

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

M. Díez-Minguito, J. Marro, and P.L. Garrido

Institute “Carlos I” for Theoretical and Computational Physics, and Departamento de Electromagnetismo y Física de la Materia, Universidad de Granada, 18071 Granada, Spain

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

$$H = -J \sum_{\langle j, \mathbf{k} \rangle} \sigma_j \sigma_{\mathbf{k}} . \quad (0.1)$$

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