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A brief comment on the modeling of flow

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Abstract

Particle-interacting models that exhibit currents, namely, lattice gases and Lennard–Jones systems with a biased hopping of particles, which mimic features of traffic and anisotropic phase segregation in simple fluids and mixtures, are compared with each other. The aim is better understanding important issues concerning theoretical and computer simulation studies of (nonequilibrium, anisotropic) particle flow. © 2008 Elsevier B.V. All rights reserved.

Keywords: Anisotropic phase transitions; Driven lattice gases; Lennard-Jones nonequilibrium fluids

1. Introduction

The constant flow of matter that characterizes a class of nonequilibrium steady states often manifests as observable welldefined stripes [1–4]. This has been reported associated to phase segregation in driven sheared systems [5–7], flowing fluids [8], shaken granular matter [9,10], nonequilibrium liquid–liquid binary mixtures [11], and it has also been reproduced by computer simulations in models of driven colloids [12,13] and fluids [4, 14–17], for instance. Further examples that share some of the relevant physics are the electric charge anisotropy in conductors [18–22], the ripples shaped by the wind in sand deserts [23,24] the transport of colloidal particles through potential wells [25, 26], and the trails and lanes formed by living organisms and vehicle traffic [27,28].

The so-called *driven lattice gas* (DLG1) [29] has served as *toy model* and ideal theoretical prototype for these anisotropic conditions during more than two decades now. In fact, this model raises a number of intriguing questions and it has been the object of many computer simulations and field theoretical studies [4,30–34]. These analyses have revealed, in particular, that the DLG1 exhibits some counterintuitive behavior and that it involves certain features that, one may argue, are hardly realistic. These facts seem to question altogether the role of the DLG1 as a prime example, and urge one to compare it with related systems. This paper reviews some recent attempts along

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these lines thus deepening on the similarities and discrepancies between four models, namely, the DLG1, a simple lattice variation of this, and two off-lattice models set up as continuum analogs of the driven lattice gas. The comparison also indicates that versions of these models, which reduce to the familiar Lennard–Jones fluid model at equilibrium, may serve as a basis to perform extensive simulations concerning anisotropic phase segregation under drives and shear conditions [35]. The models here concern two dimensions. Their three-dimensional counterparts are undoubtedly a more realistic representation of nature. However, the conclusions in this paper are not essentially affected by this restriction which is dictated by the enormous computational effort would be needed to perform the comparison in three dimensions.

2. Definition of models

2.1. DLG1

The DLG1 consists of a rectangular lattice with configurations $\mathbf{n} = \{n_i\}$, where $n_i = 1$ or 0 is a variable at the lattice site i = 1, ..., N. The two possible states of the variable are to be interpreted as having either a *particle* (1) or a *hole* (0) at site *i* or, in a binary mixture interpretation, as having particles which belong to different species. As for the standard lattice gas [36], dynamics is a stochastic process at temperature *T* consisting of nearest-neighbor (NN) particle \rightarrow hole exchanges [4]. This conserves the particle density, $\rho = N^{-1} \sum_i n_i$, and depends on **n**. A distinguishing feature of the DLG1 is that exchanges

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Table 1

The particle, represented as a filled circle at the center of each graph, can jump to NN empty sites in the DLG1 and also to next NN empty sites in the DLG2. The allowed jumps are governed by the temperature in the absence of a field (E = 0) while, for $E \rightarrow \infty$, there are thermal jumps (T), forbidden jumps (×) and jumps governed only by the field (E)—which are always performed when attempted if the targeted site is empty

E = 0						$E \to \infty$					
DLG1			DLG2			DLG1			DLG2		
×	Т	×	Т	Т	Т	×	Т	х	×	Т	Ε
Т	•	Т	Т	•	Т	×	•	E	×	•	Ε
×	Т	×	Т	Т	Т	×	Т	×	×	Т	Ε

in one of the principal lattice directions, say \hat{x} , are favored. Therefore, assuming periodic (toroidal) boundary conditions, a net current of particles sets in along \hat{x} . This is accomplished in practice by defining a biased transition probability (per unit time) or rate, ω , which is chosen to reduce to the familiar Metropolis algorithm [4] in the absence of the bias, namely,

$$\omega(\mathbf{n} \to \mathbf{n}^*) = \min\{1, \exp[-T^{-1}(\Delta H + E\delta)]\}.$$
 (1)

Here, \mathbf{n}^* stands for configuration \mathbf{n} after jumping of a particle to an NN hole; $\Delta H = H(\mathbf{n}^*) - H(\mathbf{n})$ is the change in the potential *energy* function $H = -4J \sum_{NN} n_i n_j$ brought about by the jump; and units hereafter are such that both the coupling strength J and the Boltzmann constant are set to unity. One further assumes $\delta = (\mp 1, 0)$ for NN jumps along $\pm \hat{x}$ or along the transverse direction, say \hat{y} , respectively. Consistent with this, $\vec{E} = E\hat{x}$ may be interpreted as a field driving particles, e.g., an electric field if one assumes that particles are charged. In the binary alloy interpretation, dynamics consists of interchanges between particles of different species, one of them favored along \hat{x} . Of particular interest is the case of an *infinite* field, $E \to \infty$. For any finite T, this corresponds in practice to prevent the particles from jumping against the field direction, $-\hat{x}$.

2.2. DLG2

The DLG1 may be modified along several ways. A simple variation that interests here consists in allowing for jumps to both NN and next NN holes, i.e., not only along the two principal directions but also along the two diagonal directions [15]. The nature of the jumps in this case, to be denoted DLG2 in the following, is illustrated in Table 1.

2.3. DLJF1

The simplest continuum, off-lattice analog of the DLG1 consists of N point particles located at $\vec{r_i}$, i = 1, ..., N, within an $L \times L$ square with periodic boundary conditions [15]. Each configuration, $\mathbf{c} \equiv \{\vec{r_i}\}$, has a potential energy given by $\Theta(\mathbf{c}) = \sum_{\text{pairs}} \varphi(r)$, where the sum is over all pairs of particles, rstands for the relative distance, and interactions are according to a truncated and shifted Lennard–Jones potential, namely, $\varphi_{LJ}(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ [37]. This means that any two particles do not contribute to that energy, so that $\varphi(r) = 0$, when their separation is larger than a cut-off r_c , while otherwise (i.e., for $r < r_c$) they contribute $\varphi(r) = \varphi_{LJ}(r) - \varphi_{LJ}(r_c)$. The cutoff will be set $r_c = 2.5\sigma$, and the familiar reduced variables will be used for temperature, $T^* = T/\epsilon$, length, $L^* = L/\sigma$, and particle density, $\rho^* = \rho \sigma^2$. In order to have preferential hopping as close as possible to the one for the lattice above, it is assumed that the rate is given now by

$$\omega(\mathbf{c} \to \mathbf{c}^*) = \min\{1, \exp\left[-T^{-1}(\Delta \Theta + E\hat{x} \cdot \vec{\delta})\right]\},\tag{2}$$

where $\Delta \Theta = \Theta(\mathbf{c}^*) - \Theta(\mathbf{c})$ and $\vec{\delta} = \vec{r_i}^* - \vec{r_i}$ is the particle displacement attempted at each time step. Lacking a lattice, the field is the only source of anisotropy here, and any trial move should only be constrained by a maximum displacement in the radial direction. That is, $0 < |\vec{\delta}| < \Delta$, where $\Delta = 0.5\sigma$ in the simulations reported. The model, to be denoted DLJF1 hereafter, then reduces for $E \to 0$ to the Lennard–Jones fluid which is familiar from computer simulation studies of fluids at thermodynamic equilibrium [37,38].

2.4. DLJF2

This is not the only off-lattice analog one can think of. A simple alternative consists in assuming the same interactions as for the DLJF1 but modifying the rate ω . A convenient choice [16] is

$$\omega(\mathbf{c} \to \mathbf{c}^*) = \frac{1}{2} \left[1 + \tanh(E\hat{x} \cdot \vec{\delta}) \right] \min\{1, \exp(-T^{-1}\Delta\Theta)\},$$
(3)

where symbols have the same meaning as before. This nonequilibrium model is denoted DLJF2 hereafter. Note that a main difference with the previous one is that the field does not compete here with the potential energy, which makes the case $E \rightarrow \infty$ relevant, as will be discussed. This limit corresponds to sampling only half of the circle of radius δ (the half part in the direction of the field) when attempting the particle move, and not the whole circle as for E = 0.

3. Discussion of results

3.1. Morphology and growth of order

The stable ordered configurations of the DLG1 at low T consist of one stripe, to be interpreted as a liquid (rich-particle) phase of density $\rho_L(T)$. The gas (poor-particle) phase of density $\rho_G(T)$ fills the remainder of the system. Except for some microscopic roughness, the interface is linear and rather flat, in general. Typical computer evolutions (Fig. 1) begin with a completely disordered state to simulate the system at infinite temperature. It is then simulated a sudden quench and the subsequent time evolution. With this aim, one proceeds with rate (1) that involves the temperature T at which the system is quenched. The only relevant length during this evolution is the typical width of the stripe, which may be measured in several ways. Assuming that the stripes move transversely by monomer evaporation, the prediction for late times and large systems is that this length changes with time according to $\ell(t) \sim t^{1/3}$, which is accurately confirmed by the simulations [14].

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Fig. 1. Evolution with time of the DLG1 (left to right; first upper and then lower graphs) from a random configuration (not shown) for a half-filled lattice and low temperature, namely, $T = 0.6T_{\infty}$.



Fig. 2. Snapshots during the time evolution of the DLJF2 at T = 0.275 for $\rho = 0.35$ and $E \to \infty$ (upper series); stationary configurations for the same system as *T* is increased from 0.10 to 0.35 for $\rho = 0.30$ and $E \to \infty$ (medium series); and stationary configurations for the DLJF1 when E = 1 and *T* increases from 0.25 to 0.45 with $\rho = 0.36$ (lower series).



Fig. 3. Triangular anisotropies observed at early times for E = 1 at low T in computer simulations of the DLG1 (left), in a similar simulation of the DLJF1 (center), and a comparable situation obtained from a Langevin equation description (right). The field E points in any case to the right.

Both DLJ1 and DLJF2 behave practically in the same way under equivalent conditions, as illustrated in Fig. 2. It has also been determined in these continuum cases that the relevant length changes with time as $\ell(t) \sim t^{1/3}$ during the most part of the phase segregation process [16]. There is, however, an important difference concerning this matter. As shown in Fig. 3, and first noticed in Ref. [39] (see also [40]), the DLG1 essentially differs from the other cases in one significant detail. The fact that two identical microscopic rules, namely, (1) and (2), re-



Fig. 4. Schematic phase diagrams, namely, the transition temperature as a function of the field *E*, for three models discussed, as indicated. There is (anisotropic) order only below the curve for each case. Here, $T_0 = T_{\text{Onsager}}$ and 2.35 T_{Onsager} , respectively, for the DLG1 and DLG2, and 0.459 in reduced unit for both DLJF1 and DLJF2. The saturation variables are $T_{\infty} \simeq 1.4T_{\text{Onsager}}$ ($\rho_{\text{critic}} = 0.5$) and 0.314 ($\rho_{\text{critic}} = 0.321$), respectively, for the DLG1 and DLJF2.

sult in different macroscopic symmetry is a disquieting feature of the DLG1 because the Langevin description also coincides in this respect with the Lennard–Jones systems.

3.2. Phase diagram

The DLG1 exhibits a critical point for $E \to \infty$ at $\rho = \frac{1}{2}$ and $T = T_{\infty} \simeq 1.4 T_{\text{Onsager}}$, where $T_{\text{Onsager}} \approx 2.2691$ is the Onsager critical temperature. Detailed study of the Monte Carlo data reveals what seems to be novel critical behavior [32,33], e.g., the best fits to the order parameter index indicate that $\beta \simeq 1/3$. This is, in fact, another feature of the DLG1 which lacks a fully satisfactory theoretical explanation. The DLJF2 has been shown to have a critical point for $E \to \infty$ which is characterized by $T_{\infty}^* = 0.314$, $\rho_{\infty}^* = 0.321$ and $\beta \simeq 1/8$. The picture concerning nonequilibrium universality classes might become even more complex. In fact, some preliminary analysis [41] suggests that the DLG2 might show the same critical behavior of the order parameter (at E = 12 where $T_E \simeq 1.45T_{\text{Onsager}}$) as for the DLG1.

This is very remarkable at the light of the different trends exhibited by the models for the dependence with field of the ordering temperature, T_E , as illustrated in Fig. 4. This seems to confirm that something "goes wrong" with the DLG1. That is, the microscopic dynamics in this case, as it also occurs for the DLG2 and for the DLJF1-see Eqs. (1) and (2)-is such that the role of the potential energy, as measured by ΔH or $\Delta\Theta$, becomes negligible as $E \to \infty$. Therefore, the transition should be suppressed in the three cases for large enough values of the field, which occurs for the DLG2 and for the DLJF1 but not for the DLG1. The latter behaves in this sense like the DLJF2 that was designed to have a different behavior for large fields—compare Eq. (3) with Eq. (2). I have been informed [42] that the ordering transition T_E for a half-filled hexagonal lattice falls with increasing E. The DLG1, however, is again singular in this detail. The macroscopic singular behavior of the DLG1 should perhaps be associated with the only particularity it exhibits at the microscopic level, that is, the fact that a particle cannot follow the current unless the lattice site in front of it is empty. However, one should perhaps expect different critiJ. Marro / Computer Physics Communications 179 (2008) 144-149



Fig. 5. Typical time development of the transverse structure function for the models as computed for the DLG1. Time t is in Monte Carlo steps.

cal behavior then for the DLG2 than for the DLG1, which is against the present indications [41], as mentioned above.

3.3. Correlations

A deep understanding of many of these questions is often acquired by monitoring the nature of correlations. A measure of these, which can be accessed both theoretically and in some laboratories by scattering experiments, is the structure function or Fourier transform of the two-point correlation function. For a half-filled lattice this function is

$$C(\vec{r}) = \langle n_{\vec{R}} n_{\vec{R}+\vec{r}} \rangle - \frac{1}{4},$$
(4)

where $n_{\vec{r}}$ is the occupation variable at \vec{r} and the steady average $\langle \cdots \rangle$ involves also averaging over \vec{R} . The relevant structure function in these anisotropic cases, namely,

$$S(k_y;t) \sim \left|\sum_{\vec{r}} C(\vec{r};t) \exp(ik_y y)\right|^2$$
(5)

is shown in Fig. 5 for the DLG1 [14]. As expected, this shows a well-defined peak which grows with time (as the condensed phase becomes more compact) as it shifts towards smaller values of k_{y} (as the stripe width becomes larger).

The fact that, far enough from the critical point, the phase segregation process revealed by $S(k_y; t)$ involves a unique relevant length, $\ell(t)$, suggest one to assume that this function should only depend on time through $\ell(t)$. More specifically, one expects *self-affinity* as first described in equilibrium [43], namely, $S(k_y; t) \propto \ell(t) F[k_y \ell(t)]$ in the present case. This is nicely confirmed in Fig. 6 for the DLG1 [14], and one should expect a similar behavior for the other cases. The figure describes, as one moves towards the smaller values of κ , the consequence $Z \sim \kappa^{-3}$ of the Porod law reflecting the existence of (small) isotropic clusters forming the gas phase, the analogous to this but reflecting anisotropic clusters, which results in $Z \sim \kappa^{-2}$ behavior for larger distances, and the familiar Guinier Gaussian peak [45]

$$Z \sim \exp[-\text{const.}(\kappa - \kappa_{\text{max}})^2]. \tag{6}$$

More intriguing is the behavior of Z(x) for $\kappa < \kappa_{max}$. As the figure indicates, scaling does not hold well in this region even at



Fig. 6. The time-independent function $Z \equiv S(k_y; t)/\ell(t)L$ vs. $\kappa \equiv k_y \ell(t)/L$ for the DLG1, including data from 10⁴ to millions of MC steps.

the end of long enough simulations of the DLG1. This is due to the fact that $Z(\varkappa)$ goes as $\rho^2 L/\ell(t)$ at $k_y = 0$, so that it depends on time for very small values of κ . However, a detailed study of data reveals that the scaling function near the origin tends with time towards a common envelope $Z \sim \kappa^{1+1/3}$ at very large distances, say for $\kappa_0 < \kappa < \kappa_{max}$, which has not been explained yet. This behavior breaks down closer to the origin, $\varkappa \leq \varkappa_0$, where $Z(\kappa) \to 0$ as $\kappa \to 0$ for $t \to \infty$ in a macroscopic system.

On the other hand, the DLG1 is known to display (more clearly above criticality) slow decay of two-point correlations, $C(\vec{r})$, which is associated to the violation of the detailed balance condition for E > 0 [44]. Analysis of the components of this correlation function along the field, C(x, 0), and transverse to it, C(0, y) shows that correlations are qualitatively similar for both the DLG1 and the DLG2—although somewhat weaker along the field in the latter case. That is, allowing the particle more freedom to pass one in front of it, does not modify essentially the correlations. In particular, the power-law behavior translates into a discontinuity of $S(\vec{k})$ [44], namely,

$$\lim_{k_x \to 0} S(k_x, 0; t) \neq \lim_{k_y \to 0} S(0, k_y; t),$$
(7)

which is clearly confirmed by the data for both DLG systems.

4. Conclusion

The four models that I have compared here evolve after quenching towards thermodynamic equilibrium [46–55] for E = 0, while they tend to a nonequilibrium steady state for any E > 0. The system relaxation does not seem to be essentially influenced by this conceptual difference, however. For example, all the systems exhibit—independently of the existence or not of the bias—a unique relevant length far from criticality, which increases $\ell \sim t^a$ apparently due mainly to monomer events, and self-affinity of the structure function. The bias induces a striped condensed phase, and there is as well some minor though significant reflection in the scaling function of the underlying anisotropy for E > 0. The lattice and off-lattice models considered are also qualitatively similar to each other. Perhaps the only noticeable difference from this general point of view is that, in addition to show liquid and gas phases like the DLGs, the DLJF systems fall into a solid-like phase at low enough temperature.

Closer inspection has revealed important differences between the nonequilibrium cases, however. First, the field dependence of the ordering temperature T_E . This monotonically increases for the DLG1 but decreases when one permits diagonal jumps (DLG2) and when the particles are allowed any continuum position (DLJF1), and the transition disappears in these two cases for large fields. Furthermore, comparing critical points for $E \to \infty$, one has that $T_{\infty}/T_0 \simeq 1.4$ for the DLG1 but the opposite behavior for the DLJF2, namely, $T_0/T_{\infty} \simeq$ 1.46. Concerning critical indexes, one measures "rare" behavior, namely, that $\beta \simeq \frac{1}{3}$ for the DLG1 (and perhaps also for the DLG2), and one finds consistency with the equilibrium behavior $\beta = \frac{1}{8}$ for the DLJF2. I also mention that it was reported many years ago that $\beta \simeq \frac{1}{2}$ for an actual sheared fluid [5].

There is an important difference among the DLGs and the DLJFs from the microscopic point of view, namely, the one which exists in general between lattice and continuum descriptions. However, this is not enough to understand the observed macroscopic differences. For example, the DLG1 and the DLG2 have a qualitatively different phase diagram—including that the latter has no infinite-field critical point—in spite of the fact that their correlations have essentially the same nature. The fact that particles need to travel along the two main lattice directions seems at the origin of the singular DLG1 behavior and of some (but not all) of its properties. This geometric restriction is not a realistic feature of cooperative transport and, in fact, stripes form in nature without such microscopic limitation.

Summing up, the DLG1 merits further study in order to understand the intriguing questions posed above, but it should be replaced as the prototype for anisotropy. Several possible candidates have been described which look interesting, e.g., for computer studies such as simulation of sheared conditions [35]. This indication is not trivial, because the fact that the lattice gas is a useful simplification of a Lennard-Jones fluid does not translate readily to nonequilibrium. On the other hand, concerning the development of theory, it has emerged that correlations do not necessarily determine the phase diagram. It has also emerged that the microscopic details of transverse dynamics are probably more essential than believed, e.g., to distinguish theoretical descriptions for the DLG1 and the DLG2. Finally, it is worth mentioning that I just knew of an interesting alternative to the modeling of driven lattice gases which has a simple experimental realization ([56] and references therein).

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