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Critical phenomena at surfaces in a model of non-equilibrium phase transitions

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Abstract. Critical phenomena at surfaces are studied in a simple two-dimensional model of non-equilibrium phase transitions belonging to the class of interacting particle systems Mean field renormalization group approach and numerical simulations are used to determine the phase diagram for this system and some of the critical exponents associated with ordinary, special, extraordinary and surface phase transitions

1. Introduction

Critical phenomena at surfaces have been extensively studied in the past years in the framework of equilibrium phase transition [1]. The presence of free surfaces adds a rich complexity to the bulk critical phenomena. Besides the case where both the bulk and the surface become ordered simultaneously (ordinary transition), one finds cases in which the surface is ordered while the bulk is disordered (surface transition) or more complicated situations [1].

Several predictions from scaling theories and renormalization group approach have been tested on exactly solvable models or by numerical simulations and our present understanding of the surface equilibrium transitions is quite satisfactory. The study of surface critical phenomena is related to several important physical problems such as wetting, polymer adsorption and surface reconstruction.

Although the situation is well understood for equilibrium critical phenomena, nothing is known for systems having non-equilibrium bulk phase transitions. One of the reasons is that there is no first principle theory for non-equilibrium systems. Thus, we cannot approach the problems of bulk or surface phase transitions on a general footing. Accordingly, it is of interest to investigate the surface and bulk critical behaviour of simple models having bulk non-equilibrium phase transition and investigate whether or not predictions similar to those of equilibrium scaling theory hold in the non-equilibrium case.

An interesting class of such models is the one called interacting particle systems [2]. These are Markov processes on a lattice where the sites can have two states (vacant or occupied). The enumeration of the state of occupancy of all the lattice sites defines the configuration or the state of the system. Transitions between different configurations occur via elementary processes, related to the creation, annihilation or hopping of particles. These models have one adsorbing state for which the lattice is completely empty (or full).

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A particular example of such a model, called model A, was recently introduced by Dickman [3, 4]. We shall study in this paper a semi-infinite two-dimensional version having a (one-dimensional) free surface. For sequential dynamics, for which at most one elementary process occurs per unit of time, the original A model belongs to the universality class of directed percolation [5, 6]. For parallel dynamics, the question of universality is still controversial [7, 8], so we shall mainly consider here the case of sequential dynamics.

The paper is organized as follows. In section 2 we precisely define the model. In section 3, we treat both problems of the bulk and surface phase transitions in mean field renormalization group approximation. The phase diagram shows ordinary, extraordinary, surface and special transitions. Some relations between critical exponents are also derived. Those results are compared with the ones of numerical simulation performed in section 4. Finally, conclusions are drawn in section 5.

2. The model

Model A gives a simple description of poisoning transitions similar to those observed on catalytic surfaces. One considers a d-dimensional substratum covered by a regular hypercubic lattice. Each site has two possible states: empty or occupied by a particle A. The first step of the dynamical process is adsorption. The probability for a vacant site to become occupied during a short time interval δt is $p_B \delta t$. The second step of the process is desorption. The probability for an occupied site x to become vacant is $q_B \delta t$, provided that at least one of the nearest neighbours of x is vacant. During the time interval δt, one of the two processes occurs at each site. For simplicity we shall restrict ourselves to the case $q_B = (1 - p_B)$. Moreover, we shall consider a semi-infinite system and we restrict ourselves to the two-dimensional case.

Let us first consider the bulk. Each site has four nearest neighbours. Qualitatively speaking, one expects that if p_B is large enough, an initially empty substratum will be completely covered, by A particles, after some time. This is the poisoned phase or the adsorbing state. However, if p_B is small enough, the desorbing mechanism will be efficient enough to prevent such a poisoning. Thus one may anticipate the existence of a threshold value p_{Bc} such that, in the stationary state, the covering fraction of A on the substratum X_B will be 1 for $p_B \geqslant p_{Bc}$ (poisoned phase) and smaller than 1 for $p_B < p_{Bc}$. If $1 - X_B(p_B)$ varies continuously across p_{Bc} the transition will be of second order and its behaviour near the threshold will be described in terms of the bulk critical exponent β_B:

$$\bar{X}_B(p_B) = (1 - X_B(p_B)) \sim (p_{Bc} - p_B)^{\beta_B}. \tag{2.1}$$

Let us now consider a semi-infinite system with a free surface (see figure 1). Each site on the surface has only three nearest neighbours. Moreover, we assume that the probability of adsorption on the surface, p_S, can differ from that for the bulk. The problem is thus characterized by two control parameters p_B and p_S. The probability of desorbtion on the surface is chosen as $q_S = 1 - p_S$.

Intuitively, one expects that for $p_B \geqslant p_{Bc}$, several situations can occur on the surface as a function of p_S. The surface can be poisoned for p_S large enough or not poisoned for small values of p_S.

Note moreover that for $p_B = 1$, we recover the one-dimensional bulk problem.

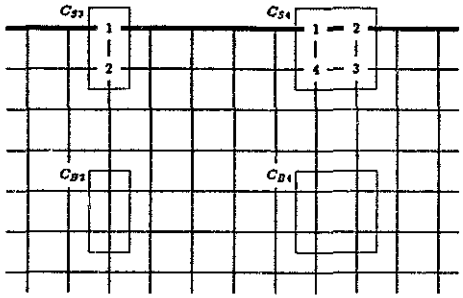

Figure 1. Semi-infinite lattice studied The bold line corresponds to the free surface C_{S2} and C_{S4} are the clusters considered to locate the surface transition, while C_{B2} and C_{B4} are the clusters considered for the bulk transition

3. Mean-field renormalization group approach

It is well established that the mean field renormalization group approach gives an efficient way to compute qualitatively correct phase diagrams. This method has been successfully applied to several problems of equilibrium phase transitions [9–11] and to non-equilibrium situations [12, 13].

The mean field renormalization group method is a combination of usual mean field strategy with scaling or renormalization group ideas. It proceeds in two steps. First, one computes the order parameter Ψ for a finite cluster of N sites and a control parameter p. To obtain a non-zero value, one has to add a symmetry breaking field b at the boundary of the cluster. One then computes the order parameter Ψ' for a smaller cluster $N' < N$ sites, with a boundary field b' and control parameter p'. As one is interested in the location of a second order transition point, one considers arbitrary small symmetry breaking fields. The equations for the order parameters Ψ and Ψ' can then be linearized in the fields. Assuming that the two order parameters rescale in the same way as the two symmetry-breaking fields, one obtains an implicit relation $p' = f(p)$ for the control parameter of the model, which can be interpreted as a renormalization group transformation. The critical fixed point of this transformation gives the critical value of the control parameter p_c.

In our problem, the order parameters are the probabilities $\bar{X}_B(p_B, p_S)$ and $\bar{X}_S(p_B, p_S)$, of a site belonging to the bulk or to the surface respectively being empty.

These quantities are expressed in terms of the stationary values of certain joint probabilities that the sites of a cluster are empty or not. Following the general strategy outlined above, we shall consider clusters of four sites and two sites. Depending on whether we are investigating the bulk or the surface transition, those clusters will be located completely in the bulk or partially in the bulk and partially on the surface as illustrated on figure 1. Let us start with the two-site cluster C_{S2} corresponding to the surface transition (see figure 1). We shall study the time evolution of $P(\sigma_1, \sigma_2, t)$, the probability that the site 1 on the surface and the site 2 in the bulk are respectively in the states σ_1 and σ_2. Let x'_B be the probability that a bulk site outside the cluster is occupied, and x'_S, the probability that a surface site outside the cluster is occupied. We make the approximation that x'_B does not depend on the depth of the site. Then the evolution rules of the model with sequential dynamics lead to the following equations of motion for the two-site probabilities (omitting to write explicitly the time

dependence):

$$\dot{P}(1,1) = P(1,0)p'_B + P(0,1)p'_S - P(1,1)[q'_S(1-x'^2_S) + q'_B(1-x'^3_B)] \quad (3.1)$$

$$\dot{P}(1,0) = P(0,0)p'_S + P(1,1)q'_B(1-x'^3_B) - P(1,0)(q'_S + p'_B) \quad (3.2)$$

$$\dot{P}(0,1) = P(0,0)p'_B + P(1,1)[q'_S(1-x'^2_S)] - P(0,1)(p'_S + q'_B) \quad (3.3)$$

$$\dot{P}(0,0) = P(1,0)q'_S + P(0,1)q'_B - P(0,0)(p'_S + p'_B). \quad (3.4)$$

In terms of the stationary solutions P_{sta}, one has

$$\bar{X}'_S(p'_S, p'_B) = 1 - X'_S(p'_S, p'_B) = P_{sta}(0,0) + P_{sta}(0,1). \quad (3.5)$$

For $p_B > p_{Bc}$ a possible surface-like transition line will be given by setting $\bar{x}'_B = 1 - x'_B = 0$ and $\bar{x}'_S = 1 - x'_S \to 0$. Then

$$\bar{X}'_S(p'_S, p'_B) = g_2(p'_S, p'_B)\bar{x}'_S + \mathcal{O}(\bar{x}'^2_S) \quad (3.6)$$

where $g_2(p'_S, p'_B)$ is a known function not given explicitly.

A similar calculation can be done for the four-site cluster C_{S4} (see figure 1). In terms of the stationary values of the probabilities $P(\sigma_1, \sigma_2, \sigma_3, \sigma_4, t)$, that the sites 1 and 2 on the surface and the sites 3 and 4 in the bulk are respectively in the states σ_1, σ_2, σ_3 and σ_4, one has:

$$\begin{aligned}\bar{X}_S(p_S, p_B) &= 1 - X_S(p_S, p_B) \\ &= P_{sta}(0,0,0,0) + P_{sta}(0,0,0,1) + P_{sta}(0,0,1,0) + P_{sta}(0,0,1,1) \\ &\quad + \tfrac{1}{2}[P_{sta}(1,0,0,0) + P_{sta}(1,0,1,0) + P_{sta}(1,0,0,1) + P_{sta}(1,0,1,1) \\ &\quad + P_{sta}(0,1,0,0) + P_{sta}(0,1,1,0) + P_{sta}(0,1,0,1) + P_{sta}(0,1,1,1)]. \end{aligned} \quad (3.7)$$

The four-site probabilities can be computed along the same line as developed for the two-site ones. We shall not give here the explicit forms which are quite heavy. After some tedious algebra, one finds:

$$\bar{X}_S(p_S, p_B) = g_4(p_S, p_B)\bar{x}_S + \mathcal{O}(\bar{x}_S^2). \quad (3.8)$$

Within the present mean field renormalization group approach, the critical line corresponding to the surface transition (line BS on figure 2) is the solution of:

$$g_4(p_{Sc}, p_B) = g_2(p_{Sc}, p_B). \quad (3.9)$$

A similar mean field renormalization group argument cannot be done for $p_B < p_{Bc}$. Indeed, in this case $\bar{x}'_B$ is finite and one would need to know its explicit transformation under renormalization to obtain an equation equivalent to (3.9). Such a transformation is not accessible within this formalism.

For the bulk transition, the strategy is the same. One works with the clusters C_{B2} and C_{B4} drawn in figure 1. These clusters are far below the surface and hence are not influenced by surface effects. Thus, it is justified to assume that the breaking fields are independent of the depth of the sites. Accordingly, the only breaking fields that appear are $\bar{x}_B$ and $\bar{x}'_B$. One finds that the bulk critical probability p_{Bc} is the solution of

$$2p_B^3 - 9p_B^2 + 4 = 0. \quad (3.10)$$

This corresponds to the ordinary transition at $p_{Bc} = 0.728$.

The complete phase diagram as determined by mean field renormalization group is shown in figure 2. As for the equilibrium case, one finds ordinary, special, extraordinary and surface transitions.

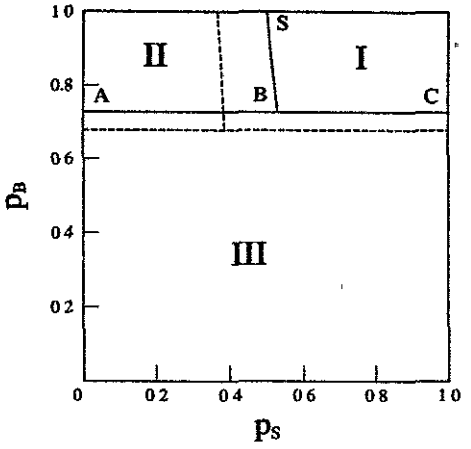

Figure 2. Phase diagram obtained by mean field renormalization group (full line) and simulation (broken line) The line BC corresponds to the ordinary transition, the line AB to the extraordinary one and the line BS to the surface transition The special transition takes place at B. The phases I, II and III are respectively the phases in which, (I) the bulk and the surface are poisoned, (II) the bulk is poisoned but not the surface and (III) both the surface and the bulk are not poisoned.

The next question to be addressed concerns the critical exponents. It is known that although the mean field renormalization group method gives generally good phase diagrams, the critical exponents are not as good, at least when small clusters are used, which is the case in the present study.

As in any renormalization group approach, the correlation length exponent is easily obtained by studying the renormalization group recursion relation in the vicinity of the fixed point solution. The value of ν for the surface transition when $p_B \to 1$ and for the ordinary transition when $p_S \to p_B$ are the ones of the one-dimensional and two-dimensional bulk models, which have already been estimated by mean field renormalization group [12].

More interesting is to study what happens in the vicinity of the special point (point B in figure 2), where simultaneous 'surface-bulk' occurs. We have computed the exponent ν [from $\mathrm{d}p'_B/\mathrm{d}p_B|_{p_{Bc},p_{Sc}} = l^{1/\nu}$, with the scaling factor $l = 2^{1/2}$] along the line of surface transition. In the vicinity of B, one gets $\nu = 0.84$. This critical line approaches B linearly, giving for the crossover exponent (defined as $p_B - p_{Bc} = (p_S^{Sp} - p_{Sc})^{1/\Phi}$) the value $\Phi = 1$. If one assumes the usual crossover argument to hold also for this non-equilibrium case, one would have $\Phi = \nu(d=2)/\nu(\text{at } B)$; and $\nu(d=2) = 0.84$, a good result if one compares with $\nu = 0.85$ of more accurate studies [14].

Other quantities of interest are the critical exponents β for the bulk and the surface. The behaviour of the order parameter $\bar{X}_S(p_S, p_B)$ along the surface transition line, at fixed value of p_B, is characterized by the surface order parameter β_1, defined by

$$\bar{X}_S(p_S) \sim (p_{Sc} - p_S)^{\beta_1}. \tag{3.11}$$

These exponents cannot be calculated in the mean field renormalization group method. However, β_B can be extracted from the results of the study of one cluster size. This leads to the known result $\beta_B = 1$, both for the one- and two-dimensional case [7]. For

the surface exponent β_1, the situation is more subtle. However, one can use a one-site mean field approximation to relate β_B with β_1.

Let $\bar{x}_n$ be the probability that a site belonging to the nth row below the surface is empty. Thus, $\bar{x}_1 = \bar{x}_S$ and $\bar{x}_{n\to\infty} = \bar{x}_B$. In the steady state, the mean-field equation for $\bar{x}_n$ reads

$$\bar{x}_n(3p_B - 2) = [\bar{x}_{n-1} + \bar{x}_{n+1} + \mathcal{O}(\bar{x}^2)](1 - p_B). \tag{3.12}$$

Going to the continuous limit, the coordinate z measures the distance of the rows from the surface. The surface is at $z = z_1$ and the surface order parameter is $\bar{x}(z_1) = \bar{x}_S$. The limit $z \to \infty$ corresponds to the bulk, with an order parameter $\bar{x}_B$. Introducing the extrapolation length λ

$$\left.\frac{d\bar{x}}{dz}\right|_{z=z_1} = \frac{\bar{x}(z_1)}{\lambda} \tag{3.13}$$

one finds after integration

$$\bar{x}_1^2[a(p_B - p_{Bc}) + c(p_B)\lambda^{-2}] = a(p_B - p_{Bc})\bar{x}_B^2 \tag{3.14}$$

where a and c are finite coefficients and $p_{Bc} = \frac{4}{5}$ in this approximation. When the extrapolation length remains finite, which is the case at the ordinary transitions, one obtains the following relation among the exponents:

$$\beta_1 = \beta_B + \tfrac{1}{2}. \tag{3.15}$$

Moreover, when approaching the special transition, the extrapolation length λ behaves asymptotically as

$$\lambda \sim (p_S^{sp} - p_S)^{-y} \tag{3.16}$$

where p_S^{sp} is the value of p_S at the special critical point. One then finds that

$$\beta_1 = \beta_B + \tfrac{1}{2}\Theta(\tfrac{1}{2} - y) \tag{3.17}$$

where Θ is the usual Heaviside function.

As will be seen in the next section, the relation (3.15) is approximately satisfied by the results of the numerical simulation, although the values of the exponent themselves are far from their mean field values.

4. Numerical simulation

The numerical simulation has been performed on a system of size 128×256 periodic in the longer direction. For such size, the finite size effects are negligible [7]. Starting from an empty surface, one waits N_i time steps per site to reach a stationary solution. Then, the stationary solutions are obtained by averaging over N_m measures each separated by N_{int} time steps over N_s different samples. The values of N_m and N_{int} are chosen in such a way that the fluctuations are negligible.

The first simulation concerns the ordinary transition at $p_B = p_S$. With $N_s = 2$, $N_i = 1000$, $N_m = 200$ and $N_{int} = 10$, one obtains

$$p_{Bc} = p_{Sc} = 0.679 \pm 0.002 \qquad \beta_B = 0.59 \pm 0.04 \qquad \beta_1 = 1.0 \pm 0.08. \tag{4.1}$$

The second simulation concerns a point on the surface transition line for which $p_B = 0.85 > p_{Bc}$. With $N_s = 5$, $N_i = 5000$, $N_m = 500$ and $N_{int} = 10$, one obtains

$$p_{Sc} = 0.376 \pm 0.003 \qquad \beta_1 = 0.25 \pm 0.05. \tag{4.2}$$

Note finally that for $p_B = 1$, one recovers the one-dimensional system for which one knows that [3]

$$p_{Sc} = p_{B,1dim} \simeq 0.365 \qquad \beta_1 \simeq 0.28. \tag{4.3}$$

This last value of the critical exponent β_1 is the one of two-dimensional directed percolation. Note that for $p_B < p_{Bc}$, one does not observe a surface transition for any value of $p_S < 1$. Thus one sees that the phase diagram obtained by simulation is qualitatively similar to the mean field renormalization group predictions. Quantitatively, the agreement is not bad.

Concerning the critical exponents, the values for β_B and β_1 are quite far from the mean field values. Note, however, that the relation (3.15) established in mean field approximation is almost satisfied by the numerical results obtained for the ordinary transition.

Another interesting feature concerns the surface transition Simulations done with parallel dynamics [15] have shown that the surface exponent β_1 was the same for several points along the surface transition line. Moreover, one notes that the value obtained for β_1 is compatible with the value of the exponent corresponding to the limit case $p_B = 1$, which is the one of the one-dimensional bulk case.

Note that such a behaviour is not necessarily present for equilibrium phase transitions. Indeed, if one introduces a surface partition function obtained by tracing out the degrees of freedom below the surface, then the associated effective one-dimensional Hamiltonian is usually not the one-dimensional Hamiltonian of the original problem.

The fact that the two exponents are the same means, in terms of renormalization group arguments, that the fixed point corresponding to the special transition is unstable and that its critical behaviour is governed by the more stable fixed point at $p_B = 1$. A similar situation has been found for the surface effects in the Potts model [16].

5. Conclusions

The study of critical phenomena at surfaces in a simple model of non-equilibrium phase transition shows that a similar richness to that found in equilibrium surface critical phenomena is present. Namely, one finds ordinary, extraordinary, special and surface phase transitions. The mean field renormalization group approach gives a good description of the phase diagram. The critical exponents ν obtained by this method are reasonable. However, the exponents β obtained by simple mean field approach are rather poor when compared with the results of the simulation.

As far as the special transition is concerned, the question of the form of the crossover for the critical exponents β_1 and β_B in the vicinity of this critical point needs also to be clarified. Several questions remain open concerning the critical exponents. More information is needed (as for example the determination of the correlation length exponent ν), to test if scaling relations exist among bulk and surface exponent as it is the case in equilibrium. These points are under investigation.

Acknowledgments

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