

Title	Critical behavior of an interacting catalysis model(New Developments in Statistical Physics Similarities in Diversities, YITP Workshop)
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Citation	物性研究 (1993), 60(4): 339-343
Issue Date	1993-07-20
URL	http://hdl.handle.net/2433/95123
Right	
Type	Departmental Bulletin Paper
Textversion	publisher

Critical behavior of an interacting catalysis model

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Abstract

We study a generalized monomer-monomer model with repulsive interactions between the same species. There exists a tricritical point at which a first-order and two continuous transition lines merge. These continuous transitions belong to the Reggeon field theory (RFT) universality class. We also suggest a model with an inactive state of doubly degenerate absorbing states. Preliminary results indicate that this model exhibits a continuous transition of a new universality class other than the RFT type.

There has been much attention recently given to nonequilibrium lattice models of catalysis exhibiting a phase transition from an active steady state into an inactive state [1-18]. One important model is the monomer-dimer model introduced by Ziff, Gulari, and Barshad [1] to describe the oxidation of carbone monoxide on metal surfaces. 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 dissociates. A nearest neighbor of adsorbates, comprised of a dissociated O atom and an CO atom, react and form a CO_2 molecule and desorb from the metal surface. In two dimensions, as the CO gas pressure is lowered, a first-order transition occurs 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 found to belong to the same universality class as Reggeon field theory (RFT) [2, 3, 4], directed percolation [4, 5], and contact process [6]. Interesting features of the monomer-dimer model necessitate the study of the monomer-monomer

model [7], where a monomer of two different species, A and B, adsorbs onto a vacant site and an adjacent A-B pair reacts and desorbs. In this model, there does not exist a reactive phase and a first-order transition occurs from the A-saturated phase to the B-saturated phase. There are also some studies about the dimer-dimer model, dimer-trimer model, and etc [10, 11].

Recently repulsive interactions between adsorbates are considered in the monomer-monomer model [12]. In this surface reaction model (dollar-dime model), size of one of the species (dollars) is greater than a lattice spacing of the substrate, so the nearest-neighbor adsorption of dollars is prohibited due to the excluded volume effect. There exists no dollar-saturated phase at finite dime-adsorption rate. As the adsorption rate of dimes are lowered, this model exhibits a continuous phase transition from a dime-saturated inactive state into a reactive steady state. The value of the order-parameter critical exponent β is obtained numerically by steady-state Monte Carlo simulations and mean-field cluster approximations in one dimension ($\beta = 0.28 \pm 0.05$) and is consistent with that of the RFT universality class.

A more generalized model is introduced subsequently where the strength of the repulsive (excluded volume) interaction is varied [13]. This interacting model interpolates the monomer-monomer model and the dollar-dime model as the interaction strength increases. When the repulsive interaction is weak, the interacting model exhibits a first-order transition between the dollar-saturated phase and the dime-saturated phase. At the critical value of the interaction strength, the first-order line terminates at a tricritical point beyond which two continuous-transition lines appear. These two continuous-transition lines separate a new reactive phase between two saturated phases. When the interaction is infinitely strong, the dollar-dime model is recovered where the dollar-saturated phase disappears and there is a single continuous transition. Nature of these continuous transitions is studied in one dimension by the complementary numerical schemes of series expansions [14] and dynamic Monte Carlo simulations [5, 9, 15]. Along both of continuous-transition lines, the steady-state and dynamic exponents β , δ ,

η , z are obtained within 1-5 % numerical accuracy [13]. The values of the exponents do not seem to vary with the interaction strength and typically $\beta = 0.274 \pm 0.003$, $\delta = 0.160 \pm 0.003$, $\eta = 0.317 \pm 0.004$, and $z = 1.26 \pm 0.01$. These values are consistent with those of the RFT universality class in one dimension. Tricritical behavior is not fully understood yet due to low numerical accuracy.

In summary, we find a tricritical point in a monomer-monomer model with repulsive interactions at the confluence of the first-order and two continuous transitions at finite interaction strength. These interactions in the monomer-monomer model do not change the universality class (RFT class) of the continuous transitions from a reactive phase into a saturated inactive phase. This may provide another evidence for the conjecture [9, 16] that a class of continuous transitions from a reactive phase into an inactive phase with a single absorbing state should belong to the RFT universality class.

It would be a natural question to ask whether a continuous transition from a reactive phase into an inactive phase with multiply degenerate absorbing states belong to a different universality class from the RFT class. Most recently a model with infinitely many absorbing states (pair contact process) is studied by steady-state Monte Carlo simulations [17]. However, this model exhibits a continuous transition of the RFT universality class again. This result seems to imply that the number of absorbing states in an inactive phase is not relevant to the universality class of nonequilibrium phase transition into an inactive phase. This shows a sharp contrast to the case of equilibrium phase transitions where the number of ground states is relevant to the universality class. It seems that the symmetry between absorbing states may be more important than the number of absorbing states in determining the universality class of a nonequilibrium phase transition, which is also true in the equilibrium case. In the pair contact process, the infinitely many absorbing states are not equivalent probabilistically. Some absorbing states can be reached more easily than other absorbing states by the dynamics of pair contact processes. It will be interesting to study a

model with multiple equivalent absorbing states. Our work is in progress for a monomer-dimer model with infinitely strong repulsive interactions between the same species, which exhibits a continuous phase transition from a reactive phase into an inactive phase of doubly degenerate absorbing states [18]. Preliminary results indicate that this transition does not belong to the RFT universality class.

Most of our work about an interacting monomer-monomer model has been done with collaboration with J. Zhuo and S. Redner [13]. We wish to thank them for fruitful collaborations and also M. H. Kim for helpful discussions. This work is supported in part by the Inha University research grant (1992), and in part by the the Korean Science and Engineering Foundation through the SRC program of SNU-CTP, and also through the Center for Thermal and Statistical Physics, Korea University.

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