Determination of the order-parameter critical exponent of an irreversible dimer-monomer surface-reaction model

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A method is proposed for the evaluation of the order-parameter critical exponent of continuous irreversible phase transitions in surface-reaction models. An application to a dimer-monomer model in two dimensions gives the best available value, namely $\beta \cong 0.578 \pm 0.010$, in excellent agreement with Reggeon field theory.

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I. INTRODUCTION

The model proposed by Ziff, Gulari, and Barshad (ZGB) [1] for a monomer-dimer surface-reaction process, which mimics the oxidation of carbon monoxide on a catalytic surface, exhibits two irreversible phase transitions into absorbing or poisoned states, in which the surface is saturated by oxygen or by CO. The ZGB model has a single parameter p, the rate of CO arrival at the surface. It has been established that for $p \leq p_1 \cong 0.3907$ [1–3] the surface becomes poisoned with O, while for $p \geq p_2 \cong 0.5256$ [1,2,4] one observes CO poisoning. A reactive steady state with CO_2 production is found for $p_1 < p < p_2$ [1–4]. The transition at p_1 is continuous and has become the focus of growing attention in order to understand its critical behavior [2,4,5]. It is now generally accepted that this transition belongs to the directed percolation (DP) or equivalently to the Reggeon field theory (RFT) universality class, as proposed by Grinstein, Lai, and Browne [5]. Evidence supporting this statement follows from time-dependent Monte Carlo simulations, which allow the precise evaluation of dynamic critical exponents [3]. In contrast, the evaluation of "static" exponents, such as the order-parameter critical exponent β and the correlation length exponent ν, is rather difficult. Close to p_1 the natural order parameter is the concentration of minority species, θ_{CO}, which is expected to behave as

$$\theta_{CO} \propto (p - p_1)^{\beta} . \tag{1}$$

The known exponent $\beta \cong 0.58$ for the RFT in two dimensions [6] is only marginally consistent with the numerical values obtained by Meakin and Scalapino simulating the ZGB model in the square lattice, namely $\beta_O \cong 0.61$ and $\beta_{CO} \cong 0.69$. Due to large fluctuations of the system, β values reported by Meakin and Scalapino have considerable uncertainties and their results suggest that $\beta_O = \beta_{CO}$ [2]. Another possibility for the evaluation of β emerges from a finite-size scaling analysis [7]. Nevertheless, systematic errors in the collapsing of the data for lattices of different sizes are believed to be the reason for the large β values obtained [7].

The aim of this Brief Report is to propose a calculation method that allows us a rather precise evaluation of β by avoiding undesired effects of both fluctuations into the poisoned state and metastabilities. The method is successfully applied to the continuous transition of the ZGB model.

II. CALCULATION METHOD

The method is based upon the ideas developed to study damage spreading at equilibrium phase transitions [8]. Let σ_1 be a steady-state configuration of the system with CO and O concentrations given by θ_{1CO} and θ_{1O}. Now a second configuration slightly away from equilibrium, σ_2, is constructed by removing a small amount of O species. After that both configurations are allowed to evolve for a long period of time using the same set of random numbers. The "damage" caused by removing O species eventually spreads and causes the concentration of CO to become different in each configuration. So, let us define the difference of CO concentration between both configurations at time t as

$$\Delta\theta_{CO}(t) = \sum |\theta_{1CO}(t) - \theta_{2CO}(t)|_{i,j} , \tag{2}$$

where $\theta_{1CO}(t)$ and $\theta_{2CO}(t)$ are 1 (0) if the $\{i,j\}$th site of the respective configuration is occupied (unoccupied) by CO species at time t, and $\Delta\theta_{CO}(t)$ is evaluated scanning all the sites of the lattice. Note that $\Delta\theta_{CO}(t=0)=0$ independently of the amount of removed O.

III. RESULTS

The method is applied to the ZGB model in the square lattice of side L ($L=150$) and results are obtained using standard Monte Carlo algorithms. For $p \leq p_1$ one has that the damage is frozen since both configurations evolve towards the O-poisoned state. Nevertheless, for $p > p_1$ one observes damage spreading, characteristic of a frozen-chaotic transition at p_1 [9]. For these p values, $\Delta\theta_{CO}(t)$ becomes stationary and saturates to a certain nonzero value after few Monte Carlo time steps [say, $t \cong (0.5-1.0)\times 10^3$]. Therefore averages of $\Delta\theta_{CO}$ are tak-

en within the long-time regime, namely, $2\times10^3 \le t \le 5\times10^3$. Let us remark that since the calculations are performed in a finite lattice of side $L=150$, the value of $\Delta\theta_{CO}$ would have vanished after a time of the order of $\tau \cong \exp(L^2)$, because eventually uncorrelated trajectories in a finite phase space will always meet [8]. So, the times considered in the evaluation of $\Delta\theta_{CO}$ are large enough to obtain reliable steady-state values but much smaller than τ, in order to avoid metastabilities of the finite system.

At criticality the concentration of CO of both configurations behaves according to (1), so one also has

$$\Delta\theta_{CO} \propto (p - p_1)^{\beta} = \Delta p^{\beta} . \quad (3)$$

Figure 1 shows a ln-ln plot of $\Delta\theta_{CO}$ vs Δp and from the best linear fit of the data one gets $\beta \cong 0.578 \pm 0.010$, in excellent agreement with the RFT value. Since a small error of measuring p_1 causes a quite big error in β, we have employed the best available value of the critical probability given by $p_1 \cong 0.390\,65 \pm 0.000\,10$ [3].

The reason why the use of the damage method gives results superior to those of standard methods stems from the fact that the former only monitors the difference between two configurations subjected to the same fluctuations, so that the noise is effectively canceled. A similar fact has been pointed out for the calculation of the susceptibility of the Ising model [8].

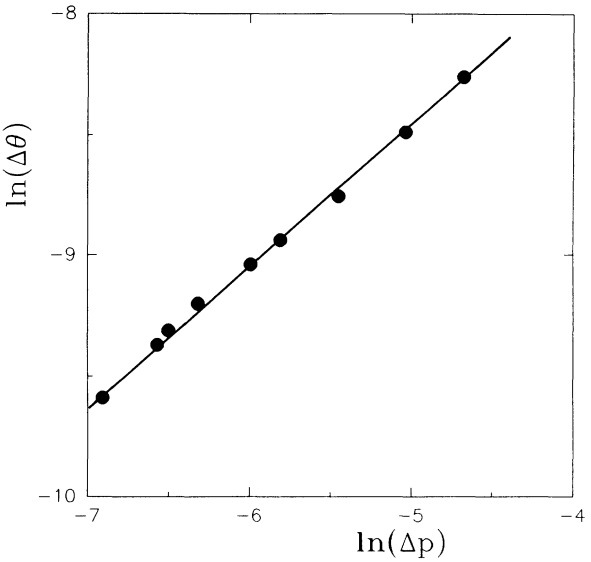

FIG. 1. Ln-ln plot of $\Delta\theta_{CO}$ vs Δp [see Eq. (3)]. Results obtained using lattices of side $L=150$. Each point is averaged within the interval $2\times10^3 \le t \le 5\times10^3$ and over 100 different samples. The straight line with slope $\beta=0.578\pm0.010$ corresponds to the best fit of the data. More details are in the text.

IV. CONCLUSIONS

A method is proposed for the evaluation of the order-parameter critical exponent of continuous irreversible phase transitions in surface-reaction models. For the ZGB model in two dimensions the value $\beta \cong 0.578 \pm 0.010$ is determined, in excellent agreement with Reggeon field theory.

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