Critical domain size in a driven diffusive system

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The homogeneous ordered state transforms into a polydomain state via a nucleation mechanism in two-dimensional lattice gas if the particle jumps are biased by an external field $E$. A simple phenomenological model is used to describe the time evolution of a circular interface separating the ordered regions. It is shown that the area of a domain increases if its radius exceeds a critical value proportional to $1/E$ which agrees qualitatively with Monte Carlo simulations.

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Lattice-gas models under the influence of an external (electric or gravitational) field are often studied as a simple model of non-equilibrium systems \cite{5,6,7}. In these models the particle jumps are biased by a driving field $E$ resulting in particle transport through the system if periodic boundary conditions are imposed. Our attention will be focused on a half-filled, square lattice-gas model supposing repulsive nearest-neighbor interaction. In the absence of a driving field ($E = 0$) the lattice gas undergoes a sublattice ordering when the system is cooled below the Néel temperature. Dividing the lattice points into two interpenetrating sublattices the ordered phases ($A$ and $B$) are usually described by the average sublattice occupations. At low temperatures one of the ordered phases dominates and its counterpart forms only small disjoint domains (islands).

In driven lattice gases a similar ordering process was predicted in earlier papers \cite{5,6}. Very recently, however, it has been demonstrated that at low temperatures a self-organizing polydomain structure of the $A$ and $B$ phases, rather than a homogeneous (monodomain) phase, is characteristic of this driven system in its stationary state \cite{5,6}. In other words, neither of the two homogeneous states ($A$ or $B$) is stable in the thermodynamic limit; the monodomain structure transforms into a polydomain structure via a nucleation mechanism. In Monte Carlo simulations the visualization of particle distributions shows clearly that in the homogeneous $A$ (or $B$) phase small domains of the $B$ ($A$) phase are created by thermal fluctuations. The size of these domains fluctuates: they can either grow or shrink, but typically collapse within some time. The size of some domains can accidentally exceed the critical domain size, in which case the growth of these domains becomes definite. As a consequence, sufficiently large domains spread throughout the system and the monodomain phase transforms into a polydomain one. In the present paper we determine the critical domain size using a simple analytical description and Monte Carlo simulations.

The decay of a metastable phase via the nucleation mechanism is well known in the theory of first order phase transitions \cite{5,6}. In such cases the critical domain size is determined by the balance of surface and bulk energies.

Namely, the free energy difference between the stable and metastable phases provides a driving force for the growth of stable regions and the surface tension causes the minor regions to shrink. The situation in the driven lattice gas is different because here the $A$ and $B$ phases are thermodynamically equivalent. Here, the driving force of growth is produced by the enhanced interfacial material transport, which causes a rearrangement of charges (extra particles and holes) along the interfaces. As a consequence, the domains are polarized and the corresponding electrostatic force drives the domain walls along the field. It will be shown that this mechanism results in a field-dependent critical domain size.

For this purpose we adopt a simple phenomenological model used previously to describe the interfacial instability \cite{7}. Neglecting noise we will concentrate on the deterministic motion. In this phenomenological model the interface thickness and particle transport in the bulk phases are also neglected. For later convenience we generalize the previous description to allow the appearance of closed interfaces in the two-dimensional system. Thus, the interface $r$ and the interfacial charge density $\rho$ are described by single valued functions of time $t$ and a parameter along the interface.

The continuity equation for the interfacial charge density obeys the following formula:

$$\partial_t \rho = -\sigma E \partial^2_{ss} r + \sigma D \partial^2_{ss} \rho \quad ,$$

where $\partial_t$ and $\partial^2_{ss}$ denote the partial and the second partial derivatives with respect to $t$ and $s$. Here it is assumed that both the interfacial conductivity $\sigma$ and the diffusivity $D$ are independent of the orientation. In the above expression we have omitted the contribution caused by the variation of interface length because it yields only a negligible correction to the solution.

The time evolution of the interface can be given as

$$\partial_t r = C \partial^2_{ss} r + \nu \rho (E - \partial_t r (E \partial_t r)) \quad ,$$

where the first term denotes the effect of surface tension and the second describes the movement induced by the driving field. Here the mobility of the interface is characterized by a parameter $\nu$. Notice that $C$ and $\nu$ are also independent of the interface orientation. In fact, the model
parameters \((\sigma, D, C, \nu)\) involve temperature-dependence while field-dependence vanishes in the low-field limit.

Starting from any initial interface and charge density at \(t = 0\) the above equations define the interface evolution. For simplicity we choose a circular domain to study the variation of its initial shape and area over a short period. In polar coordinate system conformable to the circular domain, the initial charge distribution \(\rho\) is expressed as a function of \(\phi\) angle. The polar axis is parallel to the field and its origin is the centre of the domain. The initial charge distribution is chosen to be the stationary solution of Eq. (1) for the fixed initial radius \((r = R)\). This assumption is consistent when determining the critical domain size, because the domain size remains unchanged in this state for a sufficiently long time to reach the stationary charge distribution. In the presence of a vertical field, the initial charge distribution may be expressed as a function of angle \(\phi\), namely

\[
\rho(\phi) = \frac{E}{D} R^2 \cos(\phi)
\]

where \(E\) denotes the absolute value of the vertical field. Notice that the total charge accumulated along the interface is zero and the domain is polarized, that is, charges are transported from the bottom semicircle to the top one. Substituting the above expression into Eq. (2) the time derivation of radius \(r\) at \(t = 0\) yields the following form:

\[
\partial_t r(t = 0) = \frac{\nu}{D} E^2 R \cos^2(\phi) - \frac{C}{R} .
\]

If \(E = 0\) then the circle contracts isotropically as expected. In the presence of the driving field the first term is responsible for the anisotropic increase. More precisely, in sufficiently strong fields the circular domain elongates along the field, while its transversal size is decreased by the surface tension. This anisotropic evolution of domains is clearly observable in Monte Carlo simulations. Here it is worth mentioning that the decrease of the transversal size is proportional to the curvature at \(\phi = \pi/2\) which tends to zero. In the late stage of this evolution the part of the interface parallel to the field remain unchanged [3].

Due to the anisotropic growth we can not adopt the concept of critical domain size \(R_c\) directly from the classical theories. In the present case, the definition of \(R_c\) is based on the time variation of the initial domain area,

\[
\partial_t A = \int_0^{2\pi} R \partial_t r \, d\phi .
\]

which is an increasing function of the domain radius \(R\). This quantity becomes positive if the initial radius exceeds the critical domain size given as

\[
R_c = \frac{1}{E} \sqrt{\frac{2CD}{\nu}} .
\]

As a result the critical domain size as well as the life time of the homogeneous metastable state diverge when \(E \to 0\).

It should be emphasized that \(R_c\) is directly related to the result of linear stability analysis [3]. That is, the planar interface perpendicular to the field is unstable when the wave length of the periodic perturbations is larger than \(\lambda_0 = \frac{2\pi}{R_c}\). The typical strip width was approximated by the inverse of the wave number which is characterized by the largest amplification rate [4]. However, the simple comparison of \(R_c\) and the predicted strip width is not possible because the prefactors of \(1/E\) consist of different combinations of model parameters. A more adequate picture can be drawn by finding the explicit relationship between the model parameters and the lattice-gas description. We intend to perform these calculations in the near future.

It is worth mentioning that the \(1/E\) dependence of the critical domain size has already been predicted by some authors on the basis of equilibrium free energy arguments [2,4]. Unfortunately, this approach also contains phenomenological parameters whose adequate relation to the parameters of the lattice-gas model is not known yet.

To check the above prediction we have performed a series of Monte Carlo simulations (details are given in previous works [1,5]). In our simulations the standard Kawasaki dynamics [9] was modified by taking into consideration the effect of a driving field on a square lattice with periodic boundary conditions [4]. In each run the initial state was created from a completely ordered phase \(A\) in which we generated a circular domain of \(B\) phase by shifting the inside particles along the field by one lattice site. By this means, we obtained a "polarized domain" whose surface has an extra charge distribution similar to those given by Eq. (3). After \(10-40\) Monte Carlo steps per particle we have determined the area of the circular domain. To suppress the thermal fluctuations this procedure was repeated several thousand times at a given field and radius and a temperature \((T = 0.44)\) below the peak of specific heat. The radius of the initial domains was chosen from \(8\) to \(200\) on an \(L \times L\) lattice where \(L\) was increased simultaneously with \(R\) from \(36\) to \(600\).

From an average of the data obtained for various radii we were able determine the critical domain size as a function of \(E\). The results of the Monte Carlo simulations are illustrated in Fig. 1 where the size of squares indicates the statistical error. These data confirm qualitatively the theoretically predicted \(1/E\) behavior indicated by a solid line in the figure.

If we reinterpret the early calculations [2,4] the ordered metastable states exist only below a "critical temperature" decreasing with \(E\). In other words, the number of defects (or the presence of \(B\) domains) in the metastable \(A\) phase increases with \(E\) at fixed temperatures. To avoid the discrepancy caused by the appearance of extra defects, the above simulations have been carried out for weak fields ensuring a low defect density in the metastable state. Thus, the investigated range
of the electric field may be increased by decreasing the temperature. Unfortunately, in this case we need longer run-times to have the same accuracy, which makes the simulations more time-consuming.

\[ R_{\text{crit}} \]

\[ E \]

\[ \text{slope} = -1 \]

FIG. 1. Critical domain radius vs. driving field at fixed temperature \( T = 0.44 \).

In the above mentioned simulations we have chosen the radius to be significantly larger than the interface thickness, which is comparable with the lattice constant. For smaller radii the deviation of the actual interface from the circle becomes important and causes large fluctuations. This phenomenon might have been a reason why the verification of the \( 1/E \) behavior have not been successful in the early Monte Carlo simulations [11].

In summary, we have explored the existence of a critical domain size which is required for the homogeneous (metastable) ordered phase to decay into a self-organizing polydomain structure via a nucleation mechanism. The phenomenological description of the interface evolution suggests that the area of a circular domain increases if its size exceeds a critical value. In qualitative agreement with the Monte Carlo simulations the critical domain size varies inversely with the field strength.

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[1] S. Katz, J. L. Lebowitz, and H. Spohn, J. Stat. Phys. 34, 497 (1984).
[2] For a recent review, see B. Schmittmann and R. K. P. Zia, in Phase Transition and Critical Phenomena edited by C. Domb and J. L. Lebowitz (Academic, New York, 1995), Vol. 17.
[3] K.-T. Leung, B. Schmittmann, and R. K. P. Zia, Phys. Rev. Lett. 62, 1772 (1989).
[4] R. Dickman, Phys. Rev. A 41, 2192 (1990).
[5] G. Szabó, A. Szolnoki, and T. Antal, Phys. Rev. E 49, 299 (1994).
[6] G. Szabó, A. Szolnoki, T. Antal, and I. Borsos, submitted to Europhys. Lett.
[7] J. D. Gunton, M. San Miguel, and Paramdeep S. Sahni, in Phase Transition and Critical Phenomena edited by C. Domb and M. S. Green (Academic, New York, 1985), Vol. 8.
[8] K. Binder and D. W. Hermann, Monte Carlo Simulation in Statistical Physics (Springer, 1988), and O. G. Mouritsen, Computer Studies of Phase Transition and Critical Phenomena (Springer, 1984).
[9] K. Kawasaki, in Phase Transition and Critical Phenomena edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. 2.
[10] K. K. Mon and S. Teitel, Phys. Rev. Lett. 62, 673 (1989).
[11] S. Teitel and J.-R. Lee, unpublished, some details are mentioned in Ref. [2].