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Critical behavior of an absorbing phase transition in an interacting monomer–dimer model

Hyunggyu Park, Heungwon Park

Department of Physics, Inha University, Inchon 402-751, South Korea

Abstract

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. Static and dynamic Monte Carlo simulations show that the critical behavior at the transition is different from the conventional directed percolation universality class but is consistent with that of the models with the mass conservation of modulo 2. The values of static and dynamic critical exponents are compared with those of other models. We also show that the directed percolation universality class is recovered when a symmetry-breaking field is introduced.

A monomer–dimer(MD) 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 the adsorbates, comprised of a dissociated O atom and an 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 a O_2-saturated inactive phase. This continuous transition is shown to be in the same universality class as the directed percolation (DP) [2–4]. In one dimension, there is only a first-order phase transition between two saturated phases.

Motivated by the monomer–dimer model, many related lattice models have been formed to study non-equilibrium phase transitions, e.g. the contact process (CP) [5], the A model [6], the interacting monomer–monomer model (IMM) [7,8], and so forth. The CP and A model are single-component models (there are two choices at a given

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Table 1
Numerical estimates of scaling exponents. η_d (η_i) is the exponent for the defect (interface) dynamics [17]. These estimates are taken from references [13,14,16,17,21]. Numbers in parentheses represent the errors in the last digits

Exponent	PCA	NKI	IMD	BAWe
δ	0.283(16)	0.27(2)	0.29(2)	0.285(2)
η_d	—	—	0.00(2)	0.000(1)
η_i	0.272(12)	0.30(2)	0.285(20)	0.282(4)
z	1.11(2)	1.14(2)	1.14(2)	1.141(2)
$\nu_\parallel$	3.3(2)	2.9(6)	3.17(5)	3.25(10)
β	0.94(6)	0.80(8)	0.88(3)	0.92(3)

site: vacant/occupied or healthy/diseased), while the MD and IMM model are multi-component models (three choices: vacant/monomer/dimer or the other monomer). A common feature of these models, whether single-component or multi-component, 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" [4,9] 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 done for models with more than one absorbing states. Recently Jensen and Dickman [10,11] have extensively studied some non-equilibrium 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.

This result might mislead the reader that the number of absorbing states is not relevant to the universality class of the absorbing phase transitions. This shows a sharp contrast to the case of equilibrium critical phenomena where the number of ground states plays a crucial role. 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, i.e. some absorbing states can be reached more easily than other absorbing states by the PCP dynamics. So it is important to study a model with multiple equivalent absorbing states.

A few models have appeared in the literature which have two equivalent absorbing states. Those are the model A and B of probabilistic cellular automata (PCA) introduced by Grassberger et al. [12,13], non-equilibrium kinetic Ising models with two different dynamics (NKI) [14,15], and the interacting monomer–dimer model (IMD) [16,17]. The PCA and NKI models are single-component models, while the IMD model is a multi-component model. Critical behaviors of these models are different from DP but seem to belong to the same universality class (see Table 1). This result confirms our assertion that the symmetry between absorbing states is relevant to the universality class

of absorbing phase transitions.

Recently, the branching annihilating random walks (BAW) with offsprings have been studied intensively [18–21]. The BAW models exhibit a continuous absorbing phase transition from an active steady state into a single absorbing state. According to the foregoing DP conjecture, this phase transition should belong to the DP universality class. However, recent numerical investigations of the BAW models with even number of offsprings (BAWe) reveal that the BAWe models do not belong to the DP class but the same universality class as in the models with two equivalent absorbing states [18,21] (Table 1). The BAW models with odd number of offsprings (BAWo) belong to the conventional DP class [22]. Dynamics of the BAWe models conserve the number of walkers modulo 2, while the BAWo models evolve without any conservation law. So the conservation law seems also relevant to the universality class of absorbing phase transitions.

The remaining question is why the models with two equivalent absorbing states and the BAWe models with the mass (particle number) conservation of modulo 2 exhibit critical behaviors belonging to the same universality class. Grassberger described the PCA models in terms of kinks and showed that the number of kinks is conserved modulo 2 in the PCA models [13]. The NKI model can be also described by kinks (or domain walls) and its dynamics conserve the number of kinks modulo 2 [14]. The kink representation of the IMD model is complicated due to the presence of various kinks resulting from its multi-component nature. Each type of kinks has no conservation law but the total number of kinks is conserved modulo 2 again [23]. So these models bear a close resemblance to each other, even though there is no exact mapping available between them. From the spirit of universality, one can argue that differences among the above models are just irrelevant details which do not affect the universal behavior, e.g. scaling exponents.

In this paper, we take a careful look at these details and raise the question of whether models with the same conservation law in its kink representation always belong to the same universality class. This question is intimately related to the role of symmetry between absorbing states in determining the universality class of absorbing phase transitions.

We consider the IMD model with infinitely strong repulsions between the same species in one dimension. A monomer (A) cannot adsorb at a nearest-neighbor site of an already-occupied monomer (restricted vacancy) but adsorb at a free vacant site with no adjacent monomer-occupied sites at a rate k_A. Similarly, a dimer (B_2) cannot adsorb at a pair of restricted vacancies (B in nearest-neighbor sites) but adsorb at a pair of free vacancies at a rate k_B. 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 in 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. The system has no fully saturated phases of monomers or dimers, but instead

two equivalent half-filled absorbing states. These states, *I* and *II*, comprise 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 order to study the role of symmetry between these absorbing states, we introduce a symmetry breaking field h which favors one absorbing state over the other. This can be done by differentiating the adsorption rate of monomers at an odd-numbered vacant site and at an even-numbered one. If a monomer is chosen to adsorb on an even-numbered free vacant site, the adsorption attempt is rejected with probability h ($0 \leqslant h \leqslant 1$). The case $h = 0$ corresponds to the ordinary IMD model previously studied in details [16,17]. For finite h the monomers tend to adsorb more on an odd-numbered site than an even-numbered one. Therefore the absorbing state *I* can be reached more easily than the other absorbing state *II* by this dynamics.

In this paper, we set $h = 0.5$ for convenience. 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 $q = 1 - p$. We perform dynamic Monte Carlo simulations for this model. We start with a lattice occupied by monomers at all odd-numbered 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. 5000 independent runs are made up to 5000 time steps for various values of p near the critical probability p_c. Most runs, however, stop earlier because the system gets into the absorbing state *I*. 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 [24]

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

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

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

and double-logarithmic plots of these values against time show straight lines. Off criticality, these plots show some curvatures. 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

$$-\delta(t) = \frac{\log\left[P(t)/P(t/b)\right]}{\log\, b} \tag{4}$$

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 $p_c \simeq 0.414(1)$, which is much lower than in the ordinary IMD model without the symmetry breaking field [17] ($p_c \simeq 0.5325(5)$) as expected. The

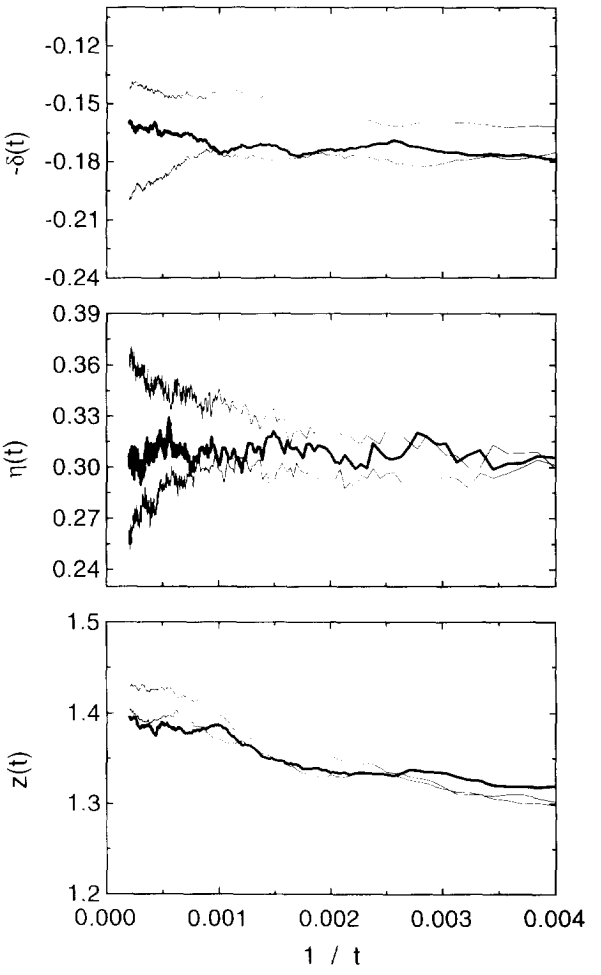

Fig. 1. Plots of the effective exponents against $1/t$. Three curves from top to bottom in each panel correspond to $p = 0.413, 0.414, 0.415$. Thick lines are critical lines ($p = 0.414$).

scaling exponent is given by the intercept of the critical curve with the vertical axis. Our estimates for the dynamic scaling exponents are

$$\delta = 0.160(5), \qquad \eta = 0.31(1), \qquad z = 1.40(20). \tag{5}$$

These values are completely different from the values in the IMD model without the symmetry breaking field (Table 1), but are in an excellent accord with those of the DP universality class; $\delta = 0.1596(4)$, $\eta = 0.3137(10)$, and $z = 1.2660(14)$ (see Ref. [21]), although the exponent z shows very slow convergence. Similar results are obtained if we set the value of the symmetry breaking field $h = 0.1$.

In summary, we have studied the IMD model with infinitely strong repulsive nearest-neighbor interactions between the same species in one dimension. This system exhibits a continuous transition from a reactive phase into an inactive phase with two equivalent absorbing states. Its critical behavior is different from the DP universality class but consistent with that of the PCA, NKI, and BAWe models. As soon as the symmetry breaking field is introduced, the two absorbing states of the IMD model become probabilistically inequivalent and this model exhibits a critical behavior in the DP universality class. It implies that the symmetry between absorbing states plays a crucial role in determining the universality class. Our numerical results indicate that the system evolves mostly into one favored absorbing state, not bothered by the other unfavored absorbing state. So the critical behavior may be governed by a fixed point with a single absorbing state, which is associated with the DP universality class. This may explain why the PCP model with infinitely many absorbing states also belongs to the DP universality class. For more numerical evidence, we are currently performing static Monte Carlo simulations for this symmetry-broken model and also studying the role of the symmetry breaking field in the PCA and NKI models. It is interesting to note that the total number of kinks in the IMD model is still conserved modulo 2 in the presence of the symmetry breaking field. So it is incorrect to say that all models with mass conservation of modulo 2 should belong to the same universality class other than the DP class.

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