Interfacial growth in driven diffusive systems

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We have studied the growth of interfaces in driven diffusive systems well below the critical temperature by means of Monte Carlo simulations. We consider the region beyond the linear regime and of large values of the external field which has not been explored before. The simulations support the existence of interfacial traveling waves when asymmetry is introduced in the model, a result previously predicted by a linear-stability analysis. Furthermore, the generalization of the Gibbs-Thomson relation is discussed. The results provide evidence that the external field is a stabilizing effect which can be considered as effectively increasing the surface tension.

I. INTRODUCTION

Driven diffusive systems (DDS) have been studied intensively[1-15] from a theoretical point of view in recent years to explore new possibilities that are open when a system is driven out of equilibrium by an external field. A simple realization of this type of system is given by a discrete model in which the particles and holes of a lattice gas not only interact with each other, via nearest-neighbor forces and have usual Kawasaki (conserved) dynamics, but also are subject to the influence of an external field which increases and reduces the rate of jumps of the particles along and in the opposite direction to the field, respectively. An interesting study, in this context, has been the characterization, by means of Monte Carlo simulation,[1] of a nonequilibrium phase transition, ocurring with periodic boundary conditions taken in the direction of the field. In such a case a high-temperature disordered phase separates at low temperature into particle-rich and particle-poor phases separated by an interface. Each phase carries a steady-state current of particles. The critical properties of this phase transition have been studied both from the discrete model[1-8] described above and from the corresponding continuum version.[9-12]

A different aspect in the study of driven diffusive systems has been brought into focus in the study of the interfacial properties.[13-15] In Ref. 13 a generalization of the above model of a driven diffusive system allows one to understand some of the features introduced by an external field on a pre-existent interfacial growth instability. Essentially, two effects are present. The first one is the change in the rate of growth of the instability. The second is the presence of new length scales which can be associated with the appearance of interfacial traveling waves. In fact, this latter result suggests connections with more complicated problems such as, the directional solidification process in the presence of convective flow,[16] for which analogous results have been obtained.

To get these results a linear-stability analysis was performed in Ref. 13 on a continuum version of a driven diffusive system.[9] But some questions remain open. There does not appear to be an easy recipe to go beyond the linear regime in the macroscopic description. Furthermore, the large external-field region is beyond the approach of Ref. 13, since nonequilibrium terms in the corresponding generalizations of the Gibbs-Thomson relation were not introduced. Generally, such nonequilibrium contributions are introduced phenomenologically. In addition, the connection between the discrete[1] and continuum[9] versions of the driven system has not been rigorously established. Hence the presence of traveling waves in a Monte Carlo simulation of such a system (and, if they appear, the required assumptions to obtain them) is a question of interest.

It is the goal of this paper to look further into these questions. We do this by means of a Monte Carlo simulation which permits us to go beyond the linear regime and also to consider large external fields. In Sec. II we present the generalized model that we use in the Monte Carlo simulation. In Sec. III we consider the symmetric version of the model, for which no interface traveling waves are present. We commment on the implications of the simulation on the nature of the nonequilibrium terms in the Gibbs-Thomson relation. In Sec. IV we consider the asymmetric case. We present evidence for the presence of traveling waves in this case, and discuss the mechanism which produces them. In Sec. V we present concluding remarks.

II. MODEL

We consider a lattice-gas model on a square lattice under the influence of an external field E.[1] The discusion is easily generalized to other lattices and higher dimension. Half the sites are occupied by particles and half by holes; Kawasaki (conversed) dynamics are used. The transition probability $W(\{n\}\rightarrow\{n_{ij}\})$ for an interchange between the occupants of sites i and j is given by

$$W=\exp[H(\{n\})-H(\{n_{ij}\})+\alpha E(x_i-x_j)] \tag{2.1}$$

if the exponent in Eq. (2.1) is smaller than zero; $W(\{n\}\rightarrow\{n_{ij}\})=1$, otherwise. $\{n\}$ and $\{n_{ij}\}$ are the configurations before and after the interchange; they only differ in the occupancies of sites i and j. $H(\{n\})=-J/kT\sum_{\langle i,j\rangle}n_i n_j$ is the reduced energy of the configuration $\{n\}$ and $\langle i,j\rangle$ indicates nearest-neighbor pairs; n_i is the occupancy variable ($n_i=1$ for particle and $n_i=0$ for hole), and x_i is the x-coordinate of the site i. We allow only nearest-neighbor interchanges. The parameter α will be specified below.

The second term in the exponential of Eq. (2.1) is due to the presence of the external field E oriented in the x-direction. This term increases (decreases) the transition probability for a particle to jump in the direction of (opposite to) E. The jumps perpendicular to E are not affected. Periodic boundary conditions are considered in the x direction. As usual, for each Monte Carlo step all potentially mobile particles are given a chance to jump to a neighboring hole.[17] For each of these particles a neighbor is taken at random. If a hole is selected, the exchange is effected with probability W. The transition probability specified by W satisfies local detailed balance.

Below the critical temperature $T_c(E)$ the system segregates into two phases,[1] rich (A) and poor (B) in particles, respectively. At low-temperature a sharp interface between the two phases oriented parallel to E is present. A net flux of particles in both phases, parallel to the interface and in the direction of E, indicates the existence of a nonequilibrium steady-state induced by the external field. In this work we are interested in the growth properties of this interface when the system is initially in the steady-state. Furthermore, we restrict ourselves to a study of the region around the interface. The top row of holes (at $y=y_{\max}$) and the bottom row of particles (at $y=y_{\min}$) are pinned to establish the two-phase system.

A linear-stability analysis indicates that a generalization[13] of the continuum model of a driven diffusive system[9] which allows for asymmetry between the two phases, opens the possibility of new interfacial behavior, the presence of a traveling wave. Here, one of our goals is to study the situation beyond the linear regime. This goal has been accomplished by means of a generalization of the discrete model[1] in the same spirit as it was done for the continuum version.[13] To understand this step it is convenient to introduce briefly the continuum model. It is described by a diffusion equation:[9]

$$\partial_t c_a=-\nabla\cdot\mathbf{j}_a\ , \tag{2.2}$$

$$\mathbf{j}_a=-D\nabla c_a+\mathbf{E}\sigma(c_a)\ , \tag{2.3}$$

where $c_a(\mathbf{r},t)$ and $\mathbf{j}_a(\mathbf{r},t)$ are the macroscopic concentration and the flux in the rich and poor phases ($a=A$ and B, respectively), D is the diffusion coefficient, $\mathbf{E}=E\hat{\mathbf{x}}$ is the external field and $\sigma(c_a)$ is the conductivity. An expansion $\sigma(c_a)\approx\sigma(c_{a0})+(d\sigma/dc)_a c_{a1}$ around the steady-state concentration $\sigma(c_{a0})$ introduces the parameter, $Q_a=E(d\sigma/dc)_a D^{-1}$. In a symmetric model, $Q_A=-Q_B$. Allowing for $Q_A\neq -Q_B$ (Ref. 13) may be a more realistic hypothesis for physical systems.

An analog of this assumption in the discrete model described by Eq. (2.1) is represented by the presence of the parameter α in the second term of the exponential. This term is directly related to the flux induced by E in this model. To introduce asymmetry we take this parameter to have a different value if the jumping particle is in the rich or the poor phase. We model this possibility by the following consideration: if the majority of the nearest neighbors of this particle are particles (holes) the parameter α takes a value α_1 (α_2).[18] The reason why this generalization of the discrete model[1] produces a traveling interfacial wave will be clarified later, but it can be intuitively related to the imbalance of fluxes across the interface.

A second aspect of the modeling is connected with the fact that an external field parallel to the interface does not, by itself, produce an interfacial instability.[13,14] To study the effects of E on interfacial growth, we have considered in Ref. 13 a second generalization of the usual DDS model. In it we assumed that the system is quenched deeper into the ordered phase. Then, as a response, a flux of particles perpendicular to the interface (in the y direction) going from the poor to the rich phase will be present.[19] To introduce this effect in our discrete model, we exchange at a regular rate a randomly chosen hole (particle) by a particle (hole) in the top (bottom) row of the poor (rich) phase.[20] Macroscopically speaking, the quench introduces a gradient of concentration perpendicular to the interface in both phases.[20] To make the modeling efficient for computational purposes it is useful to introduce an auxiliary field gradient G (like a gravitational field) in the y direction which produces a biased random walk of particles and holes. For a discussion on the fundamental differences between the auxiliary field gradient G and the external field E, see Refs. 1 and 13.

For $E=0$, a Mullins-Sekerka–type instability[21] will be present at the interface, and a growing pattern will emerge. The effect of surface tension, arising through the introduction of interaction energies at the microscopic level in Eq. (2.1), and the flux perpendicular to the interface, imagined to be induced by the quench, are the two competing effects always present in this type of instability. This has been the approach[20] in which an instability of the Mullins-Sekerka type (for $E=0$) has been studied from a microscopic point of view. Here, we are interested in a different aspect; namely, in the effects of an external field (which is not the gradient of a potential) on the pattern-formation process.

III. SYMMETRIC CASE

In this and the following sections, we present the results of our simulations. First, we consider the effects of the external field on the interfacial growth process without asymmetry. In Sec. IV we consider the asymmetric situation. In the plots to follow, except where a specific configuration is shown, typically 100–200 runs were averaged.

For this case $\alpha=1$ in Eq. (2.1). Figure 1 shows typical patterns for different values of the external field E, taken at the same time. They have been grown from a flat interface under the influence of the nonequilibrium flux of particles from top to bottom driving the instability. In Fig. 2, we plot the perimeter of the interfaces for all the patterns as a function of time.[22] In Fig. 3, we plot the height of the largest finger also as a function of time. The fastest growth in both figures is obtained for $E=0$, and it is observed that the electric field reduces the rate of growth of the pattern. Furthermore, for sufficiently large E, the number of fingers is reduced and, eventually, the growth is suppressed.

We have also considered the pure decay of a well-developed pattern in the presence of E. To do a good comparison for the different values of E, we start the decay from the same initial structure. To be realistic, we consider only values of E for which we know from the previous growth that four fingers would be present (see Fig. 1). In Fig. 4 we plot the perimeter as a function of time for the decay; a faster decay in the presence of E is observed. Then, both in growth and decay the external field behaves as a stabilizing effect. Intuitively, this can be understood in terms of the enhancement and inhibition of jumps along and opposite to the external field.

At this point, the simulation may provide some interesting information about features beyond the linear regime (and beyond the regime of small external field).[13] Consider, for example, the macroscopic treatment of the boundary conditions at the interface. Normally, the concentrations at either side of the locally curved interface are set by the Gibbs-Thomson relation embodying the requirements of local equilibrium. However, sufficiently large E might be expected to introduce a nonequilibrium term affecting concentrations at the interface. This is analogous to a nonequilibrium term of importance in directional solidification when the velocity of the solidification front is sufficiently large.[23] In the present case, there is, as yet, no microscopic derivation of the modification of the Gibbs-Thomson relation introduced by $E\neq 0$. However, on phenomenological grounds one expects a contribution proportional to E and to the curvature of the interface. (The leading effect of E, which applies even for zero curvature, has been included in the steady-state solution.) For small E, the nonequilibrium term is presumably very small in the linear regime of small curvatures. On the other hand, this term is important in the nonlinear regime as the simulation suggests. The slower growth for increased E could be connected to it. If so, the simulation suggests that this term has the same sign as that of the surface-tension term in the boundary condition., and the effect of E is equivalent to an increase in the surface tension. In the previous linear analysis,[13] only small values of E were considered. Nonequilibrium contributions to the Gibbs-Thomson relation

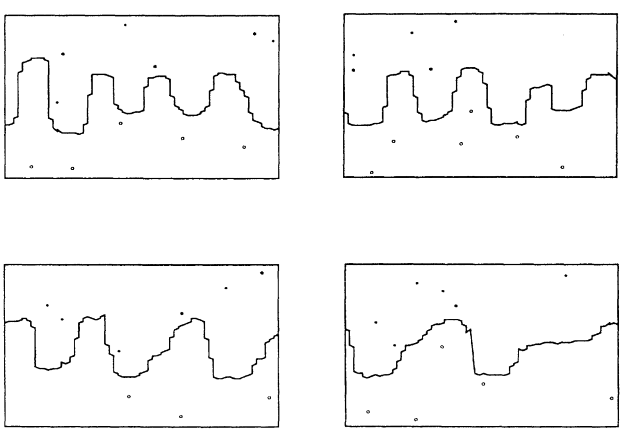

FIG. 1. Typical structures after 64 000 Monte Carlo steps for different values of external field. The structures grow from a flat interface. The temperature is $T=0.5T_c$. The perpendicular flux corresponds to a particle and a hole each 40 Monte Carlo steps (MCS). The system size in the x direction is 64. The values of E are 0, 0.05, 0.1, and 0.15. E increases from left to right and then from top to bottom.

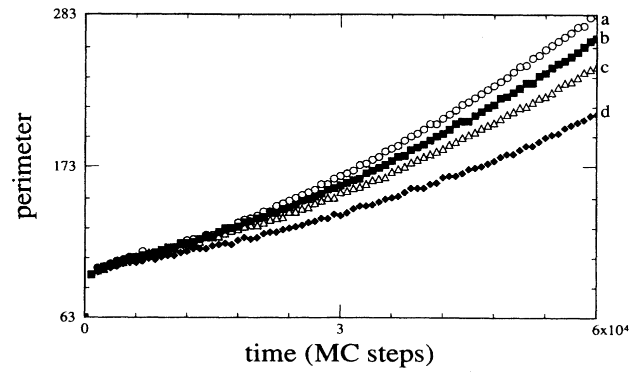

FIG. 2. Perimeter of the interfaces of Fig. 1. vs time. Curves a, b, c, and d correspond to $E=0$, 0.05, 0.1, and 0.15.

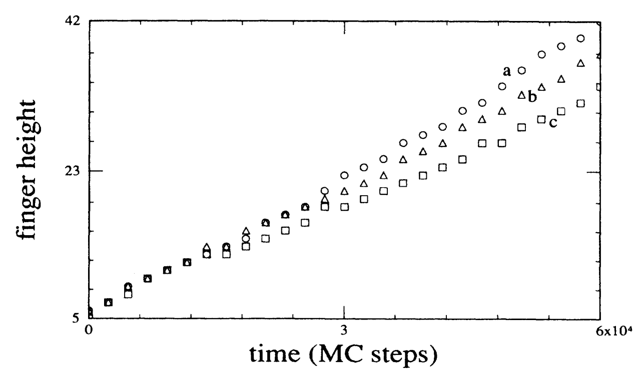

FIG. 3. Height of the fastest finger of the structures of Fig. 1. vs time. Curves a, b, and c correspond to $E=0$, 0.05, and 0.15.

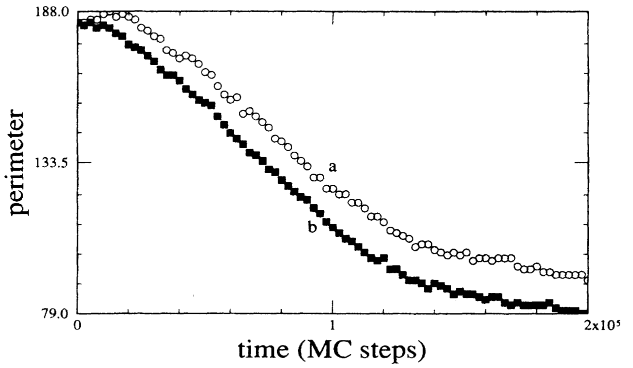

FIG. 4. Perimeter vs time for the decay of an interface. The initial structures consist of four bumps of size 8×15 on the initially flat interface. No perpendicular flux is added. Curves *a* and *b* correspond to $E=0$ and 0.05. Other parameters are the same as in Fig. 1.

were not included, and a faster growth rate for the instability was predicted for such circumstances.

IV. ASYMMETRIC CASE

In this section, we present the results for the asymmetric case. The different conductivity of the two phases is modeled as follows. The parameter α in Eq. (2.1) takes two different values (α_1 and α_2) depending on whether the majority of neighbors of the mobile particle are particles or holes, respectively.

Figure 5(a) shows the situation for the *symmetric* case in which $\alpha_1=\alpha_2=1$ ($E=0.15$); no net motion of the pattern is observed, but rather simple decay is evident. This is contrasted in Fig. 5(b), which shows (for $\alpha_1=2$, $\alpha_2=0$ $E=0.075$) how the initial pattern moves to the right, that is, in the direction of E, indicating a traveling wave. Furthermore, we have observed that if the values of α_1 and α_2 are interchanged the resulting motion is reversed. To have a quantitative measure of this behavior we have plotted in Fig. 6 the center of mass of the particles, X_c, as a function of time for different values of E.[24] From Fig. 6 we obtain a linear behavior of X_c versus time, which gives a constant velocity of the center of mass, V_c, for each E. In Fig. 7 the apparent linear dependence of V_c on the external field E is shown.

To explain this behavior we can use a simple picture. We concentrate on the particles and holes of two adjacent fingers in Fig. 5(a). E is in the direction from left to right. This means that the particles located at the right border of a finger have an enhanced probability to jump out of it. When this jump is performed, it remains more probable for the particle to continue the jumps in the direction of E. Many particles would decay to the valley, but many of them will continue until they attach to the left border of the adjacent finger.[25] The jump of a particle out of a finger leaves a hole in it. In the symmetric case considered in Sec. III the holes jump (opposite to E) inside the fingers with the same probability as the particles do out of the fingers. In this way, the increase in the number of particles due to the arrival of new ones is compensated by the arrival of holes. But in the asymmetric case an imbalance in the number of particles and holes would be present. This line of thinking suggests a net motion of the finger in the direction of E (or in the opposite direction) according to the disparity of conductivities. This suggests the mechanism for a traveling wave in the asymmetric situation. Note that a very small deviation of the center of mass from its original position in the direction opposite to E is obtained for the symmetric case, but it has no relation with the traveling wave. It can be understood from the small asymmetry in the shape of the fingers that appears in Fig. 1 when $E \neq 0$. This is related

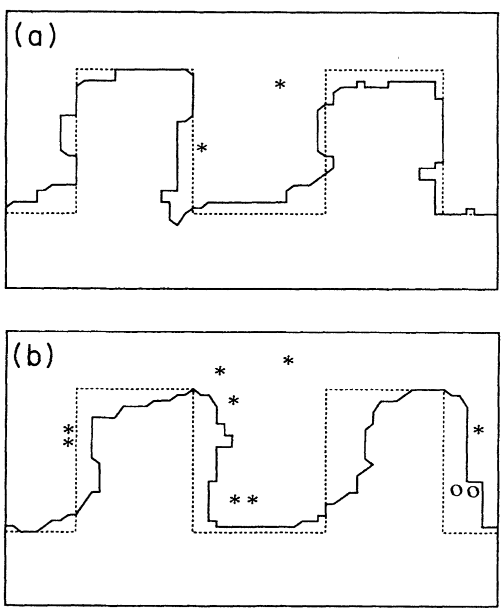

FIG. 5. Top figure (a): No traveling wave for the symmetric case, $\alpha_1=\alpha_2=1$ and $E=0.15$. Bottom figure (b): Traveling wave for the asymmetric case, $\alpha_1=2$, $\alpha_2=0$, and $E=0.075$. In each case the solid line is a typical structure after 80 000 Monte Carlo steps. The dashed line is the initial configuration. No perpendicular flux is added.

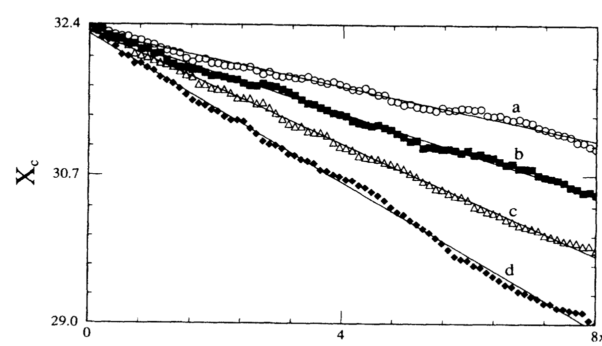

FIG. 6. x coordinate, X_c, of the center of mass of the particles vs time. Curves *a*, *b*, *c*, and *d* correspond to $E=0.08$, 0.1, 0.13, and 0.15.

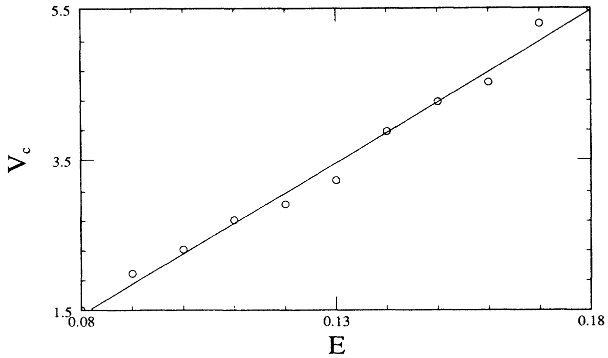

FIG. 7. V_c, the velocity of the center of mass of the particles vs the external field.

to the very disordered accumulation of particles when they attached to the adjacent finger in contrast with the systematic process of particles in line jumping out of the finger on the opposite side.

As we noted above, this possibility of an interfacial traveling wave was predicted in the linear regime by a stability analysis[13] of a model[9] that is believed to represent the continuum version of the discrete model given by Eq. (2.1). The mechanism producing traveling waves in the linear regime is associated with the existence of new length scales involving the external field E. The parameter $Q_a = E(d\sigma/dc)_a/D$ defined after Eq. (2.3) has dimensions of inverse length. These new length scales are associated with spatially modulated decay into the bulk of small perturbations in concentration (as opposed to the usual monotonic-exponential decay for $E=0$). In the asymmetric case there is, across the interface, an imbalance of fluxes induced by these gradients of concentration. The simple decay or growth of the interface in the symmetric case is now modulated. The modulation reflects itself in the appearance of the traveling wave.

The mechanism for traveling waves in the continuum version beyond the linear regime has not been investigated. In any case, the essential ingredients are presumably the difference in conductivities in both phases and then, the existence of new length scales which differ. Using these ingredients in a simple way in a discrete model of a driven system, we have observed traveling waves in the simulations.

V. CONCLUSIONS

We have studied via Monte Carlo simulations the growth of interfaces in a driven diffusive system well below the critical temperature. We have introduced two generalizations of the usual description of these systems. The first, allowing for a flux normal to the interface, permits the study of instabilities in the presence of an external field. The second introduces the possibility of asymmetry in the discrete version of this model. The results show that asymmetry in the model can give rise to an interfacial traveling wave. This latter possibility was predicted previously for the linear regime and small external field by means of a linear-stability analysis of a continuum model. Furthermore, the simulations give us clues about how to generalize the Gibbs-Thomson relation to this nonequilibrium situation. Among other results, the effect of the external field on the growth and decay of the interface is a stabilizing effect, qualitatively like an enhanced surface tension. For large external field the interfacial instability is substantially suppressed. This suggests that a kinetic term should be present in the Gibbs-Thomson relation and this term should have the same sign as the term proportional to the surface tension. Further investigation is needed to understand fully such nonequilibrium contributions in driven systems.

The model described here seems to be one of the simplest in which an external field modifies a preexistent interfacial instability in such a way that a new phenomenon occurs, e.g., the traveling wave. We believe the study of interfacial instability in a nonequilibrium steady state could have some experimental relevance, for example, in the growth of structures in the presence of a gravitational field, or in cases for which convective flow or ionic transport would be involved.

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