Driven lattice gas with nearest-neighbor exclusion: shear-like drive

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Abstract

We present Monte Carlo simulations of the lattice gas with nearest-neighbor exclusion and Kawasaki (hopping) dynamics, under the influence of a nonuniform drive, on the square lattice. The drive, which favors motion along the +x and inhibits motion in the opposite direction, varies linearly with y, mimicking the velocity profile of laminar flow between parallel plates with distinct velocities. We study two drive configurations and associated boundary conditions: (1) a linear drive profile, with rigid walls at the layers with zero and maximum bias, and (2) a symmetric (piecewise linear) profile with periodic boundaries. The transition to a sublattice-ordered phase occurs at a density of about 0.298, lower than in equilibrium ($\rho_c \approx 0.37$), but somewhat higher than in the uniformly driven case at maximal bias ($\rho_c \approx 0.272$). For smaller global densities ($\rho \leq 0.33$), particles tend to accumulate in the low-drive region. Above this density we observe a surprising reversal in the density profile, with particles migrating to the high-drive region and forming structures similar to force chains in granular systems.

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I. INTRODUCTION

An important model of interacting particles in statistical mechanics is the lattice gas. In this model the particles have nearest-neighbor interactions which can be either attractive (ferromagnetic) or repulsive (antiferromagnetic). In equilibrium, such systems have been used extensively as models of simple fluids. Nonequilibrium versions of this model have also been widely studied [1, 2], generally in the form of a lattice gas with periodic boundaries under a constant drive that biases the hopping rates along one of the principal axes of the lattice [3]. Lattice gases with biased hopping are also known as driven diffusive systems (DDS) [1]; the repulsive version [4, 5] serves as a model for fast ionic conductors [6].

The lattice gas with nearest-neighbor exclusion (NNE) is the infinite repulsion limit of the ordinary repulsive lattice gas. Here, particles are forbidden to occupy the same or neighboring sites; the minimum allowed interparticle separation is that for second neighbors. Hard-core exclusion is the only interaction between the particles. (This model also represents the zero-neighbor limit of the Biroli-Mézard lattice glass model [7].) The equilibrium version was studied in [8, 9, 10, 11, 12] both theoretically and numerically, for various lattice types. These analyses show that the model exhibits a continuous phase transition to an ordered state at a critical density \( \rho_c \) (\( \rho_c \approx 0.37 \) on the square lattice), with exponents that belong to the Ising universality class.

More recently, nonequilibrium versions of the NNE model were studied [13, 14]. In Ref. [13] (using nearest-neighbor hopping dynamics on the square lattice), it was found that the critical density varies with drive intensity: the higher the drive, the lower the critical density. The transition is continuous for low bias but becomes first order if the bias strength is \( \geq 0.75 \). Above the transition density, the system separates into regions of low and high local density, with the high-density region essentially frozen. Szolnoki and Szabó [14] extended the dynamics to include next-nearest-neighbor (diagonal) hops, and observed a similar variation of the critical density with drive strength, but with a homogeneous stationary state. Continuous phase transitions in this version of the model fall in the Ising class, as the equilibrium case.

Here we consider a hard-core DDS with nearest-neighbor hopping dynamics, in which the drive is nonuniform. The simplest case is that in which the bias, along the \( x \) direction, varies linearly along the perpendicular (\( y \)) direction. The motivation for this drive configuration
is to model a system of hard particles in a uniformly sheared fluid, or a granular system under shear. Specifically, the probability for a particle at \( y \) to attempt a jump to the right \((x \rightarrow x+1)\) is given by:

\[
P_r(y) = \frac{1}{4} \left( 1 + \frac{y - 1}{L - 1} \right),
\]

for \( y = 1, 2, \ldots, L \), on a square lattice of \( L^2 \) sites. The corresponding probability for attempting to hop to the left is \( P_l(y) = 1/2 - P_r(y) \), while hops in the \( \pm y \) directions are attempted with probabilities of 1/4. From Eq. (1) it is clear that a particle at \( y = 1 \) experiences no bias, while one at \( y = L \) cannot jump to the left. We present numerical results from Monte Carlo (MC) simulations of the model. One point to be noted is that the drive cannot overcome the repulsion between particles: attempted moves are accepted if and only if the nearest-neighbor exclusion condition is respected.

Our main objective is to obtain the phase diagram and critical properties of the model. We determine the critical density and study the behavior of the order parameter and the stationary current as functions of density. Of particular interest are the current and the density profiles as functions of \( y \). Our simulations indicate that at low densities, particles tend to accumulate in the low-drive region, and that as we increase the density, they migrate to the high-drive region. This is surprising since, in the uniform-drive case [13], a large bias is required to cause particle aggregation. The density and current profiles change dramatically at a density of about 0.33. In the following section (II) we detail the model and simulation procedure. In Section III, we present numerical results and discussions. Final considerations are reserved for section IV.

II. SIMULATIONS

We consider a square lattice of length \( L \) (\( L^2 \) sites) with \( N \) particles (\( N < L^2/2 \)). (Most of our studies use \( L = 100 \).) The initial configuration is prepared via random sequential adsorption (RSA) [15, 16] of particles, always respecting the excluded-volume condition. Once all of the \( N \) particles have been inserted, the biased hopping dynamics begins. A particle is selected at random and assigned a new (trial) position at one of the nearest neighbor sites, with probabilities as discussed above. If the trial position does not violate the exclusion constraint, the move is accepted, otherwise it is rejected. Each MC time unit corresponds to \( N \) attempted moves. We follow the evolution for a total of \( 10^6 \) MC time
units. We use 20 values of density $\rho = N/L^2$ to investigate the transition, ranging from $\rho = 0.1$ to $\rho = 0.37$.

We study two kinds of drive configuration and associated boundary conditions. The first, employed with the linear bias profile, Eq. (1), imposes rigid walls at $y = 1$ and $y = L$ (moves to $y = 0$ or $y = L + 1$ are prohibited). The second one involves a drive profile symmetric about the mid-plane ($y = L/2$), such that the bias is the same at $y = 1$ and $y = L$. In this case we apply *periodic* boundary conditions in the $y$-direction. The symmetric drive profile used in the case of periodic boundaries is piecewise linear:

$$P_r(y) = \begin{cases} \frac{1}{4} \left( 1 + \frac{y - 1}{L/2} \right), & \text{if } y \leq L/2 \\ \frac{1}{4} \left( 1 + \frac{L - y}{L/2} \right), & \text{otherwise} \end{cases}$$

This equation guarantees that particles crossing the boundary in the $y$ direction are subject to the same bias. We use periodic boundaries in the $x$-direction (parallel to the drive) in both cases.

### III. RESULTS

**A. Stationary global properties**

To characterize the behavior of the model we study the order parameter and the stationary current. The order parameter is defined as the difference in sublattice occupancies per particle,

$$\phi = \frac{N_A - N_B}{N},$$

where $N_{A(B)}$ is the number of particles in sublattice $A(B)$. The current is defined as the difference between the number of jumps along the drive less the number contrary to it, per site and unit time.

In Fig. 1 we show the average value of the order parameter and, in the inset, its corresponding fluctuation. The transition point is characterized by a sudden rise in the order parameter and by a peak in its variance. The data suggest a continuous transition to sublattice ordering at a critical density of $\rho_c \approx 0.298$. The critical density is lower than that for the equilibrium transition [9] of $\rho_c \approx 0.37$. In the uniformly driven system studied in [13], the transition (for maximal bias, for $L = 100$) occurs at a density of 0.272, and is *discontinuous*. A transition density of $\rho_c = 0.30$ in the uniformly driven system corresponds to a
FIG. 1: Order parameter (circles) versus overall density, $L = 100$. The inset shows its variance. The peak in $\langle \Delta \phi^2 \rangle$ is around $\rho = 0.298$.

bias of 0.75 ($P_r = 3/8$); at this point the transition is discontinuous. (The transition in the uniformly driven system is continuous for $\rho \leq 0.6$.) The apparently continuous transition in the presence of a nonuniform drive is likely to be due the fact that the system does not order all at once. We will return to this point later.

FIG. 2: Average stationary current versus density for $L = 100, 90, 80$ and 70.

In Fig. 2 we show the stationary current, averaged over the region $16 < y < L - 16$, for each lattice length $L$, to avoid strong wall effects. This quantity displays the same behavior as in the uniformly driven case: it increases at small densities (reflecting the increasing number of carriers) and decreases for larger densities (due to the reduction in available
FIG. 3: Stationary density profile $\rho(y)$ for various global densities. The curves for the three denser states are shifted upwards by 0.15, 0.1 and 0.05, respectively. Inset: same quantity for densities 0.33, 0.34, and 0.35 (from top to bottom). The first two curves are shifted upwards by 0.1 and 0.05.

space for movement). The maximum value of $\langle j(t) \rangle$ falls at roughly in the same density as in the uniform drive case [13]. Interestingly, the phase transition near $\rho = 0.298$ is associated with a plateau in the current.

The order parameter and the stationary current present strong fluctuations for densities above $\rho = 0.32$. The evolution of these quantities typically displays sudden jumps between the ordered and the disordered state, a fact already observed in the uniformly driven case. The drive provokes formation of organized structures while their thermal motion provides a mechanism for breaking such clusters. We will see that such behavior may find a parallel in actual physical systems.

**B. Density and current profiles**

Of interest is how the system organizes as the density increases. To understand this, we determine the stationary density and current profiles, $\rho(y)$ and $j(y)$, respectively. These quantities are shown in Figs. 3 and 4. The immediate conclusion that can be drawn from these plots is that particles concentrate in the low-drive region (lower half of the lattice), for densities up to $\rho = 0.33$.

Enhanced particle concentration in the low-drive region is in fact observed for densities as low as $\rho = 0.20$. This is surprising given the finding that, in a uniformly driven system, a
strong drive favors order, i.e., provokes a reduction in the critical density. On this basis one might expect the high-drive region to order first (i.e., at a lower global density), which would require particles to concentrate in the high-drive region. In fact just the opposite occurs: for a global densities $\rho \leq 0.32$, the density profile $\rho(y)$ (Fig. 3) is highly skewed to the region around $y = 0$, where the bias is small. Note that the local density is $\geq 0.37$ in this region (for $\rho$ between 0.30 and 0.32), that is, greater than or equal to $\rho_c$ in equilibrium. The density profile decays monotonically with increasing $y$ (except for small density oscillations induced by the wall at $y = 0$). For $\rho = 0.33$, the local density instead increases with $y$, reaching a peak near $y = 47$, after which it decays in an approximately linear fashion until $y = L$. For a certain range of global densities $\rho$, the local density near $y = 1$ actually decreases with increasing $\rho$. Note also that, as may be seen from Fig. 4, the current density in the high-drive region is zero for $\rho \geq 0.35$.

C. Ordering and jamming

Ordering occurs first in the low-drive region. The high density in this region is also reflected in the current profile (Fig. 4). The current is much smaller in the small-$y$ region (low-bias) and increases monotonically with $y$. The order parameter profile (not plotted here), follows the same pattern as the density profile. It clearly shows that ordering occurs
in the low-drive region for densities between 0.30 and 0.32, as described above.

A possible explanation for the surprising reversal of the density and current profiles with increasing global density is related to the formation of a jammed region, as observed in the uniformly driven system [13]. When the global density is too low for such a region to form, particles tend to collect in the low-drive region because a strong drive tends to destroy the local correlations needed for particles to pack to high density, even if such packing does not result in long-range order. The depletion of the high-drive region appears to be the reason for the plateau in the current observed around $\rho = 0.30$ in Fig. 2. Fig. 3 shows that as the global density increases, the local density in the high-drive region remains nearly constant, so the current hardly varies.

When, on the other hand, the global density is sufficiently high for a jammed region to form, it appears in the high-drive region, leading to an irreversible accumulation of particles there, so that the low-drive region has fewer particles than at lower global densities, for which there is no jammed region.

To illustrate these ideas, we show in Fig. 5 a configuration for $\rho = 0.31$ and $L = 100$. As expected, the low-drive region is very dense and contains few mobile particles. In the uniformly driven system (at maximum bias) one observes, at this density, formation of "herringbone" pattern of diagonal stripes, pointing along the drive, with particles in this structure essentially frozen. In the present case the low-drive region is highly ordered, with almost all particles in the same sublattice, but there is no sign of the herringbone pattern.
high-drive region is disordered, permitting the high currents and lower densities reported above. Several clusters of particles exist in the high-drive region, but they are not large enough to cause jamming.

We may now identify two factors leading to the continuous variation of the order parameter with density shown in Fig. 1. One reason is that ordering begins in the low-bias region. Studies of the uniformly driven system show that the transition is continuous under a weak bias. The second reason is that the width of the ordered region grows continuously with increasing density.

For global densities above about 0.34, the situation, as noted, is completely changed. Particles now accumulate in the high-drive region, and the density profile exhibits a maximum in the central region (intermediate drive strength). At these higher densities the current profile displays a peak in the low-drive region. The peak shifts to smaller $y$ (smaller drive intensity) and decreases in amplitude as the global density is increased.

Fig. 6 shows a typical configuration at global density $\rho = 0.35$. Evidently the long diagonal line of particles at the upper right is associated with jamming in the high-drive region. The empty triangular region implies a decrease in the local density with increasing $y$. Particles are not free to enter this region since all particles along the diagonal edge are jammed. These observations are supported by the the density and current profiles (Figs. 3 and 4). The density is roughly constant in the middle portion of the lattice and begins to decrease near $y = 78$, where the empty triangular region begins. The current is only
appreciably different from zero in the lower portion of the lattice, as signalled in Fig. 6 by the presence of particles both sublattices. The diagonal edges observed in configurations at this density (always in the high-drive region), are extremely long-lived structures, since only the particle at the tip of the line can move without violating the exclusion constraint. The particles at the tips of the diagonal are blocked by others, giving a virtually infinite lifetime to this structure.

Of note are the large number of voids and diagonal strings of particles in the high-bias region of Fig. 6. This hints at the possibility that the entire jammed structure is induced by the drive in the early stages of the evolution. To verify this conjecture, we show in Fig. 7 the distribution of $\Delta y$-displacements (averaged over all particles), during thermalization, for four different global densities. The slightly asymmetric curves are a signature of the accumulation of particles in the low-bias region; they have a higher probability to migrate downwards than upwards. For densities below 0.31, and above 0.34, no asymmetry can be detected in the curves for $f(\Delta y)$. The distribution narrows sharply with increasing global density, so that for most particles only small $y$-displacements are possible.

To study correlations between the particles, we determine the radial distribution function, $g(r)$ in the high- and low-drive regions (Fig. 8). This function is proportional to the probability of finding a pair of particles separated by a distance $r$, and is normalized so that $g \rightarrow 1$ as $r \rightarrow \infty$. For purposes of determining $g(r)$, the low-drive region is taken as the strip $6 \leq y \leq 14$, while the high-drive region comprises $86 \leq y \leq 94$.

The $g(r)$ curves for global density $\rho = 0.31$ show that the high- and low-drive structures
FIG. 8: Pair distribution function for the high- and low-drive regions, for densities $\rho = 0.31$ and $\rho = 0.35$.

are markedly different. In the low-bias region the peaks are much larger due to the sublattice ordering associated with packing of particles (as evidenced by the configuration in Fig. 5), and is compatible with the existence of long-range order. The high-drive region shows little structure; the oscillations in $g(r)$ decay rapidly with distance. The picture for $\rho = 0.35$ is quite different. The sharpness of the peaks in the curve for $\rho = 0.35$ in the high-bias region reflects the very different sublattice densities, as does the fact that $g \simeq 0$ for $r = 3, \sqrt{13}$ and $\sqrt{17}$. The radial distribution function in the low-drive region, for this density, exhibits less structure, indicating the more equal sublattice occupancies.

D. Boundary effects

The density profiles of Fig. 3 show that particles tend to accumulate in the layers in contact with the rigid walls ($y = 1$ and $y = L$). This accumulation is due to excluded volume effects [17] that entropically favor enhanced densities at rigid surfaces. (A certain fraction of the volume excluded by the particles in these layers overlaps with the volume excluded by the wall, thereby leaving more space for the remaining particles.) The effect of this accumulation shows up in the current profile (Fig. 4), as a sharp peak at $y = L$. Although the number of particles is larger in these layers, it is not yet enough to provoke a jammed structure, therefore allowing a high current. At higher global densities, the number of particles is large enough for them to block the way and there is no current at all near the boundary at $y = L$. 

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FIG. 9: Stationary density profile under the symmetric drive profile, Eq. (2). The curve with a central minimum corresponds to $\rho = 0.30$. The others are for densities (from bottom to top): $\rho = 0.31, 0.32, 0.33, 0.34, 0.35$. The last five curves were shifted upwards by: 0.1, 0.08, 0.06, 0.04 and 0.02, respectively.

The question naturally arises as to whether the surprising changes in the density and current profiles (as functions of global density), described above, are somehow induced by the rigid walls at $y = 1$ and $y = L$. To see that this is not the case, we show in Figs. 9 and 10 the density and current profiles in the system with a symmetric drive profile, Eq. (2), and periodic boundaries in the $y$ direction. We find that for $\rho \leq 0.30$, particles are concentrated the low-drive region, just as in the system with rigid walls. Above this density the pattern changes to one in which they concentrate in the high-drive region. As we increase the number of particles, they continue to accumulate in this region, and the local density in the low-drive region is smaller than observed at a global density of 0.30 (up to $\rho = 0.34$). Interestingly, around the position of maximum bias, the local density decreases in a region of approximately 15 lattice spacings. This suggests the presence of diagonal voids that prevent homogenization of the lattice. These structures become more evident with increasing density, but not as dramatically as in the presence of walls.

The behavior of the current parallels these trends, just as in the studies with rigid walls. For densities up to $\rho = 0.30$ the current profiles display a peak in the high-drive region. Increasing the value of $\rho$ beyond this point dramatically changes the profile. The peaks are now located in the region of intermediate drive strength, and the current in the maximum-bias region falls to zero. As before, the peaks decrease in amplitude and shift towards the
FIG. 10: Average stationary current profile for a system subjected to the drive of Eq. (2). The single peaked curve is for $\rho = 0.30$. The others are for the same densities as in fig. 9 (from top to bottom). The curves for $\rho = 0.31$ to $0.35$ were shifted by $0.01, 0.008, 0.006, 0.004$ and $0.002$.

low-drive region as we increase the density. The same explanation as before holds: as the density is increased more and more particles accumulate near the central region, therefore narrowing the window where particles are mobile (while decreasing the effective number of mobile carriers). Thus rigid wall are not the cause of the reversals observed in the density and current profiles.

IV. CONCLUSIONS

We studied a lattice gas with nearest-neighbor exclusion driven by a nonuniform, shear-like drive, on the square lattice, under nearest-neighbor hopping dynamics. The problem is of interest both as an example of the surprising behavior to be found in a simple nonequilibrium system, and as a toy model for a granular or colloidal system under shear. We find that the model undergoes a continuous order-disorder transition at a critical density of about $\rho_c = 0.298$. This is unlike the uniformly driven model, in which the transition is discontinuous for a bias $\geq 0.75$. The stationary current follows roughly the same trends as in the uniformly driven case, but exhibits a plateau in the neighborhood of the phase transition.

Our results show that this transition is due to the concentration of particles at the low-bias region, for global densities between $\rho = 0.30$ and $0.32$. Remarkably, the nonuniform drive induces a highly nonuniform density profile, expelling particles from the high-bias region. The effect is sufficiently strong to induce sublattice ordering in the low-bias region.
Thus the drive favors a class of configurations that, on the basis of entropy maximization, are extremely unlikely. Note that at these densities there is no jamming, i.e., the system is ergodic. Migration of particles to the low-bias region appears to derive from the destruction of short-range correlations (required for efficient packing), by the drive.

For higher densities, we observe a completely inverted picture, with formation of jammed structures in the high-drive region, while particles outside this region remain mobile. The jammed region is characterized by a dense ($\rho \geq 0.37$) strip of particles; at higher global densities this region displays long diagonal chains of particles associated with voids.

Preliminary studies show that the above-mentioned effects also appear if half the system has no bias while the remainder is subject to maximum bias [19].

The jammed diagonal structures appearing at high density may be seen as an instance of force chains in granular systems [18]. By applying a shear drive to a packing of grains, interparticle contacts are built, leading to the formation of chain structures that carry the interparticle forces, which sustain further stress in that direction. In experiments, the system yields under a sufficiently large stress, breaking the chains. Since in our model the interparticle interactions are infinite, so is the yield stress. Therefore, as long as the drive is applied, we observe such ideal force chains. For a system in which the density varies while the drive is on, such force chains can arise at much lower densities [19].

A thermal system composed of particles that have highly repulsive interactions, albeit not infinite ones, is a colloidal suspension. In fact, the experiments of Bertrand et al. [20] show a similar effect to the slow relaxation observed here. They studied suspensions at several densities under the influence of shear. The suspension presents shear-thickening at intermediate densities, where a small vibration drives the system back to a fluid state. At higher densities, after shear is applied, the suspension forms a paste, becoming trapped in this jammed state. In our case, thermal motion, or vibration, is always present, as well as shear, so we do not observe the breakdown of the jammed state at intermediary densities, but a slow relaxation towards a denser state. In a granular system, which is, by definition, athermal, effects analogous to those of thermal agitation can be produced by shaking. This raises the possibility that the behavior identified in the sheared lattice gas might also be observed in a sheared packing if, besides the shear drive, continuous shaking were applied to the grains. This suggests that the model studied here can be extended to study the dynamics of certain complex fluids, a subject we intend to explore in future work.
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