Novel Phases and Finite-Size Scaling in Two-Species Asymmetric Diffusive Processes

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We study a stochastic lattice gas of particles undergoing asymmetric diffusion in two dimensions. Transitions between a low-density uniform phase and high-density nonuniform phases characterized by localized or extended structure are found. We develop a mean-field theory which relates coarse-grained parameters to microscopic ones. Detailed predictions for finite-size (L) scaling and density profiles agree excellently with simulations. Unusual large-L behavior of the transition point parallel to that of self-organized sandpile models is found.

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There is much interest in the studies of lattice gas systems evolving under conservative stochastic dynamical rules [1]. When the rules do not satisfy detailed balance condition, intriguing properties atypical of thermal equilibrium arise [2]. Their mappings onto surface growth models and directed polymer in a random medium [3] generate further interests and development. Very recently, such connections have been exploited to shed light on the unbinding transitions of directed polymer [4].

One particularly simple class of lattice gas models consists of particles undergoing biased diffusion with no interaction except hard-core exclusion. Generally known as the asymmetric simple exclusion process (ASEP) [1], it has attracted the interests of both physicists and mathematicians for its novel phase transitions [5] and shock structures [6] under various boundary conditions. Generalizing the ASEP to a model having two species biased along *opposite* directions in an $L_x \times L_y$ system, Schmittmann and co-workers [7] observed a transition between a uniform and a nonuniform phase as the number of particles is varied, with the latter phase characterized by a compact strip of aggregated particles. However, the fundamental question of the existence of the transition in the thermodynamic limit has not been answered. This is not a simple issue to settle, since the limiting process depends crucially on *anisotropic* finite-size effects induced by making one direction special. The precise form of anisotropies is unknown. Nevertheless, a hint is provided by analogous continuous phase transitions, which typically have ensemble averages depending on L_x^p/L_y with $p \neq 1$ [8]. Depending on how $L_x \to \infty$ and $L_y \to \infty$ are taken, undesired singularities may arise from $L_x^p/L_y \to \infty$ or 0. If p is not known, it is not possible to proceed. In another context, a cellular automaton model with *orthogonal* biases has been formulated to mimic cross traffic flow [9]. A similar jamming transition has also been found. Whether the transition survives in the thermodynamic limit is likewise not investigated.

Motivated by these open questions, we study in this Letter a three-state model with two interpenetrating ASEP orthogonal to each other. By biasing the first (second) species along $+y$ ($+x$) direction, *isotropic* finite-size effects are ensured (i.e., effectively $p = 1$ above) so that no ambiguity is associated with the thermodynamic limit, whereas the essential simplicity of previous models is maintained. Specifically, we consider a model on a two-dimensional (2D) square lattice of square geometry $L \times L$, with periodic boundary conditions. Occupation numbers $\{n_{x,y}\}$ specify the configuration, where $n_{x,y} \in \{0, 1, 2\}$ represents a vacancy, a type-1 or a type-2 particle at site (x, y), respectively. Except for hard-core exclusion, the particles are noninteracting. In simulations, a site and one of its nearest neighbors are randomly picked in turn. If and only if one of them is vacant, a jump occurs with rate: p for a type-1 particle hopping along $+y$, or a type-2 particle hopping along $+x$; q for type 1 along $-y$, or type 2 along $-x$; and r for type 1 along $\pm x$, or type 2 along $\pm y$. L^2 such trials constitute one unit of time (one sweep). Note that choosing $p > q \geq 0$ introduces the asymmetry, whereas $r > 0$ provides transverse diffusions necessary for ergodicity (contrary to the traffic flow automaton [9] which has $r = 0$). Using Metropolis rules and a parametrization by an "electric field" $\mathcal{E}$ [2], the rates become $p = 1/4 = r, q = e^{-\mathcal{E}}/4$.

Simulation results.—Simulations are done on wide ranges of parameters $32 \leq L \leq 256, 0.2 \leq \mathcal{E} \leq \infty$, with equal density of particles, $\overline{\rho}_1 = \overline{\rho}_2 \equiv \overline{\rho}$. While transitions between a uniform (U) phase and a strip (S) phase are expected as $\overline{\rho}$ is varied, a novel droplet phase (D) which is not present in previous models [7,9] appears in between (see Fig. 1). The three phases are characterized by different symmetries, with the *localized* droplet breaking translational invariance along both spatial directions and drifting steadily forward along its symmetry axis. That it is not an unstable or metastable state is revealed by the behavior of an order parameter ϕ (essentially the Fourier amplitude of the density profile at a smallest wave vector [8]), which varies from one (compact strip) to zero (perfectly uniform). Figure 1(a) depicts ϕ versus time (t) in the steady state for $L = 48$, $\mathcal{E} = \infty$, showing frequent jumps among the three phases. In fact, a histogram analysis shows that with those parameters the system is at a three-phase coexistence, i.e., at a *triple point.* Deviating from this point, we find the following: (a)

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At slightly different density, the U or S phase becomes dominant. (b) For smaller bias $\mathcal{E}$ with fixed L, $\phi(t)$ plots and histograms show that the triple point splits into two transitions, e.g., $S \to D$ at ρ_{SD}, then $D \to U$ at ρ_{DU}, as $\overline{\rho}$ decreases, with gradually widening gap ($\rho_{SD} - \rho_{DU} = 0$–$0.02$ as $\mathcal{E} = \infty$–0.5, for $L = 48$). Diminishing first order characteristics—hysteresis and finite jumps in ϕ and currents—suggest that the transitions eventually turn continuous, consistent with the observation that ρ_{SD} grows with decreasing $\mathcal{E}$, making the droplet longer and fuzzier until no longer distinguishable from a strip. (c) For a larger L at fixed $\mathcal{E}$, hysteresis becomes more pronounced while the transition points shift systematically downward.

These results remind us of a pure substance which has a triple point and a first order phase boundary ending at a critical point [10]. Another possibility is to have a first and a continuous order phase boundary joining at a tricritical point. Despite the obvious interest, however, we have not been able to map out the phase diagram completely. One difficulty is due to the above-mentioned decreasing transition densities for increasing system sizes, casting doubts on the survival of the transitions as $L \to \infty$. At the same time, growing hysteresis makes it harder to locate the transitions precisely. To understand these crucial finite-size effects, we now focus our attention on a continuum theory.

Mean-field theory.—We begin by defining $P^y_{nn'n''\ldots}(x,y,t)$ as an equal-time, joint probability at time t for the locate state at sites $(x,y),(x,y+1),(x,y+2),\ldots$ to be $n,n',n'',\ldots$ where $n = 0,1,$ or 2 as above ($P^x_{nn'n''\ldots}$ likewise). Since particles only hop to nearest neighbors, it is easy to see for $P_n(x,y,t+1) - P_n(x,y,t) \equiv \dot{P}_n$, that

$$\tfrac{1}{2}\dot{P}_1 = p[P^y_{10}(x,y-1) - P^y_{10}(x,y)] + q[P^y_{01}(x,y) - P^y_{01}(x,y-1)] + r[P^x_{10}(x-1,y) - P^x_{10}(x,y) + P^x_{01}(x,y) - P^x_{01}(x-1,y)]. \tag{1}$$

The 1/2 ensures the same time scale as in simulations and lattice constant $\equiv 1$. $\dot{P}_2$ obeys a similar equation. An attempt to close this set of equations generates a hierarchy in the usual way. To proceed, we instead adopt a mean-field approximation in the following sense:

$$P^y_{nn'}(x,y) \approx P_n(x,y)P_{n'}(x,y+1)[1 + \Delta^y_{nn'}(x,y)], \tag{2}$$

with the asymmetric local correlations induced by biases accounted for by $\Delta_{nn'}$'s (similarly for $P^x_{nn'}$). Clearly $\Delta^y_{12} > 0, \Delta^y_{21} < 0$, etc. Only those with $n \neq n'$ are kept, as $\Delta_{nn} \ll 1$ is expected and well confirmed by simulation.

By taking the (naive) continuum limit of Eq. (1) via Taylor expansions, assuming smooth functions, we obtain from Eq. (1) the continuity equation $\dot{\rho}_n = -\nabla \cdot \mathbf{J}_n$ for density ρ_n, with the current

$$\begin{aligned}\mathbf{J}_1 = {} & \hat{\mathbf{x}}E_{1x}\rho_1\rho_2 + \hat{\mathbf{y}}(E\rho_0\rho_1 - E_{1y}\rho_1\rho_2) \\ & - \hat{\mathbf{x}}D_\perp\left[(1-\rho_2)\frac{\partial\rho_1}{\partial x} + \rho_1\frac{\partial\rho_2}{\partial x}\right] \\ & - \hat{\mathbf{y}}D_\parallel\left[(1-\rho_2)\frac{\partial\rho_1}{\partial y} + \rho_1\frac{\partial\rho_2}{\partial y}\right],\end{aligned} \tag{3}$$

where the parameters are completely specified by the microscopics: $E = 2(p-q)$, $E_{1x} = 2r(\Delta^x_{21} - \Delta^x_{12})$, $E_{1y} = 2(p\Delta^y_{12} - q\Delta^y_{21})$, $D_\parallel = p + q$, and $D_\perp = 2r$. $\mathbf{J}_2$ can be obtained from $\mathbf{J}_1$ by switching the labels $1 \leftrightarrow 2$ and $x \leftrightarrow y$. Before we continue, note that the terms proportional to E's and D's represent physically drifts and diffusions, respectively. There is an induced drift normal to the bias in spite of symmetric transverse jump rates. Similar but much weaker corrections in the diffusive pieces due to Δ's are omitted in (3). In the case of $p = q$, or $\rho_1 = 0$, or $\rho_2 = 0$, the stationary state is a uniform product measure and Eq. (2) becomes exact with $\Delta = 0$. Consequently, it is necessary to have *two* species *driven* to produce all the nontrivial behavior. Contrary to similar equations derived from entropy consideration [7], the microscopic origin of each term is made explicit.

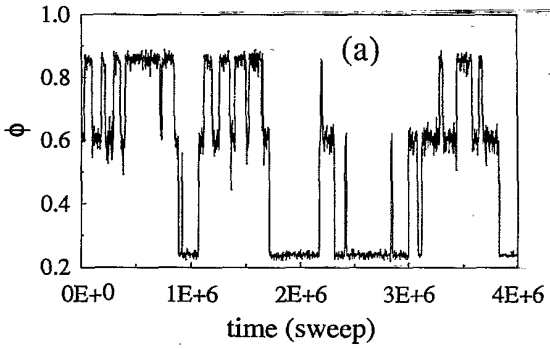
Recall that there are three different steady states in simulations. While the uniform solution is trivial to find, the droplet requires solving the full 2D problem. Since the droplet phase occupies an extremely narrow range in $\overline{\rho}$ (i.e., $\rho_{SD} \approx \rho_{DU}$), for practical purposes we may focus on the uniform and the strip phase. By setting $\mathbf{J}_n = \text{const}$, it is straightforward to show that the strip profiles satisfy

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

$$-\frac{1}{\varepsilon_0}\rho_2' = \rho_2(1 + \rho_1 - \rho_2) - \frac{1}{\rho_0}(\varepsilon_1\rho_1\rho_2 + C), \tag{5}$$

for $\overline{\rho}_1 = \overline{\rho}_2 = \overline{\rho}$, where $\varepsilon_0 = \sqrt{2}E/(D_\parallel + D_\perp) = 2\sqrt{2}(p-q)/(2r+p+q)$, $\varepsilon_1 = (E_{1x}+E_{1y})/E = [p\Delta^y_{12} + r\Delta^x_{21} - q\Delta^y_{21} - r\Delta^x_{12}]/(p-q)$, $\rho_n' \equiv d\rho_n/du$, with the u axis perpendicular to the strip at a polar angle of 135°. $C = \sqrt{2}J/E$ is a reduced current along $+u$, where $J = \mathbf{J}_1(\hat{\mathbf{y}} - \hat{\mathbf{x}})/\sqrt{2}$. u and J have the same units as in simulations.

Using the data for Δ's, we find a remarkable result: $\varepsilon_1 \approx 1 - 2\overline{\rho} = \overline{\rho}_0$ for *arbitrary* $\mathcal{E}$, L, and $\overline{\rho}$ in the uniform phase (i.e., all data fall on one *universal line*). While apparently $\Delta \to 0$ (so does ε_1) as $\overline{\rho}_0 \to 0$, we have yet an explanation for the full, universal behavior. In



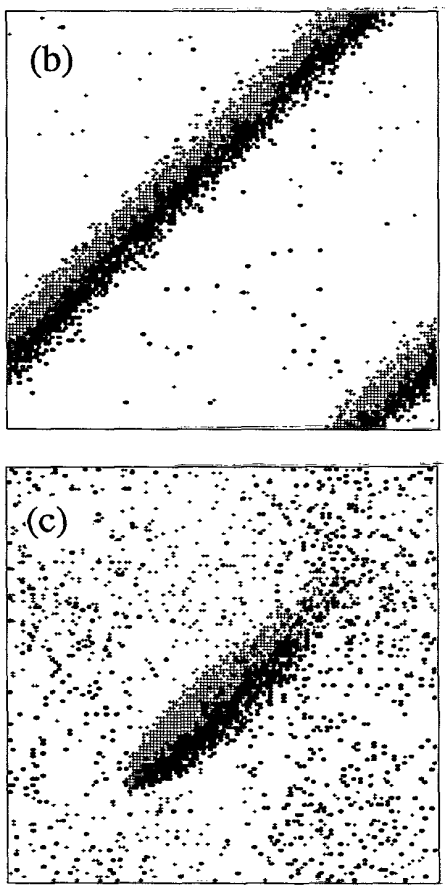


FIG. 1. (a) Order parameter at three-phase coexistence for $L = 48$, $\mathcal{E} = \infty$, and $\overline{\rho} = 0.1623$: large, intermediate, and small ϕ values correspond to strip, droplet, and uniform phase, respectively; (b) a typical strip for $L = 128$, $\overline{\rho} = 0.076$; and (c) a typical droplet for $L = 128$, $\overline{\rho} = 0.074$. Light (dark) particles drift to the right (top).

line with a mean-field approach, we assume it remains to hold locally and replace ε_1 by $\rho_0(u)$ in Eqs. (4) and (5). Agreement between the predictions and simulations provides *a posteriori* justification [11]. Then Eqs. (4) and (5) contain *no adjustable parameter* and imply the scaling form

$$\rho_n(u, J, L, \mathcal{E}) = f_n(u\varepsilon_0, J/E, L\varepsilon_0). \tag{6}$$

Unlikely to be obtained in closed forms, the functions f_n's are determined by numerically solving the coupled Eqs. (4) and (5). One stringent test of the theory is to compare these functions with those in simulations. Figure 2 shows a typical test of not only f_n but also the scaling in L. With no adjustable parameter, the agreements are impressive verifications of our approach. Deviation becomes noticeable only in the small $L\varepsilon_0$ regime. Furthermore, by (6), $(\sqrt{2}/L)\int du\, \rho_n(u) = \overline{\rho}(J/E, L\varepsilon_0)$, or equivalently

$$C = \sqrt{2}\, J/E = g(\overline{\rho}, L\varepsilon_0). \tag{7}$$

This implies the entire current-density relation (along with the transitions) is the same for different L and microscopic $\mathcal{E}$, provided $L\varepsilon_0$ is fixed. Figure 3 confirms this prediction. The $\overline{\rho}$ dependence of g also compares favorably with simulations, except at small $L\varepsilon_0$. This is consistent with the observed transitions gradually turning continuous at small biases, as fluctuations ignored in the equations become significant.

Equation (7) allows an investigation of the thermodynamic limit. The transition point $\overline{\rho}_c(L, \mathcal{E})$ is taken to be the minimum $\overline{\rho}$ allowed for the strip solution of a given $L\varepsilon_0$ (i.e., at $dC/d\overline{\rho} = \infty$; cf. Fig. 3). It is a function of $L\varepsilon_0$ alone. $\lim_{L\varepsilon_0\to\infty}\overline{\rho}_c(L\varepsilon_0)$ then decides whether the transition survives or not. Figure 4 shows, for both simulations [12] and theory that $\overline{\rho}_c \sim (L\varepsilon_0)^{-0.82(1)}$ and strongly suggests $\overline{\rho}_c \to 0$ as $L\varepsilon_0 \to \infty$.

These results have far reaching implications. If $\lim_{L\varepsilon_0\to\infty}\overline{\rho}_c = 0$ indeed holds, then *finite*-density transition will occur generically only for *infinitesimal bias* (i.e., $\mathcal{E} \propto 1/L$). It is hasty, however, to conclude that the transition would actually be extinct for finite $\mathcal{E}$. Seldom found in equilibrium, this situation is by no means unfamiliar in nonequilibrium steady states. A case of intense interest is the well-studied 1D limited local sandpile models of self-organized criticality [13]. Criticality of such models is controlled by the trough which has density ρ_t vanishing as $L^{-1/3}$ [14], but the number of

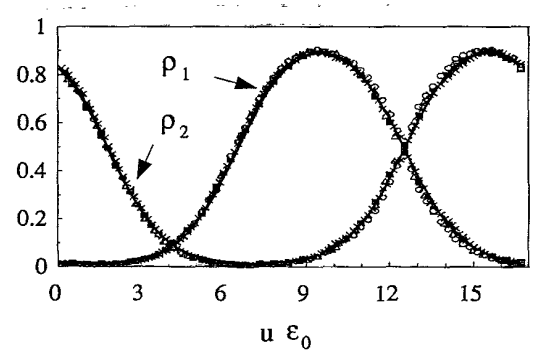


FIG. 2. Finite-size scaling of density profiles at fixed $L\varepsilon_0 = 23.65$ (or fixed C) and $\overline{\rho} = 0.36$; $L = 32$ (□), 48 (△), 64 (○) 128 (×), 256 (dashed line), and theory (solid line) [cf. Eq. (6)] with no free parameter.

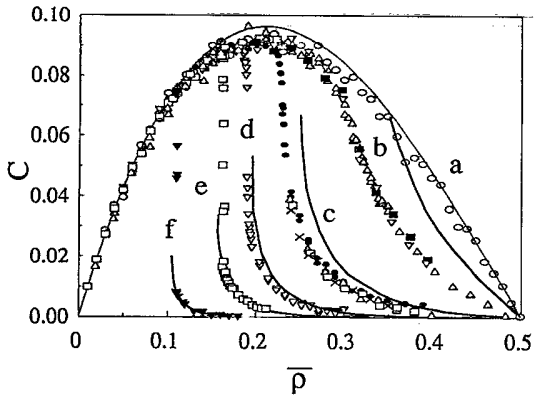


FIG. 3. Scaling of current [Eq. (7)]. Thin line is $\overline{\rho}(1-\overline{\rho})(1-2\overline{\rho})$ for uniform phase [from (4)]. Branches are for strip phase at various $L\varepsilon_0$: (a) 6.445, $L = 48$ (○) (b) 14.81, $L = 32$ (□), 48 (△), and 64 (▽); (c) 23.65, $L = 48$ (●), 64 (△), 128 (□), and 256 (×); (d) 33.84 and $L = 48$ (▽); (e) 45.26, $L = 48$ (□); (f) 75.43, $L = 80$ (▽). Note confirmed scaling in (b) and (c). Heavy lines are theoretical predictions for (b) to (f).

troughs $L\rho_t \to \infty$ as $L \to \infty$. Analogously, our model has the strip width $\xi \sim L\overline{\rho}_c \to \infty$, but $\xi/L \to 0$ (hence, ξ is a *mesoscopic* length) as $L \to \infty$, so that, like the sandpiles, the transition remains well defined for all L [15]. We suspect other models have similar features, but the corresponding analysis is hindered by anisotropies [7] or by the lack of ergodicity [9].

To conclude, we have studied systems governed by asymmetric diffusion and two-species exclusion as simple models exhibiting nonequilibrium phase transitions. Our primary results are the following: (a) There exist multiple phases in spite of their apparent simplicity; (b) a quantitatively successful theory with known microscopic dependence has been developed, which could be improved to handle fluctuations by adding noise terms and extended to more complicated models or related problems, such as with interparticle interactions; and (c) the survival of the associated transitions in the thermodynamic limit is addressed for the first time and found to be parallel to a certain class of model sandpiles. Finally, open questions such as the mechanism of stability for the droplet, details of the phase diagram, and issues of critical exponents at small biases are of significant interests to the general study of nonequilibrium phase transitions.

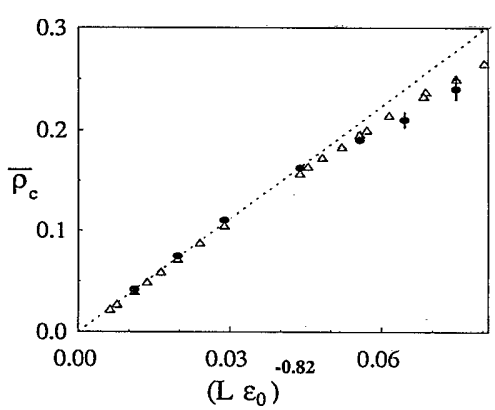


FIG. 4. Large-L behavior of transition density: theory [cf. Fig. 3] (△); data (● with error bars); linear fit (dotted line).

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Note added.—At the completion of the manuscript, we received a preprint from Vilfan *et al.* [16] who obtained mean-field exact solutions for the strip phase in the oppositely biased two-species model [7]. Their results agree qualitatively with ours, including a tentative tricritical point, but the large-L limits have not been explored.

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