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Anisotropic ordering in a two-temperature lattice gas

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We consider a two-dimensional lattice gas model with repulsive nearest- and next-nearest-neighbor interactions that evolves in time according to anisotropic Kawasaki dynamics. The hopping of particles along the principal directions is governed by two heat baths at different temperatures T_x and T_y. The stationary states of this nonequilibrium model are studied using a simple mean-field theory and linear stability analysis. The results are improved by a generalized dynamical mean-field approximation. In the stable ordered state the particles form parallel chains which are oriented along the direction of the higher temperature. In the resulting phase diagram in the T_x-T_y plane the critical temperature curve shows a weak maximum as a function of the parallel temperature which is confirmed by Monte Carlo simulations. Finite-size scaling analysis suggests that the model leaves the equilibrium universality class of the x-y model with cubic anisotropy and is described by the Ising exponents. [S1063-651X(97)09802-4]

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I. INTRODUCTION

Systems driven into a nonequilibrium steady state can reveal a number of features not characteristic of the equilibrium state. In many cases the nonequilibrium condition breaks the x-y symmetry of a two-dimensional system. The effect of this symmetry-breaking condition is especially interesting when the ground states of an equilibrium model also violate the x-y symmetry. An example is the well-known two-dimensional lattice gas model with attractive nearest-neighbor interaction and conserved density [1]. In the half-filled system the degenerate ground states violate the x-y symmetry of the system. Below a critical temperature the disordered (high-temperature) phase separates into a high- and a low-density phase with interfaces that can be oriented either horizontally or vertically if periodic boundary conditions are imposed. A simple way to introduce a nonequilibrium symmetry-breaking condition on this model is to drive the lattice gas as suggested by Katz *et al.* [2]. In the driven model, the particle jumps are under the influence of a uniform external electric field whose direction is chosen to be parallel to one of the principal axes [3]. In this case it turns out that the interface is always parallel to the driving field.

The so-called two-temperature models [4–6] imply another way to impose anisotropic dynamics. In these models the particle jumps are coupled to two different heat baths, that is, the Kawasaki (exchange) dynamics is characterized by two different temperatures, T_x and T_y, along the x and y axes, respectively. Contrary to the standard driven diffusive systems [2], these models do not exhibit macroscopic particle current through the system. The two-temperature models can be considered as a simplified description of the effect of an alternating electric field causing an increase of jump rates along the applied field [3].

In the above mentioned system with attractive interactions the symmetry breaking is represented by the orientation of the interface separating the high- and low-density phases, while the particle distribution remains isotropic in the bulk phase. Significantly different symmetry breaking can be observed in models with sublattice ordering, e.g., in square lattice gases with repulsive nearest- and next-nearest-neighbor interactions of equal strength [7]. In the half-filled system the particles form alternately occupied and empty columns (or rows). That is, here the symmetry breaking appears locally in the fourfold degenerate ground states. The ordering process is well understood in this model [8,9] and the effect of a uniform driving field on the ordering process has also been investigated [10]. It was found that the phases consisting of chains of particles perpendicular to the external field become unstable. In other words, in the stationary state the chains are oriented along the field. Consequently the chain orientation of the ordered phase can be controlled by the application of a uniform driving field with a suitable direction. A similar effect may be conjectured when using an alternating field which is technically easier to realize. This conjecture is the motivation for the present work.

The equilibrium version of the present model ($T_x = T_y$) belongs to the family of Ashkin-Teller models [11] exhibiting ground states with broken x-y symmetry on a square lattice. These models are widely used to study anisotropic ordering of adatoms on crystal surfaces [8,12,13]. In addition, the oxygen ordering in the family of YBCO superconducting oxides was successfully described with such a model [14]. In these materials the effect of an external electric field on the oxygen ordering has also been investigated [15]. It is found that the direction of Cu-O chains can be controlled by the application of an electric field. This phenomenon is generally related to the appearance of an induced electric dipole moment of the oxygen atoms. So far, a reorientation process has been demonstrated when the jump rates are affected by an external field [16]. According to the present work a similar behavior is expected when applying an alternating field (or polarized light) during a high-temperature annealing process in an oxygen atmosphere. In general, we can say that the manipulation of the ordering process with similar ''dynamical tools'' is possible for those systems which undergo spontaneous symmetry breaking accompanied by anisotropic transport properties.

In the present paper we demonstrate that the ordering process exhibiting x-y symmetry breaking can be affected by taking the jump rates to be anisotropic. For this purpose we shall study the sublattice ordering in a square lattice gas within the formalism of a two-temperature model. In Sec. II we introduce the model and investigate it by adopting a simple dynamical mean-field theory. Linear stability analysis is also performed to distinguish the stable and unstable solutions. In the light of the results obtained, the phase diagram is calculated at a higher level (four-point approximation) of dynamical mean-field theory in Sec. III. The results are compared with Monte Carlo (MC) data. In addition to the nonequilibrium phase diagram we also study the nonequilibrium critical behavior of the model by finite-size-scaling analysis in Sec. IV. Finally we summarize and conclude in Sec. V.

II. MODEL

We consider a half-filled lattice-gas model with isotropic nearest- and next-nearest-neighbor repulsive interactions with equal strength on a square lattice ($J_{\rm nn}=J_{\rm nnn}=1$). As usual, the coupling constants as well as the Boltzmann constant are chosen to be unity for convenience. The kinetics is governed by Kawasaki dynamics characterized by single particle jumps to one of the empty nearest neighbor sites [17]. To avoid the difficulties arising from the nonanalytic feature of the Metropolis rate [18], a Kawasaki hopping rate, g_α, is used for directions $\alpha=x$ or y:

$$g_\alpha(\Delta H)=\frac{1}{1+\exp(\Delta H/T_\alpha)}, \tag{1}$$

where ΔH is the energy difference between the final and initial configurations. This jump rate is anisotropic and satisfies detailed balance at temperature T_y (T_x) in the vertical (horizontal) direction.

The equilibrium model ($T_x=T_y$) undergoes a continuous phase transition at a critical temperature $T_c=0.525$ [8]. In the ground states the columns (or rows) are alternately occupied and empty, leading to fourfold degeneracy. Following the standard notation, the lattice is divided into four interpenetrating sublattices and the 2×1 or 1×2 long-range superantiferromagnetic order is characterized by the corresponding average sublattice occupation variables n_i ($i=1,\ldots,4$) [7]. In the half-filled system, the 2×1 states consisting of vertical chains are given by $n_1=n_4=(1+m_x)/2$ and $n_2=n_3=(1-m_x)/2$, where $-1\leqslant m_x\leqslant1$ is the order parameter. Notice that m_x can be either positive or negative. Its absolute value as a function of temperature may be estimated by using the standard mean-field (MF) approximation. Similar expressions are obtained for the 1×2 states of horizontal chains, namely, $n_1=n_2=(1+m_y)/2$ and $n_3=n_4=(1-m_y)/2$. It is emphasized that the four possible states are equivalent ($|m_x|=|m_y|$) in the equilibrium system. Evidently, in the high-temperature disordered phase, $m_\alpha=0$.

In the following simple dynamical mean-field approximation we will assume that the long-range order still exits under the present nonequilibrium condition. It implies that the anisotropic jump rate only results in a difference between the solutions characterized by m_x and m_y.

The time evolution of n_1 is determined by summing the contributions of the elementary jumps modifying the particle density in sublattice 1, namely,

$$\frac{dn_1}{dt}=-2n_1[(1-n_2)g_x(E_{21})+(1-n_4)g_y(E_{41})]+2(1-n_1)[n_2g_x(E_{12})+n_4g_y(E_{14})], \tag{2}$$

where E_{ij} is the average value of ΔH when a particle jumps from sublattice j to i. Similar equations can be derived for the other sublattice occupation variables. Assuming a 2×1 or 1×2 structure (vertical or horizontal chains), the stationary solution to Eq. (2) obeys the following general form:

$$\frac{1+m_\alpha}{1-m_\alpha}=\exp(3m_\alpha/2T_\alpha), \tag{3}$$

where $\alpha=x$ or y. In the equilibrium case, i.e., for $T_x=T_y$, this simple approximation predicts a continuous phase transition at a critical temperature $T_c^{(\rm MF)}=3/4$. When $T_x\neq T_y$, the jumps along the chains do not modify the particle density within the chains (and the value of the corresponding order parameter) and the particle density therefore only depends on the perpendicular jump rate (i.e., the perpendicular temperature). This implies that the chain structure remains stable even in the limit where the parallel temperature goes to infinity. The order parameter(s) as a function of perpendicular temperature can be determined numerically.

Obviously we have two different solutions for $T_x\neq T_y$ namely, $m_x\neq0$, $m_y=0$ and $m_x=0$, $m_y\neq0$. In this situation a linear stability analysis is used to determine which solution remains stable. This method has proved to be very useful when investigating the effect of a uniform driving field on these ordered structures in the same lattice gas model [10]. We shall here restrict ourselves to a survey of results obtained for the present two-temperature model leaving out the mathematical details described in the previous work [10]. It is found that the ordered structure appears when $\min(T_x,T_y)<T_c^{(\rm MF)}$ and the chains in the stable phases are parallel to the direction of the higher temperature. For $T_x,T_y<T_c^{(\rm MF)}$ the phases with chains perpendicular to the direction of the higher temperature are unstable against small perturbations in the vicinity of $T_c^{(\rm MF)}$ and become metastable at lower temperatures. This situation is similar to those found when applying a uniform driving field [10]. In the present case the chain orientation of the ordered phase may be reversed by exchanging T_x and T_y. For low temperatures this orientation process is expected to appear via a nucleation mechanism, as discussed in [10]. The detailed analysis of this reorientation phenomenon goes beyond the scope of the present work.

III. NONEQUILIBRIUM PHASE DIAGRAM

The prediction from the simple mean-field theory can be improved by using a generalized mean-field theory at the levels of two- and four-point approximations. In these calculations we have to determine the probability of all of the possible configurations on two- and four-point clusters by evaluating numerically the stationary solution of a set of

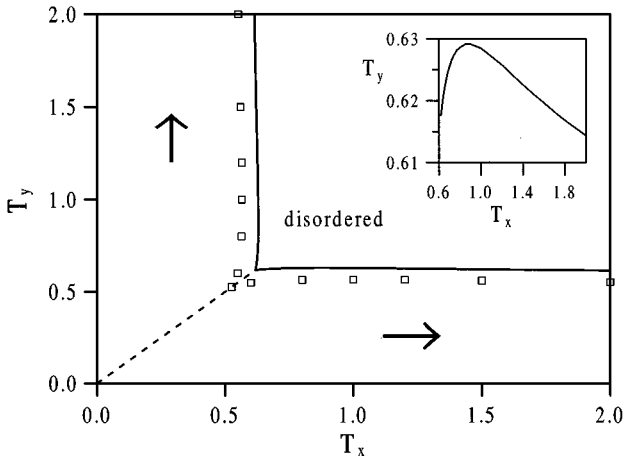

FIG. 1. Phase diagram predicted by four-point dynamical mean-field approximation (solid line). MC data are denoted by squares. The inset shows the nonmonotonous feature of the critical temperature curve.

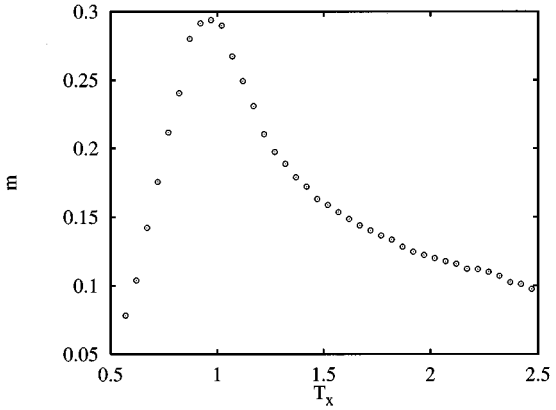

FIG. 2. Order parameter as a function of parallel temperature at a fixed perpendicular temperature ($T_y=0.56$) as obtained from Monte Carlo simulation on a square lattice of size $L\times L=100\times 100$.

equations which describe the time variation of the configuration probabilities [18,19]. The two-point (pair) approximation fails to reproduce the phase transition even in the equilibrium model ($T_y=T_x$). More precisely, this approximation predicts a first-order transition. Similar discrepancies have already been observed for other systems [18]. This shortcoming of the present technique may be eliminated by considering larger clusters.

By exploiting symmetries we have only four independent parameters to describe the probability of all the possible particle configurations on a square block. In equilibrium, this method suggests a continuous order-disorder transition and the predicted critical temperature is $T_c^{(4p)}=0.61$.

In the nonequilibrium case ($T_x\neq T_y$), the prediction of the four-point approximation agrees qualitatively with those obtained above. However, the critical temperature now depends on both temperatures. A weak but clear peak is found when T_x and T_y are close to $T_c^{(4p)}$ Namely, the perpendicular critical temperatures first *increase* when we increase the parallel temperature and after a maximum the transition temperature *decreases* monotonously as can be seen in the insert of Fig. 1. When the parallel temperature goes to infinity the transition point tends toward a constant value $T_c^{(4p)}(\infty)=0.94T_c^{(4p)}$. Hence, in agreement with the earlier approximation, the ordered state still exists even at infinite parallel temperature if the perpendicular temperature is low enough.

In order to investigate the validity of the above predictions, a series of Monte Carlo simulations [20] were carried out varying the temperatures T_x and T_y. Using periodic boundary conditions the simulations were performed on a square system with different sizes ranging from $L\times L=20\times 20$ to 200×200. We have determined the time averages of the energy and order parameter varying the perpendicular temperature at a fixed parallel temperature. As is convenient for simulation we used the order parameter

$$m=\sqrt{(m_1)^2+(m_2)^2} \tag{4}$$

derived from the two components of the sublattice ordering, $m_1=[(n_1+n_2)-(n_3+n_4)]/2$ and $m_2=[(n_1+n_4)-(n_2+n_3)]/2$ [7]. The simulations confirmed the picture obtained from the dynamical mean-field theory, that is, the ordering process remains continuous for all of the parallel temperatures studied. The complete phase diagram, shown in Fig. 1, suggests that the transition temperature depends very weakly on the parallel temperature, in a way similar to that predicted by the four-point approximation. In agreement with the theoretical approximations the critical temperature tends to a constant value which is $0.98T_c^{(\mathrm{MC})}$ when the parallel temperature goes to infinity.

The peak of the critical temperature curve implying reentrant phase behavior can also be detected if we increase T_x at a fixed suitable value of T_y. The results of a series of MC simulation are illustrated in Fig. 2, where $T_y=0.56$ and the system size is $L\times L=100\times 100$. In the case of equilibrium ($T_x=T_y=0.56$) the particle distribution is practically disordered and the nonvanishing value of the order parameter defined by Eq. (4) is due to the finite system size. Upon increasing T_x the particles arrange into a horizontally ordered chain phase leading to an increase of m. Further increase of T_x destroys the ordered structure as indicated.

The nonmonotonous behavior of the critical temperature curve may be explained by the competition of two processes. As mentioned above the ordered state with chains perpendicular to the direction of the higher temperature is unstable. Above T_c, the equilibrium system contains small ordered domains of either chain direction. However, when we impose different temperatures, the emerging small domains will prefer the direction of the higher temperature, their coalescence becomes more probable, and finally we will get larger domains of the preferred direction without changing the perpendicular temperature. This type of symmetry breaking stabilizing one type of domains on the expense of the other will, on the one hand, increase the transition temperature. On the other hand, the thermal fluctuations increase with both temperatures (T_x and T_y) and tend to destroy the order. The competition between these two effects will determine the actual phase behavior of the system. According to this explanation if the formation of chain structure is weakened by decreasing the strength of the next-nearest-neighbor coupling

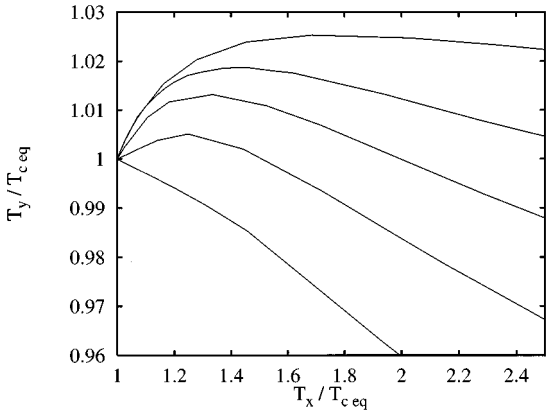

FIG. 3. Peak effect on the critical temperature predicted by dynamical mean-field approximation at different values of the next-nearest-neighbor coupling ($J_{nnn}=1.3$, 1, 0.89, 0.82, and 0.76, from top to bottom).

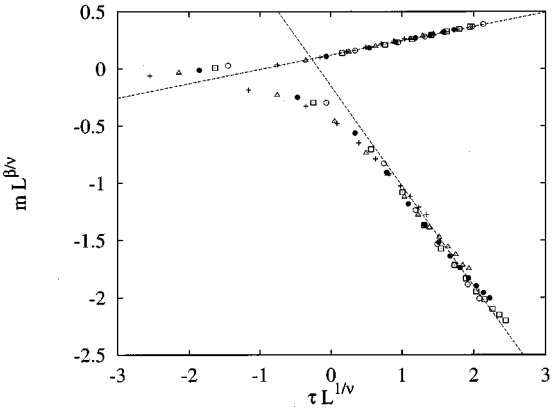

FIG. 4. Finite-size-scaling plots of MC data for the order parameter. System sizes are + 20×20, □ 30×30, ⊙ 40×40, ● 50×50, △ 60×60. The slopes of the inserted lines are 1/8 and $-7/8$.

(J_{nnn}) [21], we would expect a decrease in the transition temperature. The dynamical mean-field approximation has confirmed this prediction, i.e., by decreasing J_{nnn} the peak of the critical temperature curve becomes smaller and vanishes below a certain value of J_{nnn}, as shown in Fig. 3. In this figure we used reduced temperatures in order to facilitate the data comparison. Evidently, the effect will be opposite if we increase J_{nnn}. The MC simulations show a good qualitative aggreement with this theoretical prediction.

IV. CRITICAL BEHAVIOR

In the literature there are some examples where the critical behavior remains unchanged [22] and there are others where the universality class changes significantly under the nonequilibrium conditions [3]. We shall now study the effect of the present nonequilibrium conditions on the critical behavior of the model.

The critical behavior of the present equilibrium model has been suggested to belong to the universality class of the x-y model with cubic anisotropy [12], whose exponents are believed to be nonuniversal [23]. This expectation has been verified by finite-size-scaling analysis of the Monte Carlo data leading to the non-Ising exponents $\beta=0.1$ and $\nu=0.85$ [24] for $J_{nn}=J_{nnn}$. In the equilibrium case, $T_x=T_y$, our simulations support this result.

When the two temperatures are different a qualitative change in the critical behavior is expected because of the reduction of the ground-state degeneracy. Instead of the four possible equilibrium ground states stable for $T_x=T_y$, we have only two stable ground states for $T_x\neq T_y$. This fact implies the conjecture that the critical behavior of the nonequilibrium model is described by Ising exponents $\beta=1/8$ and $\nu=1$. To clarify this question we have performed a finite-size-scaling analysis of the Monte Carlo data in the case of infinite horizontal temperature ($T_x=\infty$). In the MC simulations the system size is varied from $L\times L=20\times20$ to 60×60. Our analysis is based on the scaling form

$$m(L,T)=L^{-\beta/\nu}\overline{m}(\tau L^{1/\nu}), \tag{5}$$

where τ is the reduced vertical temperature deviation from the critical temperature. The resulting excellent data collapse shown in Fig. 4 verifies the above conjecture. The slope of the inserted lines are 1/8 and $-7/8$. It should be pointed out that the small difference of the β values between the Ising universality class and the equilibrium behavior makes it difficult to discern the two types of behavior. It is clear, however, that the data collapse is strikingly better when Ising exponents are used. Considerably better statistics are required to settle this matter definitely.

V. SUMMARY AND CONCLUSION

In summary, we have studied the nonequilibrium ordering process in a two-dimensional lattice gas coupled to two thermal baths at different temperatures. In the equilibrium system the particles form parallel chains oriented either horizontally or vertically. Using a simple mean-field theory including linear stability analysis we have found that the ordered structure appears in the nonequilibrium case if the lower temperature is less than a certain critical value and the chains are oriented along the higher temperature. This picture has been confirmed by a dynamical four-point approximation and MC simulations. In contrast to the prediction of the simple mean-field theory, more accurate methods have indicated that the transition temperature (as well as the temperature dependence of order parameter) depends on the parallel temperature. The nonmonotonous feature of the critical temperature curve may be explained as a result of two competitive processes. It is emphasized that the ordered chain structure remains stable for sufficiently low perpendicular temperatures even when the parallel temperature tends to infinity. In this limit the isotropic finite-size-scaling analysis suggests that the critical behavior differs from the equilibrium behavior and it belongs to the Ising universality class.

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