Lattice versus Lennard-Jones models with a net particle flow

M. Díez-Minguito[1,2], P. L. Garrido[1,2], and J. Marro[1,2]

[1] Institute 'Carlos I' for Theoretical and Computational Physics
[2] Departamento de Electromagnetismo y Física de la Materia, Universidad de Granada, E-18071 - Granada, Spain

Abstract. We present several lattice and off-lattice microscopic models in which particles interact via a local anisotropic rule. The rule, which varies from one model to the other, induces preferential hopping along one direction, so that a net current sets in if allowed by boundary conditions. This may be viewed as an oversimplification of the situation concerning certain traffic and flow problems. The emphasis in our contribution will be on the influence of dynamic details on the resulting (non-equilibrium) steady state. In particular, we shall discuss on the similarities and differences between a lattice model and its continuous counterpart, namely, a Lennard–Jones analogue in which the particles' coordinates vary continuously. Our study, which involves a large series of computer simulations, in particular reveals that spatial discretization will often modify the resulting morphological properties and induce a different phase diagram (even criticality).

1 Introduction

Many physical systems out of equilibrium show up spatial striped patterns [1,2] at a macroscopic scale. In most of such systems this patterns are caused by a transport of matter, charge, or some other quantity induced by the presence of a drive, which leads the system into the heterogeneous ordering. Examples where such phenomena may occur include flowing fluids [3], and during phase separation in colloidal [4], granular [5,6], and liquid–liquid [7] mixtures. Further examples are wind ripples formed in sand [8] and the trails by animals and pedestrians [9]. Similar anisotropies also occur in high temperature superconductors [10,11], and in two–dimensional electron gases [12,13].

Studies of such instabilities, frequently described as nonequilibrium phase transitions, have focused on lattice systems [14–20], which are based in discretization of space into lattice sites, consider particles interacting via simple rules. Its simplicity sometimes allows exact calculations and are easier to be implemented in a computer. Moreover, many techniques has been developed and improved under its shadow, including nonequilibrium statistical field theory. However, lattice models are, in a sense, an oversimplification of real systems. Therefore the robustness of its behavior has to be studied carefully.

The present contribution involves Monte Carlo (MC) simulations and field theory calculations focused on how slight modifications on the dynamics at a microscopic level may influence on the resulting nonequilibrium steady state

—with special emphasis in criticality—. For this purpose we study the *driven lattice gas* (DLG) [14,15], a kinetic Ising model with conserved dynamic. This, initially proposed as a model for ionic currents, has become a prototypical model for anisotropic behavior. Here we compare its transport and critical properties with *analogue* lattice and off–lattice models. The literature offers works addressing the issue of how minor variations in the dynamics may lead to dramatic morphological changes in the early time kinetics [21] and in the stationary state [22,23]. However, this works unfortunatelly do not focus on transport and, to a lesser extent, critical properties. By concreteness we explore the robustness of those features of the DLG when extending interactions from nearest–neighbors (NN) to next–nearest–neighbors (NNN) [22].

Furthermore, we try to answer the question of how the lattice itself may condition transport, structural, and critical properties. That is, in this work we also annalize a microscopically off–lattice representation of the DLG in which the particles' spatial coordinates vary continuously. The clue is that spatial discretization changes significantly not only some morphological and early–time kinetics properties, but also critical properties, which are known to be independent of such dynamic details in equilibrium.

2 Driven Lattice Gas

The *driven lattice gas* (DLG), initially proposed by Katz, Lebowitz, and Spohn [24], is a nonequilibrium extension of the Ising model with conserved dynamics. The DLG consists of a d-dimensional square lattice gas in which pair particles interact via an attractive and short–range Ising–like Hamiltonian $H = -4\sum_{NN}\sigma_j\sigma_k$, where $\sigma_k = 0(1)$ is the lattice occupation number at site k if empty (occupied), and the sum runs over all particles and the NN sites (the accesible sites are depicted in Fig. 1). The dynamic is induced by a heat bath at temperature T and by an external driving field E which favors particle hops along one of the principal lattice directions, say horizontal ($\hat{x}$), assuming the particles are positively charged. Consequently, for periodic boundary conditions, a

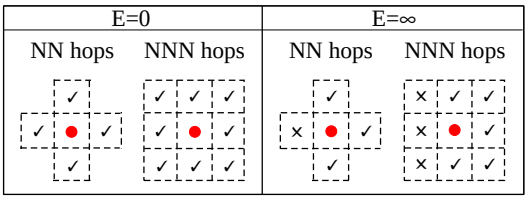

Fig. 1. Schematic comparison of the accessible sites a particle (at the center, marked with a dot) has for nearest–neighbors (NN) and next–nearest–neighbors (NNN) hops at equilibrium (left) and in the presence of a large horizontal field (right). The particle–hole exchange between neighbors may be forbidden (×) or allowed (√) depending on the strength of the field E.

nontrivial nonequilibrium steady state is reached in the system. MC simulations by using a biased *Metropolis* rate reveals that, as its equilibrium counterpart, the DLG undergoes a second order phase transition. At high temperatures the system is in a disordered state, while below its critical point (at $T < T_E$) it orders displaying anisotropic phase segregation. That is, a rich particle phase which is striped then coexists with its gas. It is also found that the critical temperature T_E monotonically increases with E. More specifically, assuming henceforth a half filled $L \times L$ square lattice in the large field limit (in order to maximize the nonequilibrium effects), $T_\infty \simeq 1.4T_0$, where the equilibrium value is $T_0 = T_{Onsager} = 2.269Jk_B^{-1}$. This limit corresponds to a *nonequilibrium* critical point. As a matter of fact, it was numerically shown to belong to a universality class other than the Onsager one, e.g., MC data indicates that the order parameter critical exponent $\beta_{DLG} \simeq 1/3$ (instead of the Ising value $\beta_{Ising} = 1/8$ in two dimensions) [14,25,26].

Other important feature may concern two particle correlation function $C(x, y)$ and its Fourier transform $S(k_x, k_y)$. As is depicted in the left graph of Fig. 2 correlations are favored (inhibited) along (against) the field direction. In fact the DLG shows a slow decay of the two–point correlations due to the spatial anisotropy associated with the dynamics [27,28]. This long range behavior translates into a characteristic discontinuity singularity at the origin ($\lim_{k_x \to 0} S_\parallel \neq \lim_{k_y \to 0} S_\perp$,) in the structure factor [15], clearly confirmed in Fig. 2.

How does all these features depend on the number of neighbors? Or in other words, while the DLG shows these peculiarities, it is natural to ask how robust is its behavior when extending interactions and accesible sites to the NNN. We wonder to what extent this slight extension in the microscopic dynamics may influence, in particular, the transport and critical properties.

Precedent works have shown that this extension in the DLG dynamics may lead to an inversion of triangular anisotropies during the formation of clusters which finally condense into strips [21]; and also dramatic changes appear in

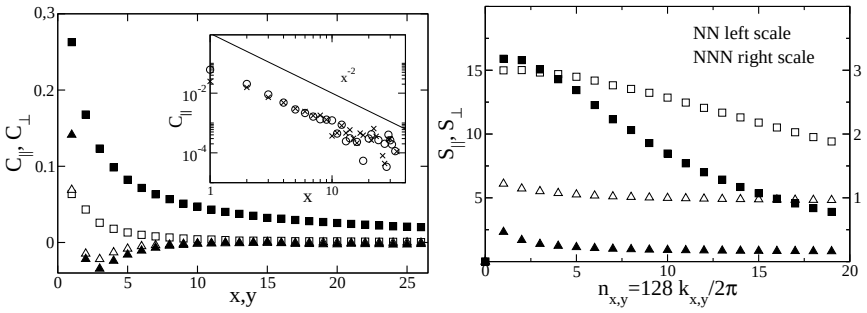

Fig. 2. Parallel (squares) and transverse (triangles) components of the two–point correlation function (left) and the structure factor (right) above criticality with NN (filled symbols) and NNN (empty symbols) interactions for a 128×128 half filled lattice. The inset shows the x^{-2} power law decay in $C_\parallel$ for both discrete dynamics.

the steady state, where contrary to the DLG with NN interactions the critical temperature decreases with increasing E [22]. However, important features as correlations and criticality remain invariant.

One one hand, analysis of the parallel ($C_{\parallel}$) and transverse ($C_{\perp}$) to the field component reveals that correlations are quantitatively similar for the DLG and for the DLG with NNN interactions (henceforth NDLG) —although somehow weaker for the NDLG. Also persists a slow decay of correlations which lead to the discontinuity at the origin in $S(k_x, k_y)$. These facts are also shown in Fig. 2. On the other hand, recent MC simulations on the NDLG confirm that the order parameter critical exponent still is $\beta_{NDLG} \approx 1/3$ [29]. The *anisotropic diffusive system* approach [30], which is a Langevin–type (mesoscopic) description, corroborates this critical behavior. In both cases the Langevin equations are derived from a coarse graining of the master equation, and lead to the above–indicated MC critical exponent. Both equations are similar, except that for the NNN case appear new entropic terms due to the presence of additional neighbors [29]. Therefore, the fact of extending particle hops and interaction to the diagonal sites modify neither correlations nor criticality, infering from this that both systems belong to the same universality class.

In this point we take the problem of robustness a step further. At what extent DLG behavior depends on the lattice? With this aim, here we present a description of driven systems with continuous variation of the particles' spatial coordinates —instead of the discrete variations in the DLG. We analyze an off–lattice representation of the DLG, namely, a microscopically continuum with the same symmetries and short–range interaction.

3 Driven Off-lattice Gas

Consider a *fluid* comprised by N interacting particles of mass m confined in a two–dimensional box of size $L \times L$ with periodic (toroidal) boundary conditions. The particles interact via a truncated and shifted Lennard–Jones (LJ) pair potential [32]:

$$\phi(r) \equiv \begin{cases} \phi_{LJ}(r) - \phi_{LJ}(r_c), & if\ r < r_c \\ 0, & if\ r \geq r_c, \end{cases} \tag{1}$$

where $\phi_{LJ}(r) = 4\epsilon \left[(\sigma/r)^{12} - (\sigma/r)^{6}\right]$ is the LJ potential, r is the interparticle distance, and r_c is the *cut-off* which we shall set at $r_c = 2.5\sigma$. The parameters σ and ϵ are, respectively, the characteristic length and energy. For simulations all the quantities were reduced according to ϵ and σ, and k_B and m are taken as unity. The choice of this potential (the widely used truncated and shifted LJ potential is one of the multiple possibilities for an attractive short–range potential) obeys to our strategy to set up the model following as close as possible the DLG.

The uniform in space and time external driving field E is implemented by assuming a preferential hopping in the horizontal direction. This favors particle jumps in the field direction, assuming the particles are positive charged (see dynamic details in Fig. 3). As defined in its lattice counterpart, we consider the

large field limit $E \to \infty$. As the stregth of the field is increased one eventually reaches saturation at $E = \infty$ and particles cannot jump against the field. This picture may be formalized in terms of the transition probability per unit time (*rate*), which reads

$$\omega(\eta \to \eta'; E, T) = s(\eta \to \eta'; E) \cdot \min\{1, exp(-\Delta\Phi/T)\}\,. \tag{2}$$

Here, a configuration at a given time is specified by $\eta \equiv \{\mathbf{r_1}, ..., \mathbf{r_N}\}$, where $\mathbf{r_i}$ is the position of the particle i, that can move anywhere in the torus. $\Phi(\eta) = \sum_{i<j} \phi(|\mathbf{r_i} - \mathbf{r_j}|)$ stands for the energy of a configuration η. The biased hopping enters in $s^{(E)}(\eta \to \eta') = \frac{1}{2}(1 + \tanh(E \cdot \delta))$, which is asymmetric under $\eta \leftrightarrow \eta'$; and $\delta = (x_i' - x_i)$ is the displacement corresponding to a single MC trial move along the field direction, which generates the subsequent increment of energy $\Delta\Phi = (\Phi(\eta') - \Phi(\eta))$. This *rate* in conjunction with the toroidal conditions violates detailed balance. It is only recovered in the absence of the driving field. In this limit the *rate* reduces to the Metropolis one and the system corresponds to the largely studied *truncated and shifted two–dimensional LJ fluid* [31,32]. Since the lattice has been removed altogether, the particle hop has to be defined carefully because the resulting steady state may depend qualitatively on this. Then, a trial move concerning any particle will satisfy that $0 < |\mathbf{r_i'} - \mathbf{r_i}| < \delta_{max}$, where δ_{max} is the maximum displacement in the radial direction (fixed at $\delta_{max} = 0.5$ in our simulations). The choice of δ_{max} differ substantially from equilibrium where how the particle move is defined is irrelevant as dictated by the detailed balance condition. In this point, we also emphasize the difference between our (nonequilibrium) model and an equilibrium system with anisotropic interactions.

MC simulations using the *rate* defined in Eq. (2) shows that the system displays highly anisotropic states below its critical point (T_∞, ρ_∞). A straight interface forms between a high density phase and its vapor: a single strip with

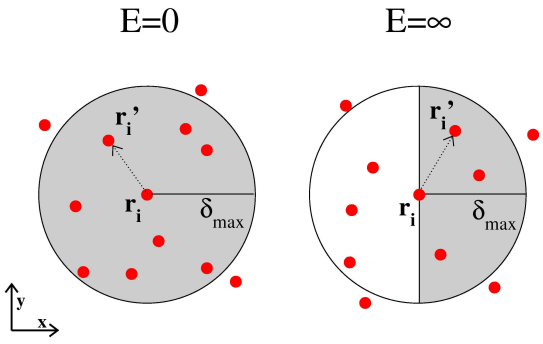

Fig. 3. Schematic representation of the accessible (shaded) region for a particle (dots) trial move at equilibrium (left) and out-of-equilibrium (right) assuming the field pointing along the horizontal direction ($\hat{x}$).

high density extending along $\hat{x}$ throughout the system separates from a lower density phase (vapor). As expected, the phase behavior is much richer (more complex structures yield to new phases) than its lattice analogue. The local structure of the anisotropic condensate changes from a strictly hexagonal packing of particles at low temperature (below $T = 0.10$), to a polycrystalline–like structure with groups of defects and vacancies which show a varied morphology (e.g., at $T = 0.12$), to a fluid–like structure (e.g., at $T = 0.30$,) and, finally, to a disordered state as the temperature is increased further. Then, skipping the microscopic structural details, the stationary striped state is similar to the lattice models.

Worthy of comparison between the off–lattice and lattice models are the transport properties. In the inset of Fig. 4 is shown the net current j upon the temperature. Saturation is only reached at $j_{max} = 4\delta_{max}/3\pi$ when $T \to \infty$. The sudden rising of the current as T is increased can be interpreted as a transition from a poor conductor (low temperature) phase to a rich conductor (high temperature) phase, which is reminiscent of ionic currents [14]. Revealing the persistence of correlations the current is nonzero for any low T, though very small in the solid–like. Additionally from the temperature dependence of j may be estimated the transitions points between the different phases (not shown), in particular, when the condensed strip changes from solid to liquid ($T \approx 0.15$) and when finally change to a fully disordered state ($T \approx 0.31$). These aspects of the current are also present in the DLG.

Due to the inhomogeneous ordering that the system exhibits, the current is sensitive to the anisotropy. The most relevant information is carried by the transverse to the field current profile $j_\perp$, which show up the differences between these two coexisting phases. Computing the transverse current profile $j_\perp$ allows us to characterize the strip state in terms of two coexisting phases (shown in

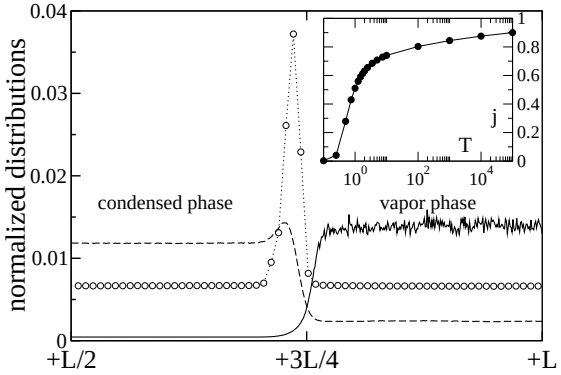

Fig. 4. Transverse to the field stationary transport distributions below criticality. The shaded (full) line corresponds to the current (velocity) profile of the off–lattice model. For comparison is also shown the current profile of the DLG with NN interactions. The inset shows the temperature dependence of the current for the driven LJ fluid.

Fig. 4). That is, a high current (or low mean velocity) phase coexists below the critical temperature with its mirror phase of low current (or high mean velocity). Above criticality, where the system is homogeneous the profile is in average flat.

The first order phase separation is clearly depicted in the current profile of Fig. 4. The current and the density vary in a strongly correlated manner: the high current phase fits with the high density phase (liquid or solid), whereas the low current phase phase matches the low density (vapor) phase. This is due to the fact that there are many carriers in the condensed phase and they yield to a higher current than in the vapor phase. However, the mobility of the carriers is much larger in the vapor phase (also depicted in Fig. 4). The maximal current appears in the interface (identifiable by the peak in Fig. 4), in which there are still a considerable amount of carriers but they are less bounded than in the particles well inside the *bulk*, and, therefore, the field drives easily those particles. This interfacial effect is more prominent in the lattice models (notice the large peak in the current profile in Fig. 4). Moreover in the lattice case there is no difference between the current displayed in the rich and poor particle phases because the particle–hole symmetry.

A main issue is the (nonequilibrium) liquid–vapor coexistence curve and the associated critical behavior. The coexistence curve may be determined from the density profile transverse to the field. This is illustrated in Fig. 5. At high enough temperature above the critical temperature the local density is roughly constant around the mean system density ($\rho = 0.35$ in Fig. 5). As T is lowered, the profile accurately describes the striped coexisting phases of density ρ_+ which coexists with its vapor of density ρ_- ($\rho_- \leq \rho_+$). The interface becomes thinner and less rough, and ρ_+ increases while ρ_- decreases, as T is decreased. As in equilibrium, one may use the difference of coexisting densities $\rho_+ - \rho_-$ as an order parameter. The result of plotting ρ_+ and ρ_- at each temperature (thus adapting the method

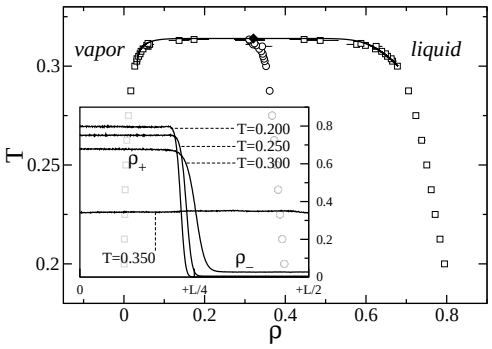

Fig. 5. Temperature–density phase diagram. The coexistence curve has been obtained from the density profile transverse to the field, shown in the inset for $N = 7000$, $\rho = 0.35$, and different temperatures. The circles are the arithmetic mean points useful to compute the critical parameters. The line is the non–linear fit using the Wegner expansion and the rectilinear diameter law with the obtained parameters.

in [33] for coexisting phases in equilibrium) is shown in Fig. 5. All the same behavior is obtained from the current (Fig. 4). It is worth notice that the estimate of the coexisting densities $\rho_{\pm}$ is favored by the existence of a linear interface, which is simpler here than in equilibrium. This is remarkable because we can therefore get closer to the critical point than in equilibrium. We also found that the rectilinear diameter law, $\frac{1}{2}(\rho_+ + \rho_-) = \rho_\infty + b_0(T_\infty - T)$, and the scaling law, (which is the first term of a Wegner expansion [34]) $\rho_+ - \rho_- = a_0(T_\infty - T)^\beta$, can be used here to estimate accurately the critical parameters. This is remarkable because these fits, which are extensively used in for fluids in equilibrium, have no justification out of equilibrium. The simulation data in Fig. 5 then yields $T_\infty = 0.314 \pm 0.001$, $\rho_\infty = 0.321 \pm 0.005$, and $\beta = 0.10 \pm 0.08$. These values are confirmed by the familiar log–log plots. Compared to the equilibrium case [31], $T_0/T_\infty \approx 1.46$. This confirms the intuitive observation above that the field acts in this system favoring disorder. On the other hand, our estimate for the order–parameter critical exponent is fully consistent with both the extremely flat coexistence curve which characterizes the equilibrium two–dimensional LJ fluids and the equilibrium Ising value, $\beta = 1/8$ (non–mean–field value). Although the error bar is large, one may discard with confidence the DLG value $\beta \approx 1/3$ as well as the mean field value. This result is striking because our model *seems* to have the symmetries and short–range interactions of the DLG. Further understanding for this difference will come from the statistical field theories, but the present state of the theory does not enable us to determine theoretically the critical exponent for this off–lattice model.

4 Final Comments

The main reason for this disagreement between the lattice and off–lattice limits may be the particle–hole symmetry violation in the driven LJ fluid. However, to determine exactly this statement will require further study. Nevertheless, this important difference between the lattice and the off–lattice cases is a unquestionable nonequilibrium effect because, as is well known in equilibrium critical phenomena, this microscopic detail is irrelevant for determine the universality class. Therefore, concerning criticality, the modeling of complex systems out of equilibrium is a more subtle task and will require a carefully study.

In summary, the present non–equilibrium LJ model in which particles are subject to a constant driving field can be a (very computationally convenient) prototypical model for anisotropic behavior in nature. This off–lattice model reduces to the familiar LJ case for zero field. Otherwise, it exhibits some arresting behavior, including currents and striped patterns as its lattice counterpart. Surprisingly, its critical behavior is consistent with the Ising one for $d = 2$ but not with the critical behavior of the DLG. This is puzzling in the context of statistical field theory given that symmetries seem to bring our system closer to the DLG than to the equilibrium Ising model. The additional freedom of the off–lattice case is likely to matter more than suggested by some naive intuition.

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