Influence of extended dynamics on phase transitions in a driven lattice gas

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Monte Carlo simulations and dynamical mean-field approximations are performed to study the phase transition in a driven lattice gas with nearest-neighbor exclusion on a square lattice. A slight extension of the microscopic dynamics with allowing the next-nearest-neighbor hops results in dramatic changes. Instead of the phase separation into high- and low-density regions in the stationary state the system exhibits a continuous transition belonging to the Ising universality class for any driving. The relevant features of phase diagram are reproduced by an improved mean-field analysis.

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The concept of universality is well established in equilibrium critical phenomena. According to this concept only just a few parameters, i.e. spatial dimension of the system and the dimensionality of the order parameter determine the critical exponents meanwhile other details like the microscopic dynamics are irrelevant. The nonequilibrium systems exhibit richer and more complex feature. One of the important questions to address is whether this concept also applies to nonequilibrium systems. There are examples when a slight extension of microscopic dynamics results in different morphology of the stationary state [1,2]. The importance of the dynamics also manifests in other problems, such as chemically reactive mixtures [3] or driven diffusive systems (DDS) [4] where the microscopic and the supposed macroscopic model yield different morphologies. The former nonequilibrium system also exemplifies that the resulting stationary state may differ significantly from that of the corresponding equilibrium model [5].

Very recently Dickman has introduced a simple driven lattice gas model with hard-core interaction between the particles which excludes the simultaneous occupation of the nearest neighbor sites on a square lattice [6]. In the absence of driving this model is equivalent to a thoroughly investigated equilibrium model discussed in connection with the theory of melting [7–10]. For this particular interaction the only (control) parameter of the model is the particle concentration. The occupation variables $\sigma_i = 0 \,(1)$ if the lattice site $i$ is empty (occupied) and the concentration is defined as $\rho = \sum_i \sigma_i/N$. The only interaction is to forbid the simultaneous nearest-neighbor occupancy. During the time evolution a randomly chosen particle can hop to one of its empty neighboring sites satisfying the condition of NNE. In the basic model studied by Dickman the particles can hop only to the nearest neighbor sites while in this extended model the next-nearest-neighbor hops are also permitted with a probability as defined in Ref. [6]. Here, the value of $P$ is varied from 0.5 to 1. The case $P = 0.5$ corresponds to the isotropic hopping rate characteristic to the equilibrium model and $P = 1$ represents the infinitely strong drive. Further details and the review of the equilibrium properties can be found in Ref. [5].

![FIG. 1. Schematic illustration of possible hopping rates of the nearest-neighbor (NN) and the extended next-nearest neighbor (NNN) hopping dynamics. The drive is horizontal and the directions are chosen with equal probability $[1/4 \,(1/8)$ for the NN (NNN) hops].](image-url)
distribution is disordered if the concentration is low enough. For sufficiently high concentration sublattice ordering can be observed, that is the particles form a chequerboard-like pattern. In other words, if the square ordering can be observed, that is the particles form a homogeneous random ordered state. Conversely, Φ = 1 (or −1) if all the particles are positioned in the sites of sublattice A (B). When decreasing the concentration the equilibrium system (P = 0.5) undergoes an order-disorder transition which is continuous and belongs to the Ising universality class [10]. In the driven system, however, this transition becomes first order if only nearest neighbor hops are permitted [6]. The present dynamics conserves the number of particles therefore the first order transition is accompanied with the coexistence of high- and low-density phases.

To explore the phase diagram of the extended model, we have performed a dynamical mean-field analysis. The most relevant details of this laborious technique are given in the Appendix of the work by Dickman [6] at the levels of two- and four-site clusters. Using this method one can determine the probability of possible configurations on a given set of clusters if the particle distribution is homogeneous. Similarly to the NN hop model, the two- and four-site approximations are not capable to describe the effect of driving as a consequence of the strong constraints of NNE. This means that the results are independent of P and equivalent to those obtained by using the traditional cluster variation method [11,12] for the equilibrium system (P = 1/2). The predictions for the phase transition point are ρcP = 0.25 at two-point and ρc4P = 0.317 at four-point level.

The failure of dynamical mean-field approximation is disappointing since previously this method gave qualitatively good phase diagrams for several nonequilibrium models [13]. To overcome this shortage we have performed a six-point approximation used successfully for a similar driven lattice gas [14]. In this case we determine the configuration probabilities on 2 × 3 clusters. Taking the compatibility conditions and symmetries into account the configuration probabilities are described by 17 parameters whose value are determined by solving numerically the corresponding set of equations of motion. At P = 1/2 this calculation has reproduced the same solution obtained at the level of four-point approximation. For the driven cases, however, the solutions (for Φ = 0 and Φ > 0) are already affected by the value of P. As an example, for infinite drive the transition appears at ρcP(P = 1) = 0.3026. The resulting phase diagram is shown in Fig. 2. We should mention that the phase transition remains continuous for any drives according to this level of approximation.

To check these predictions MC simulations are performed for L = 20, 40, 80, 160, and 320 under periodic boundary conditions varying the concentration ρ and drive P. To reach the stationary state we have used both homogeneous random and ordered initial states. In the former initial state the particles are positioned within a strip parallel to the drive.

In agreement with the expectation the modification of dynamics does not influence the stationary state if P = 0.5 (equilibrium model). The MC data of Φ(ρ) functions collapse when comparing the results obtained for the NN and NNN dynamics at any system sizes. At the same time the evolution toward the stationary states becomes faster when NNN hops are allowed. Similar effect was also reported in another driven diffusive model [14] as well as in domain growth processes [15]. In contrast, a significant difference can be observed in the stationary states when the systems are driven. While the separation of the high- and low-density phases characterizes the NN dynamics [14] leading to a jammed “herring-bone” structure then the stationary state remains homogeneous for any drive and concentration when NNN jumps are also allowed. The study of order parameter and density profiles as a function of transversal coordinate also support that the ordered phase is homogeneous in the case of extended dynamics. As a consequence, the current has no size-dependence and varies smoothly with the concentration and P. The phase diagram obtained by MC simulations confirm the qualitative prediction of the dynamical mean-field theory. Namely, the critical concentration (ρc) decreases with P and the transition remains continuous for those drives displayed in Fig. 2. The classification of the critical behavior for a nonequilibrium model requires careful analysis. The difficulties
are well demonstrated by the investigation of standard model \cite{16} whose critical behavior is even controversial \cite{17}. Here, we present a finite-size scaling analysis for the infinite strong drive ($P = 1$) in the case of extended (NNN) dynamics. For this purpose we have used the scaling form

$$\Phi(L, \rho) = L^{-\beta/\nu} \Phi_r(L^{1/\nu}) ,$$

(2)

where $\rho_r \equiv (\rho - \rho_c)/\rho_c$ is the reduced concentration. Assuming that the nonequilibrium phase transition belongs to the class of the equilibrium model (i.e. Ising exponents are supposed), nice data collapse is found (see Figure 3). Here, $\rho_{\text{MC}}(P = 1) = 0.350(5)$. This value is consistent with an alternating estimate which comes from the analysis of the fourth order cumulant of order parameter $U_L = 1 - \langle \Phi^4 \rangle_L/3\langle \Phi^2 \rangle_L^2$ \cite{13}. Similar critical behavior is found for any $P < 1$ drive.

In summary, the microscopic dynamics has been slightly extended in a previously introduced driven diffusive lattice gas where the only interaction is to forbid the simultaneous nearest-neighbor occupancy. Despite the weak modification the nonequilibrium behavior changes significantly. The stationary states are found to be homogeneous for any drives and densities if the next-nearest-neighbor hops are also permitted. In this case the system exhibits a sublattice ordering when the particle concentration is increased. The value of critical concentration decreases with the drive and this behavior can be explained by the higher level of dynamical mean-field approximation. The numerical results support that the system is in the same universality class of the equilibrium Ising model. This model exemplifies that the nonequilibrium behavior may be significantly influenced by a weak modification of microscopic dynamics.

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\begin{figure}[h]
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\includegraphics[width=\textwidth]{figure3.png}
\caption{The finite-size scaling of order parameter of NNE model with NNN hopping for $P = 1$. The slopes of the asymptote lines are indicated.}
\end{figure}

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