A Nonequilibrium Lattice Gas of Two-species: Monte Carlo Investigations

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Summary. We present the phase diagram of a far from equilibrium system, mapped by Monte Carlo simulation. The model is a lattice gas of two species and holes. The two species are biased to hop in opposite directions and interact via excluded volume and nearest neighbor attractions. Three phases are found as function of temperature and charge density.

Introduction. A comprehensive theory of nonequilibrium steady states is not yet available. This motivates the study of simple models for which analytic results can be compared to simulation data. While such models may seem far removed from physical phenomena, it is clearly easier to develop the tools for treating nonequilibrium systems in such a controlled setting before turning to the more demanding task of describing systems found in the natural world. For example, it is not yet known to what extent the idea of universality can be applied to nonequilibrium systems, or for that matter how to rigorously define a phase transition far from equilibrium. For the time being, we deal with these questions intuitively, amassing detailed descriptions of nonequilibrium systems while awaiting a general theory. In this paper we present the results of a Monte Carlo (MC) study of an interacting lattice gas driven far from equilibrium. In the first part we review the earlier work which motivates our study, and in the second part we describe the microscopic model and order parameters. Finally we describe the main results of our study, a phase diagram and a detailed finite-size scaling analysis of a particular limit of the model.

Twenty years ago, Katz et al. introduced a simple modification (the “KLS model”) of the attractive Ising lattice gas, in which particle-hole exchanges along a particular lattice direction (which we call $y$) are coupled to a bias ($E$) which favors (suppresses) particle moves in the $+y$ ($-y$) direction. With the addition of periodic boundary conditions in the $y$ direction, a nonzero particle current is established and the steady state distribution is not proportional to the Boltzmann distribution. A review of this work can be found in [3]. Simulations, field-theoretic renormalization group studies, and field-theoretic renormalization group studies indicate that the model retains a continuous transition into a low-temperature phase separated state, though the universal behavior is distinct
from the Ising class (see below). Further, in contrast to the Ising model, the hopping bias allows only interfaces parallel to $y$.

Now consider a generalization of such driven Ising models [9] to two species of particles which react in opposite senses to the bias. One type ($+$) is pushed in the $+y$ direction while the other ($-$) is pushed in the $-y$ direction. In the limit $E, T \to \infty$, while $E/T \equiv \tilde{E}$ finite the only interaction between particles is excluded volume. In this case a phase transition is found as the mass density ($m$) and $\tilde{E}$ are varied. At low $m$ and $\tilde{E}$ the system is disordered. At sufficiently high $m$ and $\tilde{E}$, the two species lock into a ‘traffic jam’: each blocks the other, and one observes a high-density strip perpendicular to $y$.

If the high $T, \tilde{E}$ constraint is lifted in the two-species model, then the attractive interactions will become significant over some range of $T$. This introduces the interesting possibility of transitions between the two types of order mentioned above. Imagine, e.g., beginning with the KLS model at half-filling. Now stay at half filling, but lower the charge density, i.e., change a few ‘$+$’ particles into ‘$-$’. At some critical charge density, $q_c(E)$, the blocking transition may become stable. This possibility is investigated in the following sections by mapping the parameter space with MC simulations. Along the way we will find that it is quite difficult to find $q_c(E)$, as we lack a detailed understanding of the appropriate scaling forms in this region of parameter space. The subtleties of scaling arguments far from equilibrium will be illustrated in the last section, where we will determine $T_c$ for the KLS model at finite $E$.

**Microscopic Model and Order Parameters.** A configuration of the model is specified by a set of occupation variables, $\{s(r)\}$, where $r \equiv (x, y)$ labels a site on a fully periodic square lattice of dimensions $L_x \times L_y$, and each $s(r)$ can take the values $+1$, $-1$, or $0$ for a positive particle, negative particle, or hole. We also introduce the mass variable $n(r) \equiv |s(r)|$. We will remain always at half-filling. The charge density is defined as $q = \frac{1}{L_x L_y} \sum_r s(r)$. All particles interact via the usual Ising Hamiltonian, $H = -4J \sum_{\langle r, r' \rangle} n(r) n(r')$, independent of charge, with $J > 0$ and the sum over nearest neighbors. $J = 1$ is chosen arbitrarily: this merely sets an energy scale. The bias, $E$, points in the positive $y$-direction and is measured in units of $J$. A configuration evolves by selecting a nearest-neighbor bond at random; if occupied by a particle-hole pair, its contents are exchanged according to the Metropolis [10] rate $\min\{1, \exp[-(\Delta H - \delta y Es(r))/T]\}$. The second term models the effect of the drive: if the particle, of charge $s$, is initially located at $r$, $\delta y$ is the change in its $y$-coordinate due to the jump. Thus, positive (negative) charges jump preferentially along (against) the field direction. The parameter $T$ (“temperature”) models the coupling to a thermal bath. The natural control parameters for our study are temperature $T$ (measured in units of the Onsager value), the drive $E$ and the charge density $q$.

Conservation laws (for $q$ and $m$) ensure spatially inhomogeneous ordered phases. We therefore select an order parameter sensitive to such structures,
i.e., the equal-time structure factor associated with the particle distribution
\[ \langle \Phi(m_x, m_y) \rangle = \left\langle \left| \frac{1}{L_x L_y} \sum_r n(r) e^{i k \cdot r} \right|^2 \right\rangle, \]
\[ k \equiv 2\pi \left( \frac{m_x}{L_x}, \frac{m_y}{L_y} \right). \]
\( \langle \cdot \rangle \) denotes a configurational average, and the integers \( m_x, m_y \) index the wave vector. For a perfect strip along the \( y \)-direction, \( \langle \Phi(1, 0) \rangle = 1 \) while a random configuration gives \( \langle \Phi \rangle = O(1/L_x L_y) \). Except where noted, all simulations are run on \( 40 \times 40 \) lattices, starting from random initial configurations. One MC step (MCS) is defined as \( 2L_x L_y \) update attempts. The first \( 2 \times 10^5 \) MCS are discarded, and measurements are taken every \( 200 \) MCS for the next \( 8 \times 10^5 \) MCS.

Monte Carlo Results: Phase Diagram. Although most detailed studies of the KLS model have considered the limit of infinite \( E \) to accentuate nonequilibrium properties, we are forced to consider finite values of \( E \). As our two-species simulation stumbles through phase space it may find itself in a blocked configuration in a region of parameter space where such states should only be metastable. At large values of \( E \) this metastable configuration will persist far beyond the time of our simulation. Initial runs indicated that metastable lifetimes at \( E = 2 \) are reasonable. Note that at this value, jumps favoring \( E \) provide only one-half the change in energy required to break a single nearest-neighbor bond. It is therefore natural to wonder whether the transition at such small \( E \) remains in the KLS universality class. This question will be answered in the affirmative in the next two sections.

![Phase diagram for \( E = 2 \) in charge density \( q \) and temperature \( T \), in units of \( T_c(E = 0) \). (+) denotes the first-order line, while the diamonds and x’s denote the continuous lines. Configurations labelled: DO for disordered, HS for horizontal strip, VS for vertical strip.](image)
Fig. 1 shows the phase diagram in $q$ and $T$ for $E = 2$. The phase boundaries are mapped by sweeping in $T$ at fixed $q$ while monitoring the order parameters $\langle \Phi(1,0) \rangle$ and $\langle \Phi(0,1) \rangle$ and their fluctuations. The far left point is the KLS transition at finite $E$. Moving right, parallel to the horizontal axis, we are changing $+$ particles into $-$; as long as the $-$ are insufficient to form a blockade the transition from disorder into a parallel (“vertical”) strip apparently remains continuous, as indicated by a peak in the fluctuations of $\langle \Phi(1,0) \rangle$. We suspect that this transition can be described by the KLS field theory, with the additional complication of a small concentration of randomly distributed (but annealed) impurities. At the far right of the phase diagram the system contains equal numbers of $+$ and $-$ particles. There, we encounter a transition into a blocked phase (“horizontal strip”) which also appears continuous, indicated here by a peak in the fluctuations of $\langle \Phi(0,1) \rangle$. At larger values of $q$ and lower $T$, we are able to observe a transition from the blocked phase into a vertical strip phase. This transition appears to be first-order, displaying hysteresis and metastability. The most interesting region in the phase diagram is where the three lines join at $q_c(E)$. Future studies will focus on scaling properties in the vicinity of this nonequilibrium bicritical point.

Anisotropic Finite-Size Scaling. We now turn to a detailed discussion of the KLS transition at finite $E$. As mentioned in the introduction, a Langevin equation for a mesoscopic version of the local spin variable has been studied in great detail [8]. The most remarkable prediction of the field theory is a nontrivial anisotropy exponent, $\Delta > 1$, so that wavevectors scale as $k_\parallel \sim k_\perp^{1+\Delta}$; physically this implies that domains of correlated spins grow faster in the field direction. In order to control finite size corrections, it is then necessary to account for this anisotropy [5]. The anisotropy introduces different correlation length exponents parallel($\nu_\parallel$) and perpendicular($\nu_\perp$) to the drive, an effect which we will refer to as *strong anisotropy*, in contrast with, e.g., an Ising model with anisotropic interactions. The values of the critical exponents are known from an RG analysis to all orders; their values in $d = 2$ are $\beta = 1/2$, $\nu_\parallel = 3/2$, $\nu_\perp = 1/2$, $\Delta = 2$ [8]. Phenomenological scaling forms [7] involve two length scales, $L_\parallel$ and $L_\perp$, so that the order parameter scales as

$$m(t, L_\parallel, L_\perp) = L_\parallel^{-\beta/\nu_\parallel} L_\perp^{\nu_\parallel/\nu_\parallel} L_\perp^{-1}$$

and the scaling function depends on a "shape factor," $S \equiv L_\parallel^{\nu_\parallel/\nu_\parallel} L_\perp^{-1}$ [7, 6]. Increasing the system size while holding $S$ fixed allows us to approach $T_c$ without cutting off parallel correlations before transverse ones. We then use the (predicted) exponents to analyze our data. The validity of this approach will be judged by the quality of data collapse for $m$. In this way we will determine $T_c(E = 2)$, as it is the only fit parameter. Detailed work on carefully defined correlation functions and lengths [5] is forthcoming.

Monte Carlo Results for $E=2$. We choose as our order parameter $m \equiv \langle \frac{1}{L_\parallel L_\perp} \sum_{x,y} n(x, y) e^{2\pi i (m x/L_\parallel)} \rangle$ since it is subject to smaller fluctuations than the structure factor. Most runs last for $1.2 \times 10^6$ MCS, though in larger
systems near criticality runs of $4.8 \times 10^6$ MCS were needed to ensure good statistics. The first $0.2 \times 10^6$ MCS were discarded and measurements were taken every 400 MCS thereafter.

Fig. 2 shows the scaling of the order parameter for three different system sizes with $S = .1575$, for both $E = 20$ (effectively infinite) and $E = 2$. From these plots we estimate $T_c (E = 2) = 1.20(2)$. Notice the systematic deviations from scaling in the $T < T_c$ branch, which may be due to a small critical region or corrections to scaling from the marginal operator. Though we have not investigated this anomaly in detail, it occurs in the $E = \infty$ model as well and has been observed in other nonequilibrium Ising models. Elsewhere, the data collapse is of the same quality as in the $E = \infty$ case. We therefore have no reason to believe that the finite $E$ transition falls into a different universality class.

**Conclusions.** We have mapped out a slice of phase space for an interacting lattice gas of two species, driven far from equilibrium by a bias which drives a particle current. The phase diagram has two continuous lines which meet a first-order line at a critical charge density $q_c (E)$. In order to make more definitive claims, we need knowledge of scaling forms in the vicinity of the bicritical point. It would be quite interesting to investigate this scaling behavior in order to learn about such points far from equilibrium.
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