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Driven Nonequilibrium Lattice Systems with Shifted Periodic Boundary Conditions

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We present the first study of a driven nonequilibrium lattice system in the two-phase region, with *shifted* periodic boundary conditions, forcing steps into the interface. When the shift corresponds to small angles with respect to the driving field, we find nonanalytic behavior in the (internal) energy of the system, supporting numerical evidence that interface roughness is suppressed by the field. For larger shifts, the competition between the driving field and the boundary induces the breakup of a single strip with tilted interfaces into many narrower strips with aligned interfaces. The size and temperature dependences of the critical angles of such breakup transitions are studied.

KEY WORDS: Nonequilibrium steady state system; interfaces; phase transitions.

1. INTRODUCTION

Recently, there has been considerable interest in studying phase transitions in a driven lattice gas system, originally introduced as a model for superionic conductors.[1] Much effort[2-5] has been devoted to the characterization of new, nonequilibrium critical behavior in the bulk. For all temperatures below the transition, this system separates into an ion-rich phase and an ion-poor one. This paper concerns properties of the interface between these phases. For interfaces in equilibrium systems, there is a host

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of well-known phenomena, e.g., roughening,[6,7],[4] wetting,[9],[5] etc. For interfaces in nonequilibrium steady states, there are also many studies in a multitude of fields, e.g., crystal growth,[6] phase separation (see, e.g., refs. 11), and the classic Stefan problem (see, e.g., ref. 12), to name but a few. However, due to the extreme diversity of nonequilibrium systems, none of these investigations apply to our case, for which only a few studies exist.[13,14]

One signal of a *rough* interface is a divergent[7,8] statistical width in the thermodynamic limit. For a three-dimensional Ising lattice gas in equilibrium, certain interfaces are known[15],[6] to have a phase transition from smooth to rough as the temperature T is raised through the roughening temperature T_R (>0). In contrast, for any two-dimensional model with periodic lattices and short-range interactions, all interfaces are rough, i.e., $T_R = 0$. However, when such a system is driven to a stationary state far from equilibrium, a *finite* interfacial width is found in recent Monte Carlo (MC) studies.[14]. Here, the driving force simulates the effect of a uniform external electric field E along one of the principal directions of the lattice. Though this suppression of the interface roughness is similar to what happens in equilibrium under the action of a gravitational field,[16] there are several differences. For example, unlike the familiar gravitational case, an interface in the driven system is *parallel* to the E field. A more subtle difference lies in the behavior of the structure factors.

In a different approach, the roughening transition can also be characterized[7,8] by the vanishing of the excess step free energy $f_s(T)$. The notion behind this definition is that steps will proliferate if there is no cost ($f_s = 0$) to their formation, leading to a divergent width. Related to f_s is the anisotropic interfacial tension $\tau(\mathbf{n}, T)$, which is the free energy (per unit area) associated with an interface with normal $\mathbf{n}$. For systems in two dimensions, $\mathbf{n}$ can be parametrized by a single angle θ corresponding to interfaces tilted with respect to a principal axis. These tilted interfaces are obtained by imposing shifted periodic boundary conditions (SPBC), also known as screw boundary conditions, in that principal direction. When normalized by the cross-sectional area, $f_s(T)$ is simply the limiting interfacial tension due to an infinitesimally small θ, i.e., $f_s = \partial\tau/\partial\theta|_0$. Thus, Monte Carlo studies of lattices with SPBC are used[15] to explore f_s in equilibrium systems. Our study of driven systems with SPBC is motivated by such an approach. Though we can only measure $u(\theta)$, the internal energy, and cannot compute the free energy, we found that $\partial u/\partial\theta|_0$ does

[4] See ref. 8 for a recent review.
[5] See refs. 10 for recent reviews.
[6] See refs. 7 and 8 for theoretical models.

not vanish when the external field is turned on. Based on observations of bulk densities and finite-size analysis, we argue that this singularity is present in the *bulk* energy. We intend to pursue a theoretically sound connection between this kind of singularity and suppression of interfacial roughness.

In the case of nonequilibrium systems driven by an external field and with periodic boundary conditions (PBC), previous numerical simulations have reported that below the new critical temperature the system attains a stationary state which is highly anisotropic, with the interfaces oriented along the field. In contrast, the existence of shifted periodic boundary conditions represents a new external agent that competes with the field to orient the system. Interesting new phenomena arise, as the system adapts new configurations to become commensurate with the shifted boundary condition. These new transitions are reflected in the plots of the energy and the current versus the shift.

2. SIMULATION METHOD

We consider an $L \times L$ square lattice-gas version of the Ising model where the sites $(i, j = 1, 2, ..., L)$ can be either empty or occupied by an ion ($n_{i,j} = 0$ or 1; also refered to as particle or hole). Restricting ourselves to the case of mutually attractive ions, we study a half-filled lattice for convenience. In the presence of an external electric field E, chosen to point in the $-x$ direction, a steady current of ions is established when the boundary conditions are periodic in x.[1,4,5] The system evolves under a particle-conserving hopping dynamics when the ions hop to nearest-neighbor (NN) empty sites according to the transition probabilities per unit time $p = \min(1, \exp[-(\delta H + \varepsilon E)/k_B T])$. Here δH is the change in the configurational energy,

$$H(\{n_{ij}\}) = -4J \sum_{\text{NN}} n_{ij} n_{i',j'}, \qquad J > 0 \tag{1}$$

produced by the jump, while $\varepsilon = 1, 0, -1$, depending on whether the ions jumps against, transverse to, or with the driving E field. In this way, we simulate a system interacting stochastically with a heat bath at a temperature T. We will measure T in units of the Onsager critical temperature $T_C = 2.2692 J/k_B$. As before,[14] the simulation for our interface is practical only for a limited range of temperatures, since T must be low enough for the interface to be well defined, but not too low for the system to evolve significantly.

As mentioned above, in the case of PBC in both the x and y directions, it is known that below $T_C(E)$ the system presents an anisotropic one-

strip stationary state, with the stirp oriented along the field. Since we are mainly interested in the study of tilted interfaces, we shall impose SPBC in the x direction, while keeping the PBC in the y direction. For a shift of h lattice spacings these conditions are explicitly

$$n_{i,j+L} \equiv n_{i,j}, \qquad \text{PBC} \tag{2a}$$

$$n_{i+L,j} \equiv n_{i,j-h}, \qquad \text{SPBC} \tag{2b}$$

so that when a particle leaves one of the lateral edges it comes back to the other edge at a shifted site. Thus, the most (energetically) favorable configuration is a single tilted strip. In fact, the SPBC can be regarded as equivalent to twisting the lattice torus, along with the field, through the angle desired.

In equilibrium ($E=0$), the SPBC with a shift of h lattice constants create a tilted interface with an angle of $\theta = \tan^{-1}(h/L)$ with respect to the horizontal axis. In our study we choose to start the simulations with a single compact strip tilted at that angle which would correspond to the state at zero T and E. Thus, the process is equivalent to performing an inverted quench to the desired temperature while switching the field on. With $E>0$, we can define θ more precisely by

$$\theta \equiv \sin^{-1}(\mathbf{n} \cdot \mathbf{e})$$

where $\mathbf{n}$ is the normal pointing into the particle-poor phase and $\mathbf{e}$ is a unit vector in the direction of E.

The main focus of our simulation is studying the behavior of the (internal) energy, which we associate with the average number of particle–hole bonds per lattice site[4]:

$$u(\theta, T) = \frac{\langle H \rangle}{2JN} + 2; \qquad u(0, 0) = \frac{2}{L}; \qquad u(0, \infty) = 1 \tag{3}$$

Another quantity often used[5] is the NN correlation function for the Ising ferromagnet, which is just $2(1-u)$. For systems in equilibrium, the free energy can be obtained from u through a thermodynamic integration. For the three-dimensional Ising model, the surface free energy τ is obtained via this route.[15],[7]

It is also interesting to study the current $j(\theta, T)$, which is defined as the number of actual jumps performed along the field during the stationary evolution divided by its duration (in MC steps). In the case of $E=\infty$, the current is related to $u_x(\theta, T)$, the "directional" energy corresponding to the

[7] See ref. 17 for review.

particle–hole bonds parallel to the field, since $j(\theta, T) = u_x(\theta, T)/4$. We will normalize the values of the current to 1/8, which is the saturation current for noninteracting ions with PBC. Notice that this quantity behaves rather smoothly, due to the fact that it results from averaging over time and all particle–hole bonds parallel to E.

3. RESULTS FOR SMALL SHIFTS

Since the concept of free energy will not be very useful in driven systems, we turn to another property characterizing the interface: *excess internal* energy, i.e., the energy difference between systems with and without an interface. In general, it is

$$\Delta u(\theta, T) = 1/2[u(\theta, T) - u_B(\theta, T)] \tag{4}$$

where $u_B(\theta, T)$ is the energy per site in a system with SPBC that has the same density of particles as the bulk well inside a strip at a temperature T. The factor 1/2 comes from having two interfaces in a system with a strip (of the dense phase). Apart from being a consequence of periodic boundary conditions in the transverse directions, such an average should provide better statistics.

For systems in equilibrium, u_B does not depend on θ and the two interfaces are equivalent. Thus, $L\Delta u$ will go to a constant in the thermodynamic limit, representing the energy per unit area associated with a single interface. Since u_B is a constant,

$$\partial \Delta u(\theta, T)/\partial\theta|_{\theta=0} = 1/2\partial u(\theta, T)/\partial\theta|_{\theta=0} \tag{5}$$

The surface tension τ (a free energy) can be obtained from Δu (an internal energy) by an appropriate integration[17] in T, so that the θ dependence is not affected. Consequently,

$$\partial u(0, T)/\partial\theta \neq 0 \Leftrightarrow \partial\tau(0, T)/\partial\theta \neq 0 \tag{6}$$

i.e., the slope of the energy–angle curve at $\theta = 0$ will determine whether the interface is rough or smooth.

Before proceeding to nonequilibrium systems, we remark that such a connection between singularities in u and smooth surfaces exists in another situation, namely, interface "smoothing" by an external gravitational field. On the one hand, the width is well known *not* to diverge with the system size. Instead, it approaches the capillary height. On the other hand, it is

straightforward to estimate that, in a simulation with *pinned*[8] boundary conditions, the energy will have a term like $|\theta|$.

For a driven system, however, our simulations show that the bulk excitations *do* depend on the shifts, increasing with h until the appearance of multistrip configurations. Thus, u_B is written as a function of θ. One might expect a bulk quantity like u_B to be *analytic* in θ, so that a term like $|\theta|$ could be assigned to Δu and both (5) and (6) would remain valid.

Convinced that the internal energy $u(\theta)$ contains physically significant, quantitative information about the interface, we have performed simulation at $T=0.8$ in a system with $L=100$ and $E=15$ (in essence, ∞). A large size is required so that one can get very small discrete values of the angles. After an initial run over 10^5 MCS, when a stationary state is reached, we average over three runs in a row, each consisting of 500 measurements taken 200 MCS apart. The energies for $h=0$, 1, and 2 are 0.1077, 0.1158, and 0.1237, respectively. A plot of just these three points will show that $u(h)$ is *linear* in h, within the accuracy of the data (± 0.0005). Naively, it is easy to jump to the conclusion that *interfacial* energies must contain a term proportional to $|\theta|$, supporting the connection between singularities in such energies and the finiteness of the interfacial width.

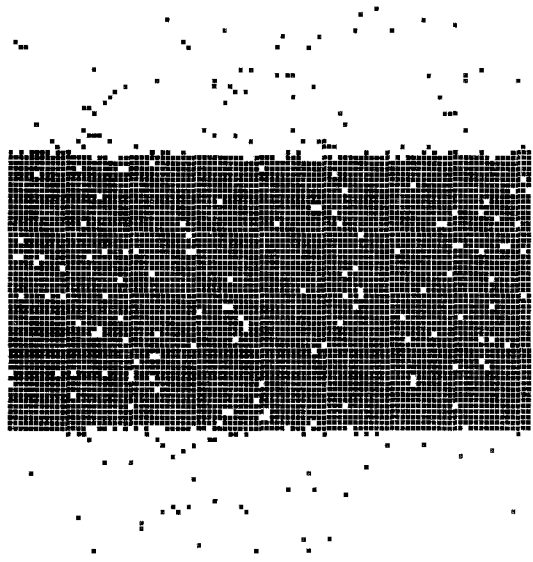
However, if we make more careful comparisons between typical configurations associated with PBC (Fig. 1a) and SPBC with small h (Fig. 1b), we find several surprising features in the latter.

1. The two interfaces are *not* equivalent. The "leading" edge (the upper interface in Fig. 1b) appears rough, while the "trailing" edge (the lower one) appears smooth.
2. The *bulk* energy density u_B and particle density certainly depend on the shift h.
3. The particle densities in the immediate vicinities of the two interfaces are *different*, inducing novel density gradients between the interfaces.

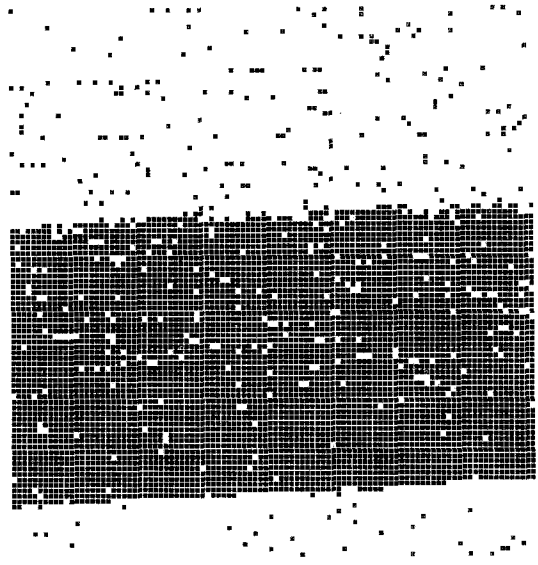
We emphasize that these features are completely unexpected, based on what is known about $E=0$ or PBC systems. In other words, *both* $E>0$ *and SPBC* must be imposed before these new phenomena could occur.

Faced with these unexpected features, we turn to systems with other L and h in an attempt to separate out the effects on the bulk and the interfaces. Data from simulations with $L=20$, 36, 48, and 100 at the same

[8] If one insists on imposing SPBC to induce a "tilted" interface, a spatial discontinuity must be introduced into the (gravity part of the) Hamiltonian. It is far from straightforward to relate this system to one with a tilted interface in uniform gravity.



(a)



(b)

Fig. 1. Typical single-strip configuration with (a) PBC and (b) SPBC shifted by 5. Here $L = 100$, $T = 0.8$. The electric field points from right to left.

$T=0.8$ for small shifts h are used. First we seek $u_B(\theta)$ and $u_I(\theta)$ from the fit

$$u(1/L, \theta) \simeq u_B(\theta) + u_I(\theta) \sec(\theta)/L \tag{7}$$

The idea behind this fit is simple. The total contribution to the energy *density* should approach a bulk term $u_B(\theta)$ for large L. Since there are no boundaries in the system, we identify the L^{d-1} contributions to the *total* energy as interfacial. In the density, these go into a $1/L$ term, the coefficient of which, $u_I(\theta)$, should be the energy (per unit area) associated with *both* of the edges. Once these coefficients are picked out, the small θ dependence can be extracted.

In practice, due to the integral nature of h, the smallest θ can be is $\approx 1/L$. Thus, a linear h term in u_B is the same order as the lowest term in u_I. To this order, $(1/L)$, we find a surprising result, i.e., u_B *is not analytic in* θ:

$$u_B(\theta) \simeq 0.08 + 0.75\,|\theta| + \cdots \tag{8a}$$

$$u_I(0) \simeq 2.68 \tag{8b}$$

Though the numerical values appear to be "scattered," they are, in fact, consistent with a visual assessment of the typical configurations. The first term in (8a) refers to the average number of particle–hole bonds (per site) in the bulk. A glance at Fig. 1a shows that the density of particles deep in the hole-rich phase is rather small, suggesting a small number like 0.08. In contrast, 2.68 measures the average number of such bonds *along* the interfaces. Since there are two interfaces, this number represents 1.34 broken bonds par lattice spacing. If there were no overhangs and bubbles ($T=0$), this number would be exactly 1. Thus, 0.34 seems consistent with an "eyeball" estimate of our interface with excitations.

The most surprising part of (8a) is surely the $|\theta|$ term. For equilibrium systems, bulk properties certainly do not depend on the existence of a single step on the interface. Though we cannot compute this term, we can offer an argument in favor of such an unexpected behavior. Consider a system with $E > 8J$ (sufficient but probably unnecessary) in the $T=0$ limit. With PBC, there would be two flat interfaces, so that $u_I=2$ and $u_B=0$. Next, consider a pair of tilted interfaces, with a single step in each. The leading edge is now unstable, since the particle at the step will be driven along the terrace, though unable to break free due to $T \to 0$. Others will follow, which is the entire story *if* there were no SPBC. With SPBC, however, the first particle will eventually come around at a higher level and find itself at the corner of a step of height 2. Now, it can break off from the bulk and wander into the "vacuum." Due to the SPBC, it has an average

drift toward the opposite edge. There, it can be absorbed, first by the terrace and finally by the step on this (trailing) edge. Thus, a step on the leading edge acts as a source for particles in the hole phase, giving a finite u_B, *even at* $T=0$. A step on the trailing edge acts as a sink to set up a steady state. Note that, due to charge conjugation, holes will leave the leading edge and drift toward the trailing edge in the opposite direction. Thus, in a steady state, both interfaces are stationary (on the average).

Finally, we remark on the important role of PBC in the other direction. Consider the evolution of the same system with a much larger extent in y. If we inspect the sample at times which are long (short) compared to a traversal in x (y), then we would find a (quasi-) steady state near the interface. Since there will be a constant flux of particles and holes away from a leading edge, we see that the bulk density (near the interface) in the particle-rich phase must be less than 1, which is the case with no shift. In contrast, we could argue that near a trailing edge, the bulk density must be higher as a result of the absorbing step. (Note that the argument for this edge must be carried out for $T\neq 0$, so that it is less transparent.) With PBC in y and for observation times much larger than periods of traversal in both directions, these differences must match somehow. We believe that this mechanism is responsible for the (average) gradient in the bulk.

The conclusion that bulk densities depend (asymmetrically) on the tilt of an interface away from the field direction echoes a previous finding.[18] Work is in progress[19] toward developing a complete and clear picture of this phenomenon. For example, we have preliminary evidence, from a continuum model, that density gradients in the bulk are confined to a boundary layer near the trailing edge. This scenerio is supported by arguments due to van Beijeren.[20] Further, we hope to study finite-size effects so that an expansion like (7) can be justified and useful information can be extracted from the higher order terms in (8).

4. RESULTS FOR LARGE SHIFTS

We have also performed a simulation with $L=20$, 36, 48, and 100 at $T=0.8$ for values of shifts h ranging up to 10, 18, 16, and 20 respectively, measuring the energy $u(h)$ and the current $j(h)$. The effect of the competition between the E field and the SPBC is even more dramatic. In the absence of E, the stable configuration always[9] consists of a single strip (of, say, the particle-rich phase), with a pair of interfaces tilted at the angle $\tan^{-1}(h/L)$. In marked contrast, when $E=\infty$, this configuration is stable

[9] Since a multistrip configuration consists of a longer interface than a single strip one, the total energy is higher, though the surface tension of the latter (tilted) interface is higher.

only for small shifts. As the shift increases, the single strip evolves into multistrip configurations; an example is shown in Fig. 2. Whenever h equals an exact divisor of L, the number of strips, denoted by n, appears to be an integer near L/h. Clearly, we could think of the n-strip configuration as a single unbroken strip wrapped n times around a torus, so that n plays the role of a winding number. The case of integer L/h might be interpreted as commensurability with SPBC. For this reason, we have chosen L values with many divisors.

To describe this "splitting" transition, we roughly identify a critical angle θ_c above which a single strip is unstable and evolves into many strips. Now, θ_c depends on L, decreasing in larger systems. It *appears* to converge to approximately 6° as $L \to \infty$, though we cannot conceive of a convincing theoretical basis for such a result. If θ_c indeed converges to this constant, the implications are startling, namely, stable configurations do not consist of more and more strips, while the first multistrip case has less than ten strips, regardless of L. If true, such a result suggests that there is some form of balance between interfacial (internal) energy, which favors smaller numbers of strips, and interfacial alignment with E, which favors more and more strips as $L \to \infty$ with h held fixed. Since interface energy is involved, we expect T to play a nontrivial role in a convincing theory of θ_c. Before developing such a theory, however, we face a daunting task, namely, mapping out $\theta_c(E, T)$.

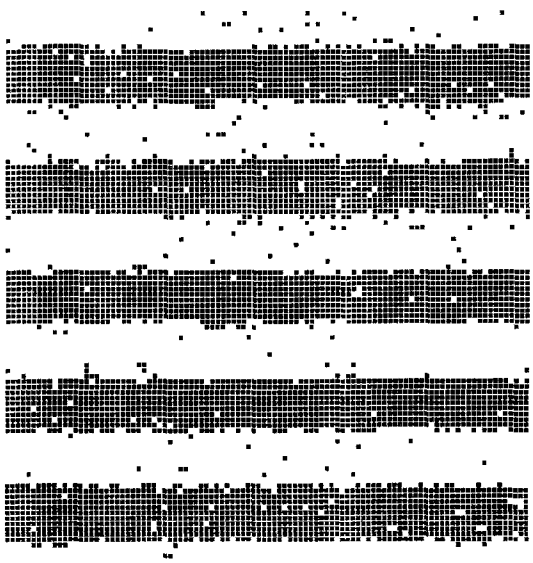


Fig. 2. A typical multistrip configuration with SPBC shifted by 20. Here $L = 100$, $T = 0.8$.

For angles slightly larger than θ_c, multistrip configurations consist of three, four, five, and six strips for $L = 20$, 36, 48, and 100, respectively. As θ is increased further, L/h decreases and the system adopts a more stable configuration with a *smaller* number of strips. We observe a sequence of "merging" transitions, from n-strip configurations to $(n-1)$-strip ones. If L/h is an integer, then the stationary state has L/h strips parallel to E. If L/h is slightly smaller than an integer, then the strips tilt *against* the direction of shift. On the other hand, they tilt in the direction of shift for L/h slightly larger than integral, as a single strip does for small h. In either case, the tilt causes an increase in u. In view of the findings of Section 3, we can also expect u to be nonanalytic at commensurate shifts.

These results are summarized in Fig. 3, where u is plotted against θ for various L. The data show that all curves resemble a series of ridges and valleys. Each valley is associated with a distinct multistrip configuration. The position of the first ridge is identified as θ_c and locates the "splitting" transition. Subsequent ridges locate "merging" transitions, since n strips evolve into $n-1$ strips. Similar behavior can be observed in a plot of the current versus the shift, shown in Fig. 4.

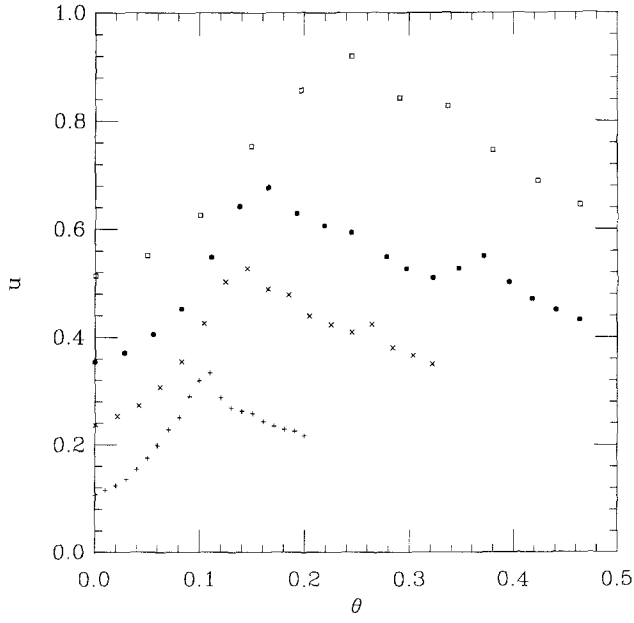


Fig. 3. Energies per site vs. $\theta = \tan^{-1}(h/L)$ for $T = 0.8$ in systems of $L = (\square)\,20$, $(\bullet)\,36$, $(\times)\,48$, and $(+)\,100$. For clarity, the first three sets of points have been shifted by 0.3, 0.2, and 0.1, respectively.

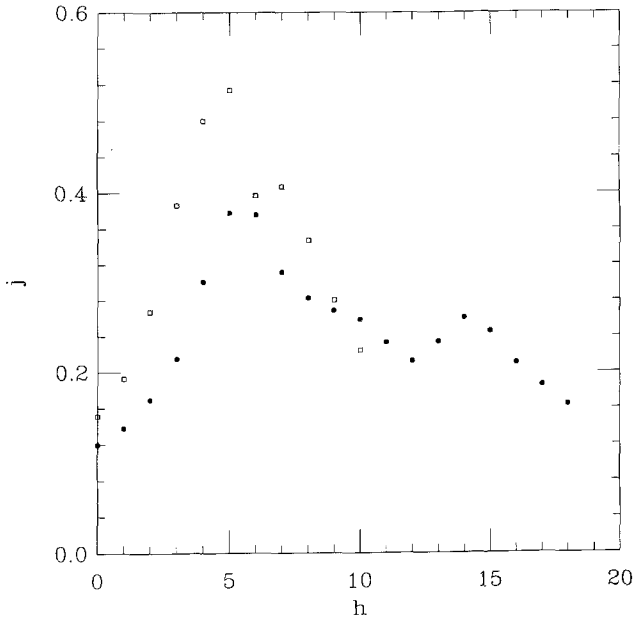


Fig. 4. Average current (in the direction of E) vs. shift for $T = 0.8$. Same symbols as in Fig. 3.

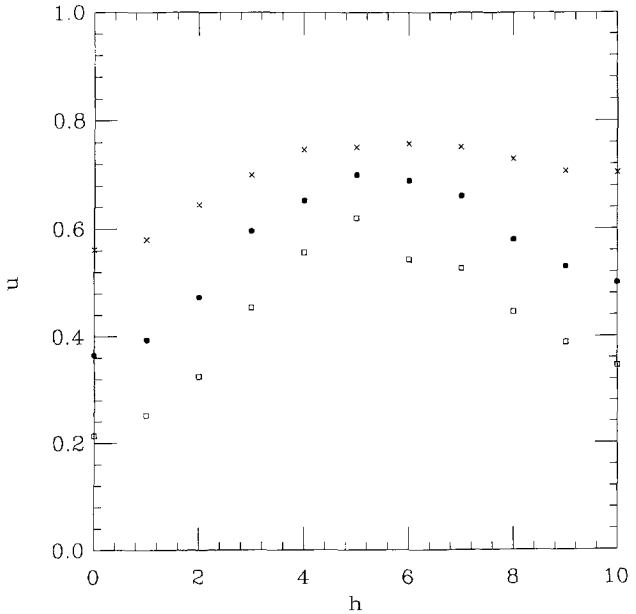


Fig. 5. Energies per site vs. shift for $T = (\square)\, 0.8$, $(\bullet)\, 1.0$, and $(\times)\, 1.2$ in a system with $L = 20$.

To probe the temperature dependence, we have performed simulations for $L = 20$ with three temperatures: $T = 0.8$, 1.0, and 1.2. Figure 5 displays the energy versus the shift. Observe that the critical angle is less and less well defined at higher T, when the interface becomes more diffuse. The flattening of the curves suggests that the change of stabilities among different configurations is less pronounced.

5. SUMMARY AND OUTLOOK

This study goes beyond previous studies on the driven lattice gas by demonstrating the much more significant role played by boundary conditions in determining the details of steady states. In particular, we believe that all thermodynamic properties, both steady-state and dynamic, will depend on *a combination of E and boundary conditions*, rather than on E alone. We found that SPBC introduces a host of new phenomena, as well as directions for future research:

1. The dependence of interfacial structure on orientation is *asymmetric* about the axes of lattice symmetry. The origin can be traced to E, which supplies the symmetry-breaking factor $\mathbf{n} \cdot \mathbf{e}$ $(= \sin\theta)$. An interface with a small, positive θ,. i.e., a leading edge, is more diffuse. On the other hand, interfaces with small, negative θ, i.e., trailing edges, display sharper profiles. Once discovered, it is easy to argue that this behavior should have been expected, since E drives particles away from a leading edge and into a trailing one. We believe that this phenomenon can be understood as an analog of those associated with crystal growth and evaporation,[6] in which interfaces are facetted and rough, respectively. However, interfaces in our system do not advance or recede, as noted previously. Unlike the bulk of a grown crystal, the bulk here is not "static," since there is a steady current of particles leaving the trailing (growing) edge by diffusion into the particle-rich bulk phase.

2. The steps on a leading edge acts as sources of particles (and holes) flowing into the bulk. Similarly, they act as sinks at the trailing edge. In this sense, the analogy with crystal growth and evaporation is strengthened. Perhaps it can be exploited in the formulation of a quantitative theory. Certainly, these sources and sinks lead to bulk densities that differ from those near an aligned $(\theta = 0)$ interface. In turn, these lead to bulk *energy* densities that depend on θ.

3. In our simulations, steady states are set up with *both* edges present. Thus, the average energy density u will not display any asymmetry in θ. Further, we decompose this total into a bulk part u_B and an interfacial part u_I. Surprisingly, we found that a term linear in θ appears in the *bulk*

u_B, forcing us to conclude that it must be a nonanalytic contribution $|\theta|$. For u_I, our data do not allow us to draw a confident conclusion on the θ dependence, though we believe that nonanalytic behavior is likely. Beyond these averages, we would like to distinguish contributions coming from the *inequivalent* edges. However, it is not clear how this can be achieved precisely.

4. For large θ, i.e., if large shifts in the SPBC were imposed, the single-strip configuration becomes unstable, evolving into multistrip ones. There appears to be a positive critical angle θ_c where this splitting transition occurs. More extensive runs with larger systems are necessary before we could confirm or disprove the conjecture that θ_c does not vanish in the thermodynamic limit. As θ is increased beyond θ_c, we observe a sequence of merging transitions, characterized by n strips evolving into $n-1$ strips. If we define Fourier components of particle density as order parameters, these transitions would be classified as first order. Again, much more studies are needed to determine the L dependence of these transitions if they survive the thermodynamic limit and, finally, a phase diagram in the E–T plane.

Though our data were collected on a two-dimensional system, there is every reason to believe that such phenomena will persist in higher dimensions.

Despite the lack of an appropriately defined "free energy," the internal energy u appears to be very useful for quantitative descriptions of interface behavior in this nonequilibrium system. Nonanalyticity in $u(\theta)$, together with the result[14] of field suppression of interfacial width, suggests that the connection between singularities in u and interface smoothness may be valid in a context broader than systems in equilibrium. Further, $u(\theta)$ appears to have many branches, each related to a different multistrip phase, while transition angles can be accurately identified solely from the high points in $u(\theta)$. If they can be established, such connections are clearly of great significance.

At a more refined level, the issue of inequivalent interfaces is pressing. A measure should be devised to distinguish, clearly and quantitatively, the leading edge from the trailing one. We emphasize that E is the sole agent responsible for the apparent smoothness of a trailing edge, since a tilted interface is always rough in both two- and three-dimensional equilibrium systems. We plan to explore means to induce only one interface in the system. Since E differentiates particles and holes, we cannot blindly follow the standard trick used in equilibrium systems, namely antiperiodic boundary conditions.[17]

In this work, we used only one value of E ($15 = \infty$, essentially) with

a very limited range of T and L. The next step would be a large-scale, systematic study, exploring finite-size effects as well as temperature and field dependences. Apart from availability of computer time, there are several difficulties to overcome. One is the long relaxation times for small E. Due to conservation of local particle density, these should follow the typical diffusive behavior and increase at least as L^2 for the equilibrium ($E=0$) case. Relaxations of the interface are even slower,[21] i.e., L^3. Estimated from time correlation measurements in the PBC case,[14] these times were found to be still extraordinarily long for systems driven by a small E. Another difficulty is the lack of a sound theoretical foundation for finite-size analysis for a nonequilibrium system.

At present, our understanding of driven systems with SPBC is largely phenomenological. The theoretical development is lagging far behind. Much of the difficulties can be traced to the lack of an undisputed concept of a free energy for nonequilibrium systems in steady states.[22] Furthermore, in stark contrast to systems in equilibrium, there is a subtle interplay among the external driving field, the boundary conditions, and the lattice. In this sense, our problem is a global one, with effectively long-range interactions. To comprehend such phenomena poses a significant and interesting challenge to theorists.

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REFERENCES

1. S. Katz, J. L. Lebowitz, and H. Spohn, *Phys. Rev. B* **28**:1655 (1983); *J. Stat. Phys.* **34**:497 (1984).
2. H. van Beijeren and L. S. Schulman, *Phys. Rev. Lett.* **53**:806 (1984); J. Marro, J. L. Lebowitz, H. Spohn, and M. H. Kalos, *J. Stat. Phys.* **38**:725 (1985); H. van Beijeren, R. Kutner, and H. Spohn, *Phys. Rev. Lett.* **54**:2026 (1985); J. Krug, J. L. Lebowitz, H. Spohn, and M. Q. Zhang, *J. Stat. Phys.* **44**:535 (1986).
3. K.-t. Leung and J. L. Cardy, *J. Stat. Phys.* **44**:567 (1986); H. K. Janssen and B. Schmittmann, *Z. Phys. B* **64**:503 (1986); K. Gawadzki and A. Kupiainen, *Nucl. Phys. B* **269**:45 (1986).

4. J. L. Vallés and J. Marro, *J. Stat. Phys.* **43**:441 (1986).
5. J. L. Vallés and J. Marro, *J. Stat. Phys.* **49**:89 (1987); J. Marro and J. L. Vallés, *J. Stat. Phys.* **49**:121 (1987).
6. W. K. Burton, N. Cabrera, and F. C. Frank, *Phil. Trans. R. Soc.* **243**:299 (1951); R. L. Dobrushin, *Theor. Prob. Appl. (USSR)* **17**:619 (1972); J. Weeks, G. H. Gilmer, and H. J. Leamy, *Phys. Rev. Lett.* **31**:549 (1973); H. J. Leamy and G. H. Gilmer, *J. Cryst. Growth* **24/25**:499 (1974).
7. S. T. Chui and J. D. Weeks, *Phys. Rev. B* **14**:4978 (1976); H. van Beijeren, *Phys. Rev. Lett.* **38**:993 (1977); H. J. F. Knops, *Phys. Rev. B* **20**:4670 (1979).
8. H. van Beijeren and I. Nolden, in *Topics in Current Physics, 43*, W. Schommers and P. von Blanckenhagen, eds. (Springer, Berlin, 1987), pp. 259–300.
9. J. W. Cahn, *J. Chem. Phys.* **66**:3667 (1977); C. Ebner and W. F. Saam, *Phys. Rev. Lett.* **38**:1486 (1977).
10. D. E. Sullivan and M. M. Telo de Gama, Wetting transitions and multilayer adsorption at fluid interfaces, in *Fluid Interfacial Phenomena*, C. A. Croxton, ed. (Wiley, New York, 1985); P. G. de Gennes, *Rev. Mod. Phys.* **57**:827 (1985).
11. J. S. Langer, *Rev. Mod. Phys.* **52**:1 (1980); J. D. Gunton, M. San Miguel, and P. S. Sahni, in *Phase Transitions and Critical Phenomena*, Vol. 8, C. Domb and J. Lebowitz, eds. (Academic Press, London, 1983), p. 287.
12. L. I. Rubinshtefin, *The Stefan Problem* (American Mathematical Society, Providence, Rhode Island, 1971).
13. K.-t. Leung, *J. Stat. Phys.* **50**:405 (1988); A. Hernandez-Machado and D. Jasnow, *Phys. Rev. A* **37**:626 (1988).
14. K.-t. Leung, K. K. Mon, J. L. Vallés, and R. K. P. Zia, *Phys. Rev. Lett.* **61**:1744 (1988), and preprint (1988).
15. K. K. Mon, S. Wansleben, D. P. Landau, and K. Binder, *Phys. Rev. Lett.* **60**:708 (1988), and preprint (1988).
16. J. D. Weeks, *Phys. Rev. Lett.* **52**:2160 (1984).
17. K. Binder, in *Applications of Monte Carlo Methods in Statistical Physics*, K. Binder, ed. (Springer, Berlin, 1984).
18. K.-t. Leung, Ph.D. thesis, University of California at Santa Barbara (1987), unpublished.
19. K.-t. Leung, G. A. Hagedorn and R. K. P. Zia, to be published.
20. H. van Beijeren, private communication.
21. L. A. Turski and J. S. Langer, *Phys. Rev. A* **22**:2189 (1977); *Acta Metal.* **25**:1113 (1977); K. Kawasaki and T. Ohta, *Physica* **118A**:175 (1983); *Prog. Theor. Phys.* **68**:129 (1982); D. Jasnow and R. K. P. Zia, *Phys. Rev. A* **36**:2243 (1987); R. K. P. Zia, R. Bausch, H. K. Janssen, and V. Dohm, *Mod. Phys. Lett. B* **2**:961 (1988).
22. J. Keizer, *Statistical Thermodynamics of Nonequilibrium Processes* (Springer, New York, 1987).