Stationary state in a two-temperature model with competing dynamics

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A two-dimensional half-filled lattice gas model with nearest-neighbor attractive interaction is studied where particles are coupled to two thermal baths at different temperatures T_1 and T_2. The hopping of particles is governed by the heat bath at temperature T_1 with probability p and the other heat bath (T_2) with probability $1-p$ independently of the hopping direction. On a square lattice the vertical and horizontal interfaces become unstable while interfaces are stable in the diagonal directions. As a consequence, particles condense into a tilted square in the novel ordered state. The p dependence of the resulting nonequilibrium stationary state is studied by a Monte Carlo simulation and dynamical mean-field approximation as well.
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Nonequilibrium phase transitions have been studied extensively in the past decade. One of the important questions to address is how nonequilibrium constraints influence the order-disorder phase transition and the stationary state. A widely studied example is the celebrated kinetic Ising model where the nonequilibrium stationary states are produced by competing dynamics [1]. The competing dynamics can be combined Glauber (spin-flip) processes at different temperatures [2], competition of the Glauber and the Kawasaki (spin-exchange) dynamics [3], or spin exchanges in different directions with different probabilities. The latter case (*anisotropic* Kawasaki dynamics) may be interpreted as a driven diffusive [4] or a two-temperature lattice gas model [5] depending on whether the spin exchanges in different directions are governed by an external field or two different temperatures. One can introduce the *isotropic* version of two-temperature lattice gas model in which the hopping of particles (spin exchange) is governed by randomly applied heat baths at different temperatures independently from hopping directions.

Although it is one of the simplest models with competing dynamics, it has not been studied yet. One can suspect that this kind of mixture of Kawasaki dynamics does not result in relevant nonequilibrium behavior and the system can be described by introducing the concept of an effective temperature. In fact, an earlier study of the Ising model with competing Glauber dynamics [2] has concluded a similar result.

In the present paper we study a two-dimensional lattice gas model where particles are coupled to two thermal baths at different temperatures independently of the hopping direction (isotropic Kawasaki dynamics). The Monte Carlo simulations demonstrate that the stationary state differs completely from those of the corresponding equilibrium model. In spite of the mentioned expectations the model shows relevant nonequilibrium behavior.

We consider a two-dimensional lattice gas on a square lattice with $L\times L=N$ sites under periodic boundary conditions. The occupation variable n_i at site i takes the values 0 (empty) or 1 (occupied) and half-filled occupation ($\Sigma_i n_i = N/2$) is assumed. The energy of the system is given by

$$E=-J\sum_{(i,j)} n_i n_j, \tag{1}$$

where the summation is over the nearest-neighbor pairs and $J>0$. The particles can jump to one of the empty nearest-neighbor sites with the hopping rate

$$W=pw(\Delta E,T_1)+(1-p)w(\Delta E,T_2), \tag{2}$$

where ΔE is the energy difference between the final and initial configurations. The probability $w(\Delta E,T_\alpha) = \min[1,\exp(-\Delta E/T_\alpha)]$ is the familiar Metropolis rate ($\alpha = 1,2$) where the lattice constant and the Boltzmann constant are chosen to be unity. The hopping rate defined in Eq. (2) may be interpreted as a randomly chosen contact to a thermal bath at temperature T_1 with probability p and another thermal bath at temperature T_2 with probability $1-p$.

In the case of $T_1=T_2$, evidently, the above-defined model is equivalent to the standard kinetic Ising model which undergoes an order-disorder phase transition at $T_c=0.567$. In this half-filled system the particles condense into a strip below T_c to minimize the interfacial energy. It should be noted that in the ordered state the interface can be oriented either horizontally or vertically; thus this ordered phase violates the x-y symmetry. A suitable order parameter for characterizing the transition to striplike order is the anisotropic squared magnetization [4]

$$m=\sqrt{|\langle M_y^2\rangle-\langle M_x^2\rangle|}, \tag{3}$$

where

$$M_y^2=\frac{1}{L}\sum_x\left[\frac{1}{L}\sum_y (2n_{xy}-1)\right]^2. \tag{4}$$

Henceforth we will restrict ourselves to the case of $T_1=0$ and $T_2=\infty$. Obviously, for a small value of p the hopping of particles is mostly governed by the heat bath at temperature T_2; therefore the stationary state is expected to be disordered. In the opposite case, the stationary state becomes ordered in the $p\to 1$ limit. To calculate the critical value p_c of the order-disorder transition point, we employ the dynamical mean-field approach suggested by Dickman [6]. This method has been applied successfully in a number of other nonequilibrium models [7–9]. The value of p_c can be ob-

tained by the linear stability analysis of the spatially homogeneous disordered phase. In this approach the first step is to set up the master equations which describe the time evolution of the probabilities of the clusters, where the size of the clusters characterizes the level of approximation. Next, we determine the stationary solution of the master equations by assuming a disordered phase. In the following a small density gradient is applied and the current generated in response to the density gradient is calculated. Decreasing the parameter p the sign of the current changes is changed at a given value which can be identified as the critical point. The results of these approximations are $p_c^{(2p)}=0.893$ at the two-point and $p_c^{(4p)}=0.907$ at the four-point levels.

A Monte Carlo simulation has been carried out to check the validity of the above predictions. We have used independent random numbers for choosing what heat bath to couple the particle to and for comparing with the corresponding hopping probability during an elementary Monte Carlo step. However, the qualitative behavior remained unchanged if the same random number was used for the above-mentioned two steps. The simulation was started from a perfectly ordered strip in the presumed ordered region (at $p=0.97$). During the simulation we have monitored the relaxation of order parameter defined in Eq. (3). Comparing the results of different system sizes, a puzzling behavior is observed. Namely, the stationary value of the order parameter decreases and tends to zero if we increase the system size. To clarify this feature we have written a computer program displaying the time evolution of configuration.

This visualization of the particle configurations has indicated that the nonequilibrium condition influences the stability of interfaces. Namely, the interface in the (01) and (10) directions became unstable. At the same time, the interfaces in the (11) and three other symmetrically equivalent directions proved to be stable. Consequently, the particles condense into a tilted square contrary to the strips observed in equilibrium system. In Fig. 1 some typical configurations are shown at different values of the control parameter p. The titled square is the real stationary state because the system evolves into this state from either a vertically or horizontally oriented strip. The opposite evolution has never been observed. However, the necessary time (τ_E) to evolve from ''strip configuration'' to the ''tilted square'' may be rather long. As an example, $\tau_E \approx 4\times 10^6$ Monte Carlo (MC) steps for a system size $L\times L=100\times 100$ and at $p=0.97$.

We have concluded that the order parameter defined by Eq. (3) cannot describe the novel type of ordering process which becomes striking especially for large systems. An adequate order parameter for the new nonequilibrium state can be defined as

$$\rho = m_x m_y , \tag{5}$$

where

$$m_x = \frac{4}{L^2} \sum_y \left| \sum_x \left(n_{xy} - \frac{1}{2} \right) \right| . \tag{6}$$

Using this definition we can describe the ordering process as demonstrated in Fig. 2. As the new ordered state differs from the corresponding equilibrium ordered phase, our system

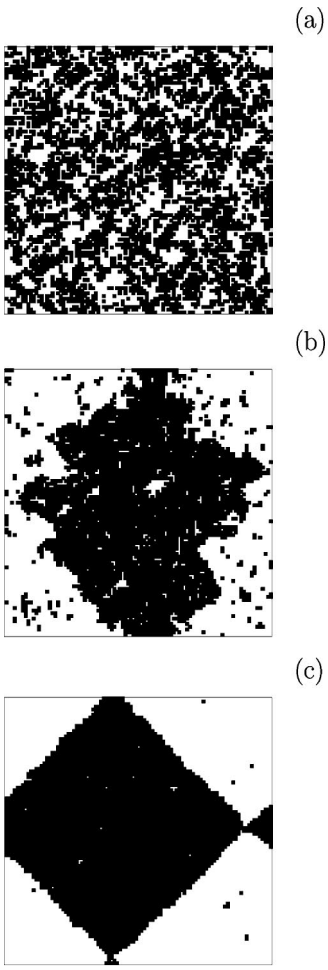

FIG. 1. Typical configurations for a 100×100 system, at $p=0.85$ (a), $p=0.95$ (b), and $p=0.99$ (c).

cannot be described by the equilibrium model with an effective temperature. The explanation of instability of horizontal (vertical) interface is related to the material transport along the domain interface. To understand the microscopic mechanism for this effect, it is instructive to compare a horizontal and a diagonal oriented interface. Suppose, a particle jumps out from a horizontal interface in consequence of fluctuations and leaves a hole in the initial site. This particle can easily move along the horizontal interface since there is no energy difference between an initial and a final site. If the

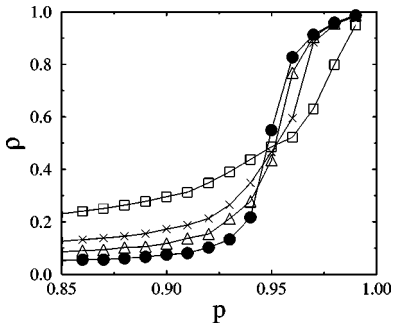

FIG. 2. The ''new'' order parameter as a function of p for different system sizes. System sizes are 20×20 (□), 40×40 (×), 60×60 (△), and 100×100 (●).

system size is large enough, the particle (hole) may meet another particle (hole) and it initiates the breakup of the interface. A significant difference has been detected in the movement of particles along the diagonal oriented interface. Here, jumps are blocked and the material transport is reduced, leaving the interface unchanged. It is an interesting question as to how a modification of the dynamics influences the stability of the diagonal interface. The movement along the interface can be reduced to only one jump by allowing for a next-nearest-neighbor jump as well. Now, the move along the interface occurs with probability 1 (since $\Delta E = 0$), similarly to the case of a horizontal interface. As a consequence, the diagonal orientation is not selected by the interfacial mobility and the horizontal (or vertical) direction, which contains lower interface energy, may be preferred. To test this argument, we have performed a MC simulation on the modified model and the equilibrium striplike state is found to be stable. We should mention that a diagonal oriented interface, which ensures minimum excess interfacial energy on a square lattice, has been obtained in a phase separation in chemically reactive mixtures [10]. A new type of stationary state, as a consequence of nonequilibrium conditions, has already been observed in other systems. For example, in a ferromagnetic Ising system with competing Glauber and Kawasaki dynamics the stationary state is identified with the antiferromagnetic state in a special parameter regime [11].

Returning to our model, we can define the derivative of energy with respect to the control parameter p similarly to the specific heat for equilibrium models. The quantity $C_p = \partial E/\partial p$ behaves like the equilibrium specific heat. The location of the maximum in C_p can be identified as a transition point for a finite lattice. Plotting the location of the C_p peak against L^{-1}, the linear fit yields $p_c = 0.947(5)$ in the thermodynamic limit. This numerical result agrees very well with the prediction of a dynamical mean-field approximation at the four-point level (the difference is only 4%).

Finally, we turn now to the problem of critical behavior briefly. A possible method to determine the critical indexes of a continuous phase transition is the finite-size scaling which has often yielded useful results for nonequilibrium models [12–14]. In the following we assume that the order parameter depends on the system size and the distance from the critical point as

$$\rho \sim L^{-\beta/\nu} f((p - p_c) L^{1/\nu}), \tag{7}$$

where β and ν are the exponents of the order parameter and correlation length. Monte Carlo data for the order parameter are fitted to the scaling form (7) with the Ising exponents and we have found good data collapse. This result is in agreement with the conjecture of Grinstein *et al.* for nonequilibrium ferromagnetic spin models with up-down symmetry [15].

In summary, we have shown that the isotropic combination of the Kawasaki dynamics for two temperatures on a square lattice can result in nontrivial behaviors in nonequilibrium stationary state. At a critical value of the control parameter p_c the system segregates into a high-density ''liquid'' and a low-density ''gas'' phase. However, in the stationary state the energy of the interface is higher than those of the corresponding equilibrium model. In the stationary state the diagonal interfaces become preferred to the horizontal and vertical ones. The phase transition describable by using a new suitable order parameter belongs to the Ising universality class. The stability of interfaces is related to the mobility of particles along the interfaces, where the diagonal orientation minimizes the influence of the energy flow between the two heat baths. Although the stability of interfaces may be tied to the type of lattice, the study of the corresponding coarse-grained macroscopic model would be useful. However, there is no straightforward way to find the macroscopic counterpart of a microscopic model. There are examples where the microscopic and supposed macroscopic model yield different morphologies [16]. Nevertheless, we believe that the behavior of our model is part of the general phenomenon where the external energy input results in interfacial effects modifying the morphology of the resulting stationary state[17,18]. Further work is required to clarify the connection between the suggested model and the abovementioned driven nonequilibrium models.

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