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Critical behavior in nonequilibrium phase transitions

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The nonequilibrium phase transitions occurring in a fast-ionic-conductor model and in a reaction-diffusion Ising model are studied by Monte Carlo finite-size scaling to reveal nonclassical critical behavior; our results are compared with those in related models.

Nonequilibrium states in macroscopic systems[1] are, almost by definition, more complex and consequently varied than equilibrium states. This prevents, in practice, their study within the simple and well-defined framework of statistical mechanics. Actually, the study of nonequilibrium phenomena is based nowadays on a collection of *ad hoc* methods, most of them approximate, for particular problems. The situation cannot be said to be much better in the simplest case of stationary nonequilibrium states, namely, when the system of interest is coupled to a subsidiary system in such a way that both systems are not in mutual equilibrium, but rather, there is a net steady flow of some extensive quantity through them. The main difficulty here again is that, excluding some trivial systems (with no interactions between their constituents),[2,3] there is no *a priori* knowledge of what the appropriate Gibbs ensemble is; moreover, the number of relevant exactly soluble models at hand is rather scarce.[3–6]

The increasing interest in stationary nonequilibrium states comes partially from the fact that, as was made clear recently, they may show instabilities;[4–9] these produce a kind of phenomenon so similar in principle to the corresponding ones in equilibrium statistical mechanics that they may be termed as *nonequilibrium phase transitions.* Initially, given that most familiar tools such as canonical averages and fluctuation-dissipation theorems are questionable here, most effort was directed towards the study of the microscopic mechanisms of the various instabilities in steady states. However, recent concern has concentrated[10–12,4] on the general properties of nonequilibrium phase transitions.

Concerning this point of view, there is a rather common belief in the literature (see, for instance, Refs. 7, 9, 4, 5, and 11–15) that nonequilibrium phase transitions bear basically a classical character, i.e., that they can be described, even exactly for present-day experimental data, on the basis of the classical Landau theory of phase transitions and critical phenomena. On the contrary, we present in this article some clear evidence that the phase transitions occurring in two models of stationary nonequilibrium states are basically nonclassical. The first case refers to a fast-ionic-conductor model, namely, to the lattice-gas version of the Ising model, where the particles are interpreted as ions under a strong uniform external electric field;[10] an extensive finite-size scaling analysis reveals that the corresponding critical exponents for the infinite system have neither equilibrium nor classical values. The second case refers to a reaction-diffusion Ising model;[5] this is shown to present a discontinuous phase transition when the (infinite-temperature) diffusion predominates over the reaction (spin-flip) dynamics, and a continuous one with equilibrium critical exponents at lower diffusion. Our results, when compared with the situation concerning some related models,[4,5,11,14,15] suggest some "unexpected" diversity which is important to the definition of universality classes in nonequilibrium phenomena. They also indicate, in particular, that nonequilibrium versions of the Ising model may provide a rich ground for the study of these matters: probably the situation here is much richer, more varied and interesting than in the familiar equilibrium counterpart. Further results on the behavior of our models and details of the corresponding analysis will be published elsewhere.

The first model of interest has been described extensively before.[17,13,10] It consists in the present case of a square lattice with periodic boundary conditions whose sites can be either empty ($n_i=0$) or occupied by an ion ($n_i=1$); $i=1,2,\ldots N=L^2$. The mean system density $N^{-1}\sum_i n_i$ equals $\frac{1}{2}$. The evolution proceeds by hopping ions to NN empty sites according to the transition probabilities per unit time $p_M=1$ if $\delta H'\leq 0$ or $\exp(-\delta H'/k_B T)$, otherwise, which satisfy locally a detailed balance condition.[17] Here $\delta H'=\delta H+E$, where δH is the change in the configurational system energy produced by the jump and $E=\pm\infty$ for jumps in the directions $\pm\hat{x}$, respectively, and $E=0$ for jumps in the perpendicular directions $\pm\hat{y}$. The existence of the uniform electric field $E\hat{x}$ induces a preferential hopping along one of the principal directions of the lattice, $\hat{x}$, leading to a stationary nonequilibrium state with a net steady current of particles. The jumps in the direction of the field may also be enhanced, as compared to those perpendicular to it, by performing the former with a frequency Γ times larger than the latter. The model solved in Ref. 4 essentially corresponds to the present one in the limit $\Gamma\to\infty$. We shall mainly refer here to the case $\Gamma=1$, however. The natural order parameter for the two-dimensional phase transition is $m=(\langle M_x^2\rangle-\langle M_y^2\rangle)^{1/2}$, where

$$M_{x(y)}^2\equiv L^{-1}\sum_{y(x)}\left[L^{-1}\sum_{x(y)}(2n_{xy}-1)\right]^2$$

and $\langle\ \rangle$ denotes the "canonical" ensemble average at temperature T produced by the transition probability p_M defined above; m is a measure of the density difference between fluid and vapor phases.

That is, as it was reported before,[10] the system segregates below some critical temperature $T_c(E)$ [$> T_c(0)$, the Onsager critical temperature] into a vapor, ion-poor phase and a liquid, ion-rich phase, the latter being highly anisotropic with striplike configurations along the field direction; that study, however, is prevented from quite definite conclusions concerning critical behavior due to finite-size effects. We report here on the results from an extensive Monte Carlo finite-size scaling analysis for $L \leq 100$ (including also some "confidence" runs for $L=300$). Most data for m as a function of L and T are presented in Fig. 1. A conclusion from Fig. 1 is that, excluding small L, one has linear behaviors of m with L^{-1} for $T<T_c(E)$ and with $L^n, n \approx -0.2$, for $T>T_c(E)$; this is confirmed later on [e.g., after Eq. (1) where we give a physical significance to n]. This allows the computation of m_∞, the order parameter for the infinite system or limit of m_L as $L \to \infty$.

We first performed plots of $m_\infty^{1/\beta}$ versus T for different values of β; these definitely show that neither $\beta=\frac{1}{8}$ nor $\frac{1}{2}$ is able to produce linear behavior near the temperature axis ($m_\infty=0$) and critical temperatures (intercepts with the temperature axis) in agreement with the rest of the data (e.g., with the behavior of the energy or the currents, with the scaling behavior we report later on, etc.). Instead, we find by using those criteria that $\beta=0.230\pm0.003$ and $T_c(E)=(1.355\pm0.003)T_c(0)$ for the infinite system. These values also produce the best linear fit in a log-log plot; cf. Fig. 2 and notice that small changes in β and/or $T_c(E)$ would not produce such clear evidence at all.

The shift we observe in the critical temperature is caused by the field-enhancing correlations (along $\hat{x}$) and thus producing phase segregation at a temperature which is otherwise (in the absence of the electric field) only characterized by short-ranged correlations; this also seems the cause for the appearance of a (new) universality class halfway between the Onsager and classical ones. Intuitively, one may argue that the effect should be less pronounced in three dimensions; this is certainly confirmed by the corresponding critical temperature which is $T_c(E) \approx 1.1 T_c(0)$.[13,18] Were that the case, one should probably expect $0.313 < \beta < \frac{1}{2}$, β perhaps being closer to the lower limit. This is also consistent with some data on the three-dimensional version of the above model[18] which seems to prefer $\beta \approx 0.4$. While the above facts for $d=2$ seem consistent with some renormalization-group (RG) computations[11,14,15] predicting a critical dimension of 2, our suggestions for $d=3$ are apparently not. One should notice, however, that the RG computations are approximate, and that they also reveal that the global behavior is not quite described by the classical, mean-field theory ignoring all effects of the fluctuations; see also later on. We are presently performing a similar finite-size analysis for $d=3$ (the only available data in three dimensions refer to 30^3 simple cubic lattices[18]) which might clear up somewhat this question.

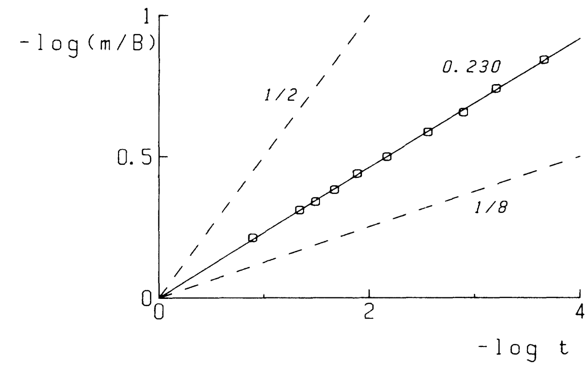

FIG. 2. Logarithmic plot of the order parameter for the infinite system, as obtained from Fig. 1 (see also the text) versus $t \equiv 1-T/T_c(E)$ showing $\beta=0.230$ and $T_c(E)=1.355T_c(0)$. The numbers identifying the lines are the corresponding slopes.

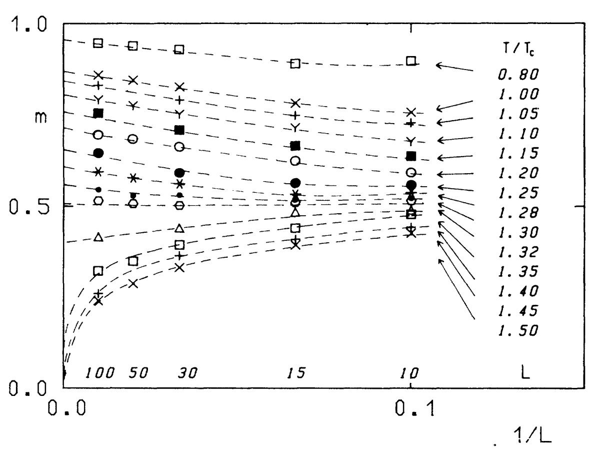

FIG. 1. Dependence of the order parameter on temperature and size for the fast-ionic-conductor model; $T_c \equiv T_c(0)$. Notice the extrapolation as $L \to \infty$.

The above conclusions for β and $T_c(E)$ in two dimensions are indeed confirmed by a global finite-size scaling analysis. For instance, Fig. 3 is a definite evidence that

$$m_L = \begin{cases} L^{-\beta/\nu}(Bz^{\beta}+B_s z^{\beta_s}), & T<T_c(E) \\ B_s'(z')^{\beta_s'}, & T>T_c(E) \end{cases} \tag{1}$$

with $z=tL^{1/\nu}$, $z'=t'L^{1/\nu}$, $\nu=0.55\pm0.2$, $\beta_s=\beta-\nu$, and $\beta_s'=n\nu$. The result in Eq. (1) is also noticeable. It reveals that the surface contributions in the present problem, which are described by the exponents β_s [for $T<T_c(E)$] and β_s' [for $T>T_c(E)$], are much more important (cf. also Fig. 1) than in the usual Ising problem with periodic boundary conditions (where, in particular, $B_s=0$). Actually, it seems that the existence of striplike configurations produces surface effects which are, at least approximately, similar to the ones in the case of the two-dimensional Ising model with free edges.[16] On the other hand, we find no evidence that ν has different values for the $\hat{x}$ and $\hat{y}$ directions; some crude Monte Carlo RG computation is roughly consistent with this fact.[19] The analysis of the specific heat by the same method (i.e.,

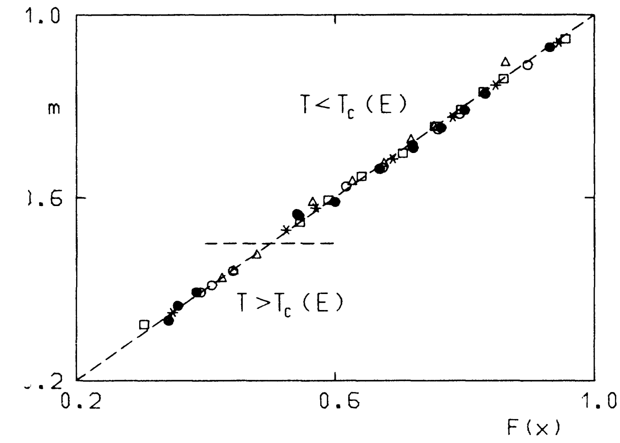

FIG. 3. Order parameter $m(L,T)$ vs $F(x)$, where $F(x)=L^{-\beta/\nu}(Bx^{\beta}+B_s x^{\beta_s})$ when $T<T_c(E)$ and $F(x)=B_s'(x')^{\beta_s'}$ when $T>T_c(E)$ to demonstrate Eq. (1). [Notice the definitions $x=tL^{1/\nu}$, $x'=t'L^{1/\nu}$, $t'=1-T_c(E)/T$, and the fact that it follows $m=F(x)$ from the figure.] The values used for the parameters are $\beta=0.23$, $\nu=0.55$, $B=1.186$, $B_s=-0.77$, $\beta_s=\beta-\nu, B_s'=0.52$, $\beta_s'=n\nu$, and $n=-0.2$. Different symbols correspond to different values of L, $10\leq L\leq 100$.

separating the bulk and surface contributions) is more involved, e.g., due to the failure of the fluctuation-dissipation theorem in this nonequilibrium case; we shall report on it elsewhere.

One should probably expect, as suggested at the beginning of this article, more variety concerning nonequilibrium phase transitions than in the equilibrium counterpart. For instance, relevant or marginal parameters affecting critical behavior, which are seldom present, in practice, in the case of equilibrium phase transitions, might be more frequent here; this is apparently the case for Γ in the above model, i.e., small values of Γ ($\Gamma=1$ and perhaps also $\Gamma\leq 20$) produce the above universality class while increasing Γ may finally lead to classical critical behavior.[10,4] That variety also makes the comparison between the behaviors of closely related models difficult. For instance, it is not quite clear, the relation between the fluid under shear model by Onuki and Kawasaki[11] and the fast ionic conductor model with $E=\infty$; actually, the shear flow in the former tends to cut off the lifetime of large fluctuations with small wave numbers, which is an effect essentially different from that of the electric field we mentioned before; there is a finite rate of shear flow acting as a continuous parameter, etc. Even the models by Leung and Cardy[14] and by Janssen and Schmittmann[15] are difficult to compare with ours, e.g., they involve field theoretic (i.e., continuous) approximate RG treatments. Finally, in order to illustrate further that variety, we describe the critical behavior in another interesting nonequilibrium version of the Ising model.

The model is now an Ising lattice whose configurations change with time according to a competition between two familiar mechanisms: a "Kawasaki (conserved order parameter) dynamics" in which unequal spins at neighboring sites exchange with a constant rate, as if the system were at an infinite temperature, and a "Metropolis (nonconserved order parameter) dynamics" in which a spin flips at a site according to the transition probabilities p_M defined before, with $\delta H'=\delta H$, however, at a finite temperature T; these two mechanisms are attempted in practice with probabilities p^* and $1-p^*$, respectively. This competition attempts to model the "reaction-diffusion" situations characterizing chemical reacting systems, spin diffusion in magnets, population genetics, etc.;[20] in particular, it maintains the system far from equilibrium thus producing nonlinear stationary nonequilibrium states undergoing phase transitions at low temperatures T, even in one dimension where essentially the same model was solved in the limit $p^*\rightarrow 1$ and for some observation time scale.[5]

The main interest here is on the nature of the expected nonequilibrium phase transition as one varies p^*; for simplicity, we refer to $d=2$ and ferromagnetic interactions. The case $p^*=0$ corresponds to the familiar equilibrium ferromagnet with critical temperature $T_c(0)$. The solution for $d=1$ and $p^*\rightarrow 1$, on the other hand, is reported[5] to have a mean-field behavior in the sense that the magnetization below $T_c(p^*\rightarrow 1)=2J/k_B\ln 3$ has two symmetric stable solutions at both sides of an unstable solution. The situation for $d=2$ and $p^*=0.95$ is not quite consistent with the latter: We observe clear discontinuities in the curves for the spontaneous magnetization and energy as a function of T, the specific heat presents a (lambda) finite discontinuity, and there are long-lived metastable states. That is, there is a first-order phase transition occurring around $T_c(p^*=0.95)=0.90T_c(0)$. The other limit is also quite interesting because we find that the behavior for $p^*\leq 0.80$ is practically the same as for $p^*=0$; that is, we observe then a typical continous phase transition, with continuous magnetization and energy as a function of T, the familiar Onsager divergence for the specific heat as computed from the fluctuations of the energy data, and (by considering lattice sizes $L\leq 100$) we find $\beta=\frac{1}{8}$, independently of $p^*(\leq 0.80)$. The critical temperature, however, changes with p^*; e.g., $T_c(p^*=0.80)=0.93T_c(0)$, $T_c(p^*=0.60)=0.96T_c(0)$, and $T_c(p^*=0.10)=0.99T_c(0)$. Figure 4 is clear enough evi-

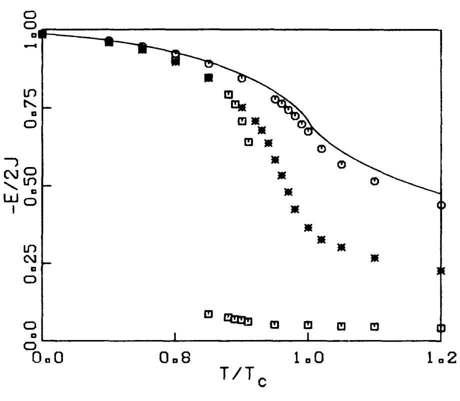

FIG. 4. Energy versus temperature in the case of the reaction-diffusion Ising model for different values of the parameter p^*: $p^*=0.10$ (circles), 0.60 (asterisks), and 0.95 (squares); the solid line is the Onsager equilibrium case ($p^*\equiv 0$).

dence that there is a change in the order of the phase transition as one varies p^*, i.e., some sort of tricritical point at $p^* \approx 0.83$.

Summing up, the finite-size Monte Carlo study of two different versions of the Ising model, both characterized by stationary nonequilibrium states, reveals nonclassical critical behavior in nonequilibrium phase transitions. In particular, one of the models seems to belong to a new universality class, and the critical behavior of the other is apparently characterized by a tricritical point and equilibrium exponents. This, when compared with the situation concerning some related models, strongly suggests a great diversity concerning nonequilibrium critical phenomena. It also indicates that stationary nonequilibrium versions of the Ising model may provide a very rich and interesting ground to analyze nonequilibrium phase transitions.

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