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Title	PHASE TRANSITIONS IN TWO-SPECIES ASYMMETRIC DIFFUSIVE LATTICE GASES(Session IV : Structures & Patterns, The 1st Tohwa University International Meeting on Statistical Physics Theories, Experiments and Computer Simulations)
Author(s)	Leung, Kwan-tai
Citation	(1996), 66(3): 606-609
Issue Date	1996-06-20
URL	http://hdl.handle.net/2433/95755
Right	
Type	Departmental Bulletin Paper
Textversion	publisher

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PHASE TRANSITIONS IN TWO-SPECIES ASYMMETRIC DIFFUSIVE LATTICE GASES

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Despite their ubiquity in nature, nonequilibrium phase transitions and critical phenomena are far less well understood in comparison with their equilibrium counterparts[1]. A major obstacle is that the Gibbs method in equilibrium statistical mechanics no longer applies. Tractable theoretical models are therefore very valuable in gaining a deeper understanding.

A sensible way to start our exploration is to generalize the equilibrium Ising model to nonequilibrium situations with steady state transports[2]: Using the lattice-gas representation of the Ising model, we imagine that particles are being driven by some external mechanism (e.g., 'charged' particles acted on by 'electric' field $\mathcal{E}$). Several questions may be posed as to the effect of $\mathcal{E}$ (or of being nonequilibrium): E.g., how are the phase transitions in Ising model modified? Or, in view of the 'charged particle' picture, does the drive lead to new phenomena when more than one kind of 'charges' are present? The former kind of questions have been investigated extensively over the last decade with an accumulation of a wide range of interesting results[3]. The latter question motivates this study.

Specifically, we consider a two-dimensional (2D) model with two types of particles driven along mutually orthogonal directions[4], on a square lattice of square geometry $L \times L$ under periodic boundary conditions. To keep things simple, we assume the particles are noninteracting except being hard cored (thus effectively at infinite temperature). Since the system is isolated, the number of particles is conserved and the dynamics is diffusive. The type-1 particle hops to its vacant nearest neighbor at a rate p along $+y$, $q(< p)$ along $-y$, and r along $+x$ and $-x$. The corresponding rates for a type-2 particle are r, r, p and q respectively. So an average type-1 (or type-2) particle drifts along the $+y$ (or $+x$) direction. We adopt the Metropolis jump rates $p = 1/4 = r$, $q = e^{-\mathcal{E}}/4$ which defines $\mathcal{E}$, and restrict ourselves to equal numbers of the two types of particles. The parameter space is spanned by $\mathcal{E}$ and the mean particle density $\bar{\rho} \equiv \bar{\rho}_1 = \bar{\rho}_2$. Hole density is denoted by $\bar{\rho}_0 = 1 - 2\bar{\rho}$.

Similar two-species models have been studied before. When the two species are driven in opposite directions, Schmittmann et al[5] observed the particles lock up in a strip normal to the drive when $\bar{\rho} > \bar{\rho}_c$. But since $\bar{\rho}_c$ decreases with system sizes, the existence of the transition in the large-L limit is in question. To address this, one must first understand the effects of finite system sizes. At first sight, the system behaves almost as 1D, being insensitive to the dimension normal to the drive. Later results[6], however, reveal that the probability of forming an *inclined* strip is finite and dependent on L_x/L_y. This implies the presence of highly anisotropic finite-size effects that are hard to quantify. In contrast, while our model with orthogonal drifts also displays a jamming transition, it is setup to have *isotropic* finite-size effects. The model is therefore in a suitable position to address the issue of the survival of the transition. In a different context, when cast in the language of traffic flow (cf. [7]), our model represents vehicles moving along crossed streets and traffic jams as the vehicle density reaches a critical value.

In addition to the uniform and strip phase found in other models[5, 7], our model shows another inhomogeneous, 'droplet' phase in between (Fig. 1). The three phases are characterized by different symmetries. The droplet is *localized* and it breaks translational invariance along both directions. It drifts steadily forward as a result of the migration of particles along its
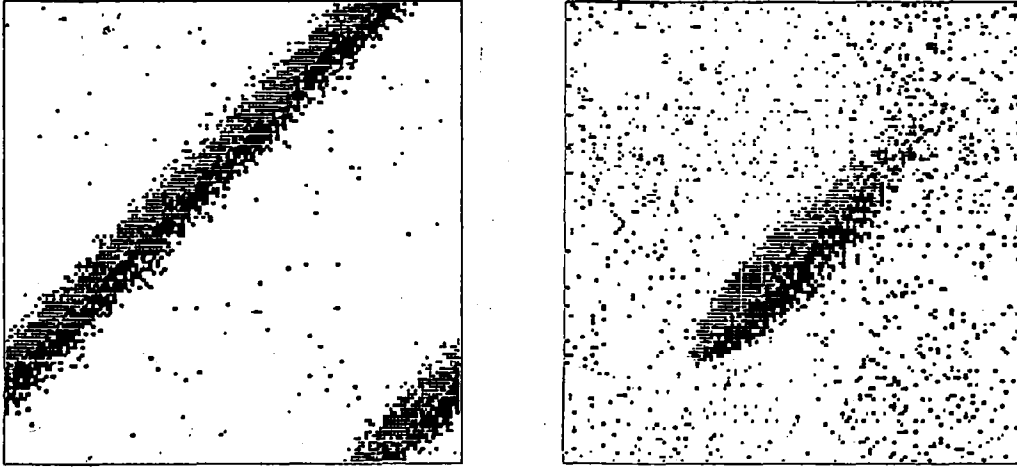
Figure 1: Typical inhomogeneous jammed phases, $L = 128$, $\bar{\rho} = 0.076$ and 0.074 respectively. Light (dark) particles drift to the right (top).

symmetry axis (Fig. 2(a)). As $\bar{\rho}$ is increased, the system goes through the uniform, droplet and strip phase in sequence (since the droplet is stable for a very limited range of $\bar{\rho}$, hereafter $\bar{\rho}_c$ is used to label the transition density between homogeneous and inhomogeneous phases). The nature of the transitions appears to be first order at large $\mathcal{E}$ or L, and continuous at small $\mathcal{E}$ or L. Although the full phase diagram has not been determined due to problems associated with strong hysterisis, there are hints of a tri-critical point separating a branch of first-order phase boundary from a continuous-order one[8, 4].

The fact that $\bar{\rho}_c$ decreases with L (cf. Fig. 2(b)) invites an investigation of the finite-size effects. For this purpose, we have developed a coarse-grained continuum theory[4]. Since the numbers of particles are conserved, the local dynamics obeys a set of continuity equations into which local hopping rules and exclusion interaction are incorporated ($n = 1, 2$ labels the species):

$$\frac{d\rho_n}{dt} = -\nabla \cdot \mathbf{J}_n \tag{1}$$

where the current density is given by

$$\mathbf{J}_1 = \hat{x} E_{1x} \rho_1 \rho_2 + \hat{y}(E \rho_0 \rho_1 - E_{1y} \rho_1 \rho_2)$$
$$- \hat{x} D_\perp [(1 - \rho_2)\frac{\partial \rho_1}{\partial x} + \rho_1 \frac{\partial \rho_2}{\partial x}] - \hat{y} D_\parallel [(1 - \rho_2)\frac{\partial \rho_1}{\partial y} + \rho_1 \frac{\partial \rho_2}{\partial y}]. \tag{2}$$

Here $\hat{x}, \hat{y}$ are the unit vectors, and the coarse-grained parameters are determined by the microscopics ones: $E = 2(p - q)$, $D_\parallel = p + q$, $D_\perp = 2r$, and E_{1x} and E_{1y} are related to nearest neighbor correlations (see [4]). A similar equation holds for $\mathbf{J}_2$. The important point to note is that the terms $\propto D$'s describe diffusive process, whereas those $\propto E$'s describe drift.

Before we discuss the solutions of Eq. (1), notice that the two species become degenerate in the case of $\mathcal{E} = 0$, and the system is reduced to the Ising model at infinite temperature which has no phase transition as $\bar{\rho}$ is tuned. On the other hand, particles without hard-core interaction would 'go through' each other and no jam would be possible. These are captured by Eq. (1) for which the only steady state solutions (i.e., $d\rho_n/dt \equiv 0$) in these limits are uniform
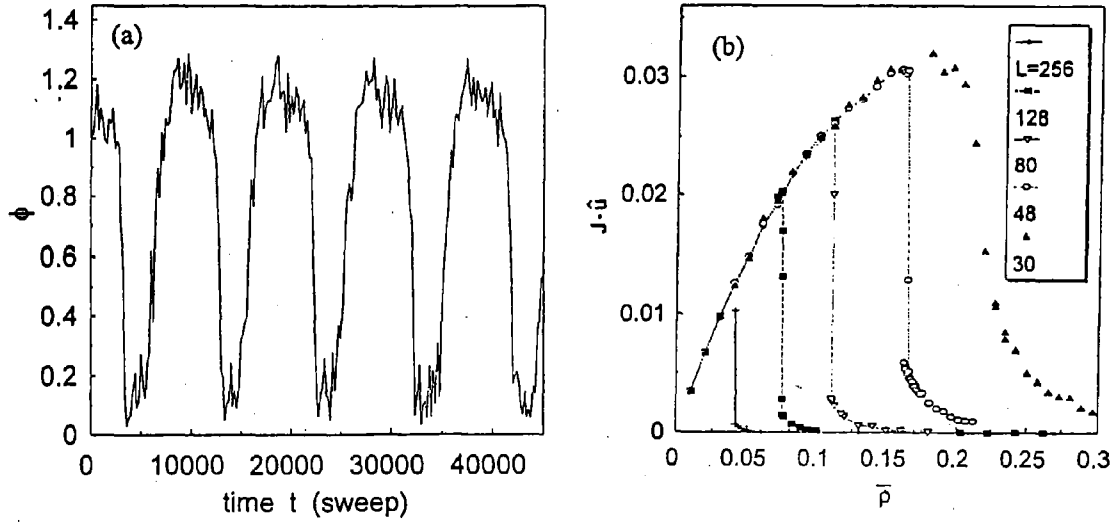
Figure 2: (a) The forward motion of a droplet is shown by $\phi(t) \propto |\sum_y \rho(L_x/2, y; t) e^{i2\pi/L_y}|$, where $\rho = \rho_1 + \rho_2$, for $L = 256, \bar{\rho} = 0.07, \mathcal{E} = 50$. Speed=1/period. (b) Current density $\mathbf{J}_1 \cdot \hat{u}$ vs $\bar{\rho}$ for $\mathcal{E} = 50$ and a wide range of L. Upper branch: uniform phase, lower branch: strip phase.

solutions. Thus, we conclude that *spontaneous pattern formation is a joint effort of the drive and hard-core exclusion.*

In this article, we will not consider the droplet phase further as it requires solving the full 2D problem. While the uniform phase is trivially described by $\rho_n = $ const, the one-dimensional steady-state strip profiles obey

$$\frac{1}{\varepsilon_0} \frac{d\rho_1}{du} = \rho_1(1 - \rho_1 + \rho_2) - \frac{1}{\rho_0}(\varepsilon_1 \rho_1 \rho_2 + C) \tag{3}$$

$$-\frac{1}{\varepsilon_0} \frac{d\rho_2}{du} = \rho_2(1 + \rho_1 - \rho_2) - \frac{1}{\rho_0}(\varepsilon_1 \rho_1 \rho_2 + C) \tag{4}$$

for the case of $\bar{\rho}_1 = \bar{\rho}_2 \equiv \bar{\rho}$, where $\varepsilon_0 = \sqrt{2}E/(D_\parallel + D_\perp) = 2\sqrt{2}(p-q)/(2r + p + q)$, $\varepsilon_1 = (E_{1x} + E_{1y})/E$. The u axis is normal to the strip, and $C \equiv \mathbf{J}_1 \cdot \hat{u}/\sqrt{2}(p-q)$ is a reduced current along $+u$.

Numerically we find that the correlation factor $\varepsilon_1 \approx 1 - 2\bar{\rho} = \bar{\rho}_0$ for *arbitrary* $\mathcal{E}$, L and $\bar{\rho}$ in the uniform phase. This prompts us to replace ε_1 by $\rho_0(u) = 1 - \rho_1(u) - \rho_2(u)$ in Eqs. (3) and (4). Since no adjustable parameter is left, the solution satisfies a simple scaling

$$\rho_n(u, \mathbf{J}_1 \cdot \hat{u}, L, \mathcal{E}) = f_n(u\varepsilon_0, C, L\varepsilon_0). \tag{5}$$

The functions f_n's are determined numerically. Agreements with simulations are impressive[4]. Now we may relate $\bar{\rho}$ to the current (cf. Fig. 2(b)) via $(\sqrt{2}/L) \int du\, \rho_n(u) = \bar{\rho}(C, L\varepsilon_0)$, or by inversion

$$C \equiv \mathbf{J}_1 \cdot \hat{u}/\sqrt{2}(p-q) = g(\bar{\rho}, L\varepsilon_0). \tag{6}$$

The scaling variable $L\varepsilon_0$ dictates how data for different L and $\mathcal{E}$ may be collapsed; it is the finite-size scaling we seek. Simulation data (cf. Fig. 3) fully support this prediction.
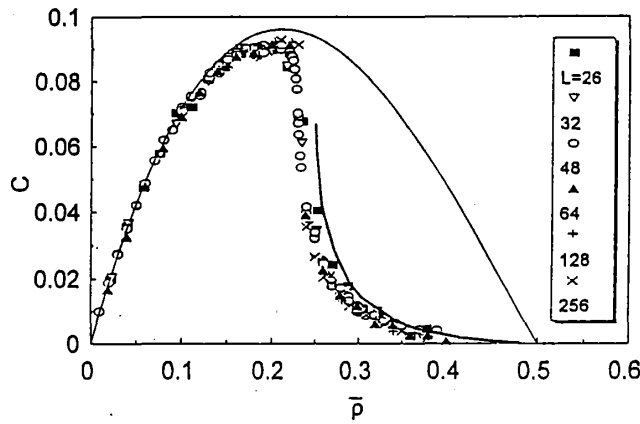
Figure 3: Finite-size scaling as predicted by Eq. (6). All data have the same $L\varepsilon_0 = 23.65$ but different combination of $(L, \mathcal{E})$. Solid lines are theoretical results for the two phases.

Finally, defining $\bar{\rho}_c(L, \mathcal{E})$ by $dC/d\bar{\rho}|_{\bar{\rho}_c} = \infty$, we find $\bar{\rho}_c \sim (L\varepsilon_0)^{-0.82(1)}$ for large $L\varepsilon_0$. This asymptotic behavior implies that the transition takes place at $\bar{\rho}_c \to 0$ as $L \to \infty$ for any *finite* $\mathcal{E}$. Although $\bar{\rho}_c$ vanishes asymptotically, the strip width $L\bar{\rho}_c$ *diverges*. This means that the strip and hence the phase transition remain well-defined in the thermodynamic limit. This situation is reminiscent of the 1D limited local sandpile model[9]. It would be interesting to exploit the intriguing connection between these two apparently different nonequilibrium problems.

Acknowledgments: Support from the National Science Council of ROC is gratefully acknowledged.

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