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On the similarities and differences between lattice and off–lattice models of driven fluids

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Abstract

Microscopic modeling of complex systems by cellular automata, which deal with particles at lattice sites interacting via simple local rules, involves some arbitrariness besides a drastic simplification of nature. Here we briefly report on some recent work on the influence of dynamic details on the morphological and critical properties of one of such model systems. In particular, we discuss on the similarities and differences between a kinetic nonequilibrium Ising model —which is a prototype for nonequilibrium anisotropic phase transitions— and its off–lattice counterpart, namely, an analogue in which the spatial coordinates of the particles vary continuously. We also pay attention to a related driven lattice model with nearest-neighbor exclusion.

A sensible approach to the modeling of complex systems consist in investigating model systems that being as simple as possible, they capture the microscopic essentials of macroscopic ordering [1, 2]. These systems often consider space as discrete by allowing particles to be only at lattice sites. However, lattice models may involve some arbitrariness, a fact which is seldom pointed out, and they result too crude to be compared directly with experiment. As a matter of fact, they often do not account for important features of the relevant (nonequilibrium) phase diagram concerning structural and morphological properties. On the other hand, theoreticians often tend to consider them as prototypical models for critical behavior, a fact which is in some cases not justified.

This seems to be the case of the *Driven Lattice Gas* (DLG) [3]. This exhibits an anisotropic nonequilibrium phase transition which is of interest to theoreticians [2, 4]. However, it is unlikely that one may observe the model behavior in nature, at least as generally as it has been believed. The DLG is a kinetic Ising model with conserved dynamics in which particles diffuse at temperature T on a (generally two-dimensional) lattice under an external driving field E, and interact via an attractive and short–range Ising Hamiltonian

$$H = -J \sum_{\langle \mathbf{j},\mathbf{k} \rangle} \sigma_{\mathbf{j}} \sigma_{\mathbf{k}} \, . \tag{0.1}$$

Here, $J > 0$, $\sigma_{\mathbf{k}}$ is the lattice occupation number at site $\mathbf{k}$, and the sum runs over all the nearest-neighbor sites (connectivity 4). Each lattice site has two possible states, namely, a particle ($\sigma_{\mathbf{k}} = 1$) or a hole ($\sigma_{\mathbf{k}} = 0$) may occupy each site $\mathbf{k}$, and half–occupied lattices are assumed.

Monte Carlo (MC) simulations (using a biased *Metropolis* rate, namely, the transition probability per unit time is $\min\{1, exp[-(\Delta H + \mathbf{E} \cdot \delta)/T]\}$ where δ is the attempted displacement)

reveal that the DLG undergoes a second order phase transition. At high enough temperature T, the system is in a disordered state while, below a critical point at $T = T_E$ it orders displaying anisotropic phase segregation. That is, an anisotropic (strip-like) rich–particle phase then coexists with its gas. It is also found that the critical temperature T_E monotonically increases with E, which is counter-intuitive, and eventually saturates as $E \to \infty$ at $T_\infty \simeq 1.4\,T_0$, where the equilibrium value is $T_0 = 2.269 J^{-1}$. It is also known that this nonequilibrium critical point belongs to a universality class other than the Ising one, e.g., MC data indicates that the order parameter critical exponent is $\beta_{DLG} \simeq 1/3$ [2,5] instead of $\beta_{Ising} = 1/8$.

In order to study the influence of microscopic details on dynamics, and also trying to provide a realistic model for computer simulation of anisotropic fluids, we recently proposed an off-lattice analogue of the DLG [6,7]. This is a nonequilibrium model fluid with continuous variation of the particles' spatial coordinates —instead of the discrete variation in the DLG. In this case, the attractive and short–range interactions consists of *truncated and shifted* Lennard–Jones (LJ) $6-12$ potential [8]. We argued that the DLG behavior is not robust enough against such a *minor* modification of the dynamics, which sheds doubts on the practical relevance of the DLG. In the present contribution, we develop this argument based on extensive recent and new MC simulations; in particular, we focus now on the system interfacial properties.

Computer, MC simulations show that the off-lattice, LJ model closely resembles the DLG in that both depict a particle current, the corresponding anisotropic (striped) interface, and an order-disorder phase transition [7]. However, the two models differ in some essential features. The additional particle freedom in the continuous case gives rise to a much richer phase diagram. Concerning the phase segregation process, we observed in the off-lattice case the formation of triangular clusters after a rapid MC (subcritical) quench from an homogenous state pointing along the field direction [6]. This result —which has been involved in field–theoretical arguments concerning driven fluids— is contrary to the case in the discrete DLG, where the triangles point against the field direction (see also [9]). Once in the steady state, MC simulations show that, for any $E > 0$, typical configurations of the anisotropic condensed phase changes from a solid–like hexagonal packing of particles at low temperature —the whole phase orders according to a perfect hexagon with one of its main directions along the field direction— to a polycrystalline structure. The latter phase further transforms, with increasing temperature, into a fluid–like structure and, finally, into a disordered, gaseous state [7].

We now report on the fact that there are also some remarkable differences concerning the interfacial properties. In the continuum model, the current profile (perpendicular to the applied field) reveals that, above criticality, the current density in the condensed phase is higher than in its mirror phase. This was expectable due to the fact that there are many carriers in the condensed phase, which allows for a higher current than in the vapor phase. The maximal current occurs at the interface, where one observes a considerable amount of carriers less bounded than well inside the bulk and, therefore, the field drives particles more easily. However, this enhanced current effect along the interface is much more prominent in the DLG, where the conduction is mainly "interfacial". On the other hand, there is no difference between the current displayed by the coexisting phases because of the particle–hole symmetry (as a consequence of Eq. 0.1), which is absent in its off-lattice counterpart. In addition, except for some microscopic roughness, the interface in the DLG is linear and rather flat [10] whereas the roughness manifests itself in its continuum counterpart at a macroscopic level [12].

Interestingly enough, the continuum model exhibits a remarkable oscillatory instability — altogether absent in the DLG case— which is more evident at temperatures well below the critical point. The interface, which on the average parallels the field, increases its length forming periodic waves in order to maximize the particle transport. Such an interfacial oscillations are so strong that induce a cooperative motion even inside the bulk. This peculiar behavior is

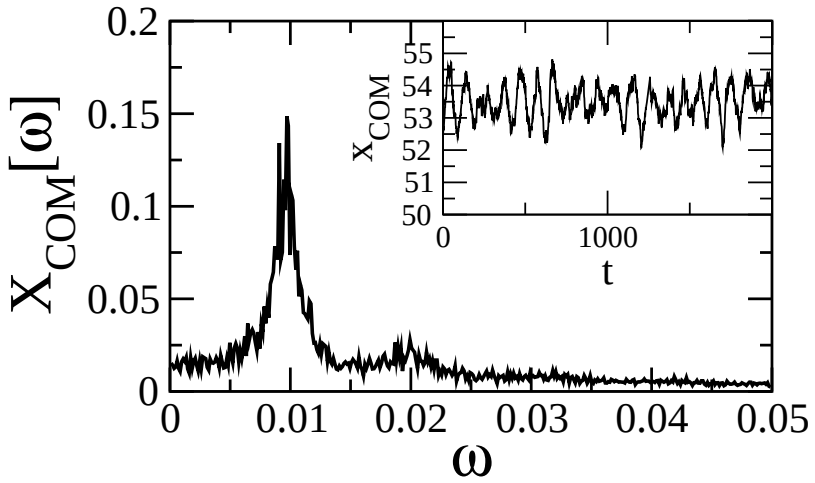

Fig. 1. Fourier Transform (main graph) of the trajectory of x_{COM} (inset) in the stationary regime for $N = 4000$, $\rho = N/L^2 = 0.35$ and $T = 0.1375$, given in LJ reduced units [8]. The spectrum was averaged over 10 independent runs, and data points of x_{COM} were sampled every 1000 MC *step*.

revealed by the time evolution of the position of the center of mass in the field direction (x_{COM}), and its Fourier transform ($X_{COM}[\omega]$). The well-defined oscillations of x_{COM} (see inset in Fig. 1) takes the form, translated into the momentum space, of a large peak (the first harmonic) in the spectrum (main graph in Fig. 1). We observe that the fundamental Fourier mode in $X_{COM}[\omega]$ increases with the temperature (due to the thermal noise) and decreases with the number of particles (because of the increase in the bulk inertia). Notice also in Fig. 1 the second harmonic. We are presently performing further analysis of these interfacial properties, which are important for microfluids [11], and will be the subject of a separate report [12].

Regarding criticality, additional, crucial differences between both cases arise. A main observation noticed before in MC simulations is that, contrary to the DLG case, for which the critical temperature T_E increases with E, the off-lattice case shows a decreasing T_E with increasing E. This confirms that the field acts in the non–equilibrium LJ system favoring disorder. Moreover, a detailed analysis of the MC data for the coexistence curve shows that the order parameter critical exponent (in the large field limit, i.e., $E \to \infty$) is $\beta \approx 0.10(8)$ [7]. That is, the critical behavior is consistent with the Ising universality class, and neither with the critical behavior of the DLG [2, 5] nor with the mean field class.This important difference between the lattice and off-lattice cases also occurs in other related models. For instance, Szolnoki and Szabó [13] showed, in an antiferromagnetic version of the DLG ($J < 0$ in Eq. 0.1), that assuming nearest-neighbor interactions under a driving field [14] and extending the dynamics to next-nearest-neighbor hops (connectivity 8 in a squared lattice), the order–disorder transition which the model undergoes becomes second order for all drive, and belongs to the Ising universality class. Furthermore, if one allows the spatial coordinates of the particles to vary continuously, then the model reduces to a *hard-disks* gas under a driving field [12], and the second order phase transition vanishes. The transition becomes similar to the melting transition for systems in equilibrium, which is described by the so-called KTHNY scenario [15].

Summing up, we remark that an increase in the spatial degrees of freedom of the particles tends to make these (nonequilibrium) driven models to exhibit Ising-like critical behavior. This fact is rather surprising, and merits further study. As a matter of fact, simple familiar

arguments concerning symmetries would rather suggest that these models criticality should differ from the corresponding equilibrium case. This is a new specific evidence that the question of what are the most relevant symmetries which determine the universal properties in driven diffusive systems is still open. More generally, the fact that microscopic details are irrelevant for universality concerning equilibrium critical phenomena cannot be simply extrapolated to the nonequilibrium case. On the other hand, our observations above altogether suggest the exceptionality of the DLG due to the fact that its behavior is highly conditioned by the lattice geometry, i.e., associated with the fact that the drive on a particle is essentially conditioned by the fact that it may find another particle in its way. This may be relevant for certain situations of restricted traffic, but it does not seem realistic for most conditions in the physics of matter.

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