}$  in a double-logarithmic plot. From Eqs. (4) and (6), it follows that for small  $x$  the curve converges to a constant value, while for large  $x$  it should follow a straight line with slope  $\beta$ . We find that the data for the various system sizes are best collapsed to a curve with choices  $p_c = 0.5815(5)$ ,  $\nu_{\perp} = 1.83(3)$ , and  $\beta/\nu_{\perp} = 0.48(2)$ , from

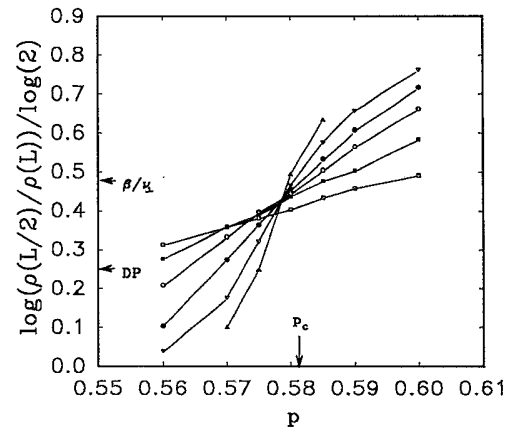


FIG. 1. Plots of  $\log[\bar{\rho}(L/2)/\bar{\rho}(L)]/\log 2$  versus  $p$ . Open squares are for  $L = 64$ , solid squares are for  $L = 128$ , open circles are for  $L = 256$ , closed circles are for  $L = 512$ , open triangles are for  $L = 1024$ , and closed triangles are for  $L = 2048$ .

which we get  $\beta = 0.88(3)$ . The straight line in Fig. 2 is a line with slope 0.88, which is in excellent accord with asymptotic behavior of  $x$  in Eq. (6).

By analyzing the decay characteristic of dimer concentrations  $\bar{\rho}(t, L)$ , we can determine the value of another correlation exponent  $\nu_{\parallel}$ . First the finite-size behavior of the characteristic time  $\tau$  is investigated. At  $p = p_c \approx 0.5815$ , we measure  $\tau$  for the various system sizes. The double-logarithmic plot (see Fig. 3) for the characteristic time  $\tau$  versus the system size  $L$  shows a straight line from which we obtain the value  $\nu_{\parallel}/\nu_{\perp} = 1.734(3)$ . This gives the value of  $\nu_{\parallel} = 3.17(5)$ , combined with the value

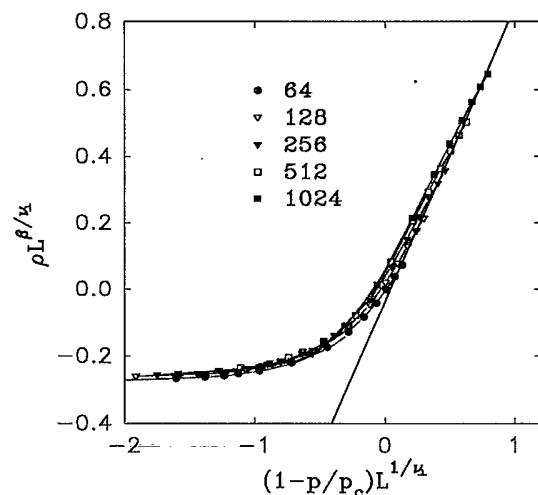


FIG. 2. The double-logarithmic plot for the data of  $\bar{\rho}L^{\beta/\nu_{\perp}}$  against  $x = (1 - p/p_c)L^{1/\nu_{\perp}}$  for the various system size  $L = 64-1024$ . With  $p_c = 0.5815$ ,  $\nu_{\perp} = 1.83$ , and  $\beta/\nu_{\perp} = 0.48$ , the data are collapsed to a curve. The solid line is of slope 0.88 ( $= \beta$ )

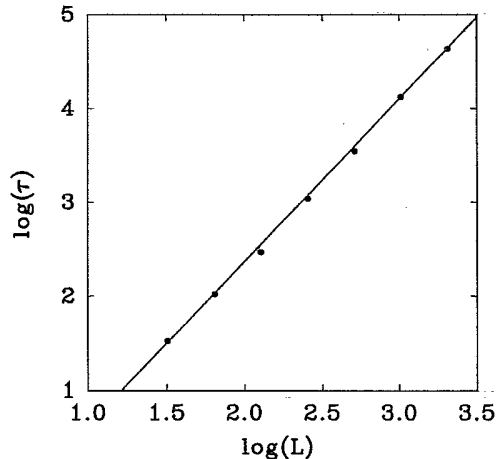


FIG. 3. The characteristic time against the system size  $L$  in a double-logarithmic plots for the various system size  $L = 32-1024$ . The solid line is of slope  $1.734 (= \nu_{\parallel}/\nu_{\perp})$ .

$\nu_{\perp} = 1.83(3)$ . We also can check the value of  $\nu_{\parallel}$  independently by measuring the decay exponent of  $\bar{\rho}$  at  $p = p_c$ . From the double-logarithmic plot for  $\bar{\rho}(t)$  versus the time  $t$  in Fig. 4, we estimate  $\beta/\nu_{\parallel} = 0.276(2)$ , which is in excellent agreement with the above results. We summarize our results for the critical exponents as

$$\beta = 0.88(3), \quad \nu_{\perp} = 1.83(3), \quad \nu_{\parallel} = 3.17(5).$$

In summary, we have numerically studied the interacting monomer-dimer model with infinitely strong repulsive nearest-neighbor interactions between the same species in one dimension. In contrast to the interactionless model exhibiting a discontinuous transition, this system exhibits a continuous transition from a reactive phase into an inactive phase with two equivalent absorbing states. This model

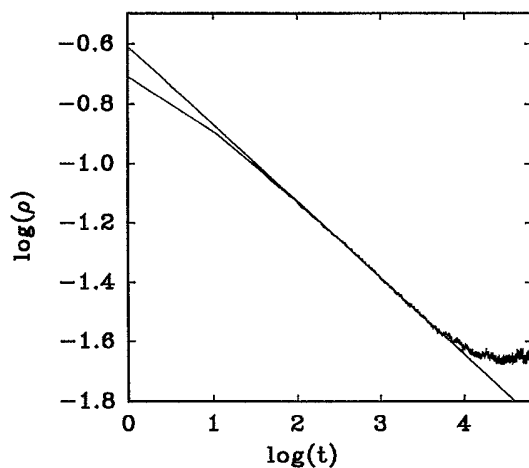


FIG. 4. The time dependence of the concentration of dimers at  $p_c = 0.5815$ . The slope of the curve gives the value of  $\beta/\nu_{\parallel} = 0.276(2)$ .

does not involve the dynamical processes with the mass conservation of modulo 2. Nevertheless, the values of the critical exponents are clearly different from the DP values and seem to be consistent with the values of the PCA and the BAW, in which the mass conservation of modulo 2 governs the dynamics. Therefore, we conclude that the symmetry between absorbing states as well as the mass conservation law are equally important in determining the universality class for nonequilibrium phase transitions. It is not yet clear why the model with two equivalent absorbing states and the one with the mass conservation of modulo 2 seem to be in the same universality class. Dynamical exponents and hyperscaling relations of the IMD will be discussed elsewhere [18].

This work is supported in part by the Korean Science and Engineering Foundation (Grant No. 931-0200-019-2), by the BSRI, Ministry of Education (Grant No. 94-2409), and by the Inha University research grant (1993).

- [1] R. M. Ziff, E. Gulari, and Y. Barshad, Phys. Rev. Lett. **56**, 2553 (1985).
- [2] P. Meakin and D. J. Scalapino, J. Chem. Phys. **87**, 731 (1987).
- [3] R. M. Ziff and K. Fichtorn, Phys. Rev. B **34**, 2038 (1986).
- [4] E. V. Albano, Phys. Rev. Lett. **69**, 656 (1992).
- [5] J. Zhuo and S. Redner, Phys. Rev. Lett. **70**, 2822 (1993).
- [6] H. Park, J. Köhler, I.-M. Kim, D. ben-Avraham, and S. Redner, J. Phys. A **26**, 2071 (1993).
- [7] J. Zhuo, S. Redner, and H. Park, J. Phys. A **26**, 4197 (1993).
- [8] H. K. Janssen, Z. Phys. B **42**, 151 (1981).
- [9] P. Grassberger, Z. Phys. B **47**, 365 (1982).
- [10] G. Grinstein, Z.-W. Lai, and D. A. Browne, Phys. Rev. A **40**, 4820 (1989).
- [11] I. Jensen, Phys. Rev. Lett. **70**, 1465 (1993).
- [12] I. Jensen and R. Dickman, Phys. Rev. E **48**, 1710 (1993).
- [13] P. Grassberger, F. Krause, and T. von der Twer, J. Phys. A **17**, L105 (1984).
- [14] P. Grassberger, J. Phys. A **22**, L1103 (1989) (errors for the value of  $\beta$  seem to be underestimated).
- [15] H. Takayasu and A. Yu. Tretyakov, Phys. Rev. Lett. **68**, 3060 (1992).
- [16] I. Jensen, Phys. Rev. E **47**, 1 (1993).
- [17] Some other types of interacting monomer-dimer models have been introduced in F. Bagnoli, B. Sente, M. Dumont, and R. Dagonnier, J. Chem. Phys. **94**, 777 (1991); J. J. Luque, F. Jiménez-Morales, and M. C. Lemos, J. Chem. Phys. **96**, 8535 (1992).
- [18] M. H. Kim and H. Park (to be published).
- [19] T. Aukrust, D. A. Browne, and I. Webman, Phys. Rev. A **41**, 5294 (1990).
- [20] The dynamic Monte Carlo method gives more systematic and accurate value for the critical point  $p_c$ . The obtained value is  $p_c \approx 0.5815(5)$  which will be reported in details in [18].