Dynamic behavior of anisotropic non-equilibrium driving lattice gases.

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It is shown that intrinsically anisotropic non-equilibrium systems relax to a non-equilibrium stationary state. An anisotropic scaling ansatz was introduced for the dynamics, which is proposed and tested numerically. Relevant critical exponents can be evaluated self-consistently using both the short- and long-time dynamics frameworks. The obtained results allow us to clarify a long-standing controversy about the theoretical description, the universality and the origin of the anisotropy of driven diffusive systems, showing that the standard field theory does not hold and supporting a recently proposed alternative theory.

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The development of a theoretical framework for the study of non-equilibrium systems is of vital importance for a wide range of disciplines in both science and technology. In order to overcome such a difficult problem, it is useful to study models capable of capturing the essential physical features of the real system. The statistical mechanics of interacting lattice gases, driven into nonequilibrium steady states (NESS) by external fields, has attracted growing attention. Some remarkable characteristics of the NESS observed in driven diffusive systems are, among others, their non-Hamiltonian nature, the violation of the fluctuation dissipation theorem and the fact that the steady-state distribution is determined by the dynamics.

The prototypical DDS has early been proposed by Katz, Lebowitz and Spohn (KLS) as a generalization of the Ising model. Then, the KLS model is a kinetic Ising model with conserved dynamics. Using the lattice gas language, particle hopping in the direction parallel to the applied drive is favored (unfavored), while jumps perpendicular to the field are unaffected by it. For half-filled lattices and high enough temperatures the KLS model exhibits a disordered phase. However, at low temperatures an anisotropic ordered NESS emerges and is characterized by strips of high particle density crossing the lattice in the direction parallel to the applied drive. So, at some critical temperature (T_c) the KLS model undergoes a second-order non-equilibrium phase transition. The issue of the universality class of the KLS model is of general interest because it will contribute to the rationalization of non-equilibrium critical phenomena. However, this task is elusive and has become the subject of a long-standing debate. A detailed discussion of such conceptually rich debate is beyond the aim of this work. Instead, we will briefly comment their theoretical and numerical aspects.

The theoretical controversy. Aimed to analyze the critical nature of DDS and determine their universality, a Langevin equation has been proposed. This equation describes the stochastic evolution of the local particle density \( \rho(x,t) \) in terms of \( \partial_t \phi = 2\rho - 1 \), it reads

\[
\partial_t \phi(r) = -\nabla_\perp^4 \phi + \tau_\perp \nabla_\perp^2 \phi + \frac{g}{6} \Delta_\perp \phi^3 + \tau_\parallel \nabla_\parallel^2 \phi + \epsilon \nabla_\parallel \phi^2 + \zeta(r,t),
\]

where \( \zeta(r,t) \) is a conserved noise term that reflects the fast degrees of freedom, \( \epsilon \) denotes the coarse-grained drive, and \( \tau_\perp, \tau_\parallel, \) and \( g \) are model parameters. This field theory leads to anisotropic scaling wave vectors in the critical region, with non-trivial correlation length exponents \( \nu_\perp, \nu_\parallel \). The current term \( \epsilon \nabla_\parallel \phi^2 \) is the most relevant nonlinearity and source of anisotropy.

Another Langevin equation, which is a coarse-grained version of the master equation, has been proposed. Although such equation has been criticized, after healing some flaws, the new equation, which is valid in the limit of an infinite driving field, reads

\[
\partial_t \phi(r) = -\nabla_\perp^4 \phi + \tau_\perp \nabla_\perp^2 \phi + \frac{g}{6} \Delta_\perp \phi^3 + \tau_\parallel \nabla_\parallel^2 \phi + \zeta(r,t).
\]

Comparing Eqs.(1) and (2) it follows that they only differ in the current term \( \epsilon \nabla_\parallel \phi^2 \) that vanishes in (Eq.(2)). This difference has deep consequences, including: i) The critical dimension of Eq.(2) is \( d = 3 \) instead of \( d = 5 \) in Eq.(1). ii) Renormalization group analyses give different critical exponents (see Table I). iii) It has been argued that the most relevant non-equilibrium effect is the anisotropy generated by the driving field and not the current. iv) In Eq.(2), the current term vanishes in the infinite driving limit, as shown rigorously in.

Another piece of heavy debate is the disagreement in the interpretation and evaluation of numerical data. Valles and Marro have concluded that \( \beta \) seemed to be close to \( \beta \approx 0.3 \), as predicted by Eq.(2). In view of the anisotropic nature of the system, Leung has developed an anisotropic finite-size approach. Extensive computer simulation results give data collapsing when the shape of the lattice \( S = L_y^{\nu_\parallel/\nu_\perp}/L_x \) and \( \beta \) are taken in accordance with Eq.(1). However, a subsequent
analysis of Leung’s data [10], discussed in [12], shows that they may also be consistent with β close to 0.3. Also recent simulations give β ≈ 0.33 [13].

We note that the analysis of numerical data obtained under NESS conditions may be biased by some assumptions such as anisotropic vs isotropic scaling, the shape S of the lattice, the method used to estimate $T_c$ in the thermodynamic limit, the quality of data collapsing, etc.

The aim of this work is to provide an unambiguous clarification of the existing controversy, based on extensive numerical studies of both the short- and the long-time dynamics of four variants of the KLS model. In their work, Janssen et al. [12] have shown that a system relaxing by a dynamic process exhibits universal behavior close to $T_c$. Since the extension of this concept to the field of non-equilibrium [13] states. This idea has been verified in many models exhibiting critical behavior under equilibrium [13] conditions. Since the extension of this concept to the field of non-equilibrium critical behavior and to anisotropic systems has not been performed yet, the present work has additional ingredients of general interest.

The KLS model [3] is defined on the square lattice assuming a rectangular geometry $L_x, L_y$, using periodic boundary conditions. A lattice configuration is specified by the set of occupation numbers $n_{i,j} = \{0,1\}$, corresponding to each site of coordinates $(i,j)$. Nearest-neighbor (NN) attraction $(J > 0)$ is considered. So, in the absence of a field the Hamiltonian $H$ is given by

$$H = -4J \sum_{<i,j,i',j'>} n_{i,j} n_{i',j'},$$

where the summation runs over NN sites only. The driving field $E$ acts along the $y$-direction. The coupling to a thermal bath at temperature $T$ and the action of the field are considered through Metropolis rates, i.e. $\min[1, \exp -(\{\Delta H - \eta E\}/k_B T)]$, where $k_B$ is the Boltzmann constant, $\Delta H$ is the change in $H$ after the exchange, and $\eta = (-1,0,1)$ for a particle attempting to hop (against, orthogonally, along) the field, respectively.

Monte Carlo simulations are performed using lattices of different sizes, with $240 \leq L_x \leq 960$ and $30 \leq L_y \leq 480$. $T$ is reported in units of $J/k_B$ and $E$ is given in units of $J$. In all cases the density is $\rho_o = 1/2$. One Monte Carlo time step (mcs) involves $L_x \times L_y$ trials.

Four variants of the KLS model are studied, namely: i) the infinite driving limit (IKLS) with $E = \infty$, ii) a finite driving case (FKLS) with $E = 0.5$, iii) the random field KLS model [14] in the infinite driving limit (IRKLS) and iv) the oscillatory KLS model [15] in the infinite driving limit (IOKLS). In the IRKLS (IOKLS), the driven field takes values $E = \pm \infty$ at random (with a period $\tau_0$), generating anisotropy but not an overall current. So, the study of the IKLS model is aimed to determine the validity of either Eq.(1) or Eq.(2). Also, the FKLS is studied to check the validity of Eq.(1) in the finite driving case. Finally, the comparison of the results of the IKLS model and those of both the IRKLS and the IOKLS models will help to clarify the role of the current.

In order to observe universality in the dynamics the system has to be initialized with configurations far from the NESS. For this purpose two different initial states have been employed, namely: i) Fully disordered configurations (FDC) as expected for $T \to \infty$ and ii) The ground state configuration (GSC) as expected at $T = 0$, which is a single strip parallel to the drive [13].

The order parameter ($OP$) is defined as the excess density in the direction parallel to the applied field, namely

$$OP \equiv (RL_x)^{-1} \sum_{i=1}^{L_x} |P(i) - \rho_o|,$$

where $P(i) = (L_y)^{-1} \sum_{j=1}^{L_y} n_{ij}$ is the density profile along the $x$-direction (perpendicular to the drive) and $R = (2\rho_o(1 - \rho_o))$ is a normalization constant. For simulations starting from the GSC the OP given by Eq.(4) and that proposed by Leung [10] give the same results. However, in contrast to Leung’s OP, that given by Eq.(4) is suitable to detect the onset of multi-stripped ordering during the short-time dynamics when simulations start from the FDC. Since $OP$ involves the calculation of the absolute value of the excess density, it is not suitable for the observation of the expected critical initial increase in the order parameter [13]. Instead, $OP$ can be identified with the square root of the second moment of the excess density. So, using FDC starting configurations, the proposed scaling anzats, which generalizes the standard one [13], reads:

$$OP(t,T,L_y,L_x) = b^{-\beta/\nu o} OP^*(b^{-z_t} t, b^{1/\nu o} \tau, b^{-1} L_y, b^{-\nu_{\parallel}/\nu o} L_x),$$

where $T = T - T_c$, $\nu o$ is the spatial rescaling factor, $\beta$ is the order parameter critical exponent, $\nu_{\parallel}$ ($\nu_{\bot}$) is the correlation length exponent in the direction parallel (perpendicular) to the drive, and $z$ is the dynamic critical exponent, respectively. In order to generate the FDC the lattice is filled at random with probability $p = 1/2$.

While a procedure is used to ensure that the whole density of the sample is exactly $\rho_o = 1/2$, density fluctuations of the order of $L_y^{-1/2}$ are present along the columns parallel to the drive. These tiny fluctuations add up according to Eq.(4), so that the amplitude of the OP depends on $L_y$ as $L_y^{-1/2}$. Taking $b \propto t^{1/2}$ in Eq.(5), it follows

$$OP(t,L_y) \propto L_y^{1/2} t^{c_2} OP^0(t^{1/\nu o} \tau), L_x, L_y \to \infty,$$

with $c_2 = (1 - 2\beta/\nu o)/2z$. [13]

Figure 1(a) shows log-log plots of $OP(t)L_y^{1/2}$ vs $t$ for the IKLS model obtained at $T = 3.20$. It should be noticed that a tiny downward (upward) deviation from linearity is obtained for $T = 3.21$ ($T = 3.19$) (not shown here). So, our estimation of the critical temperature is
\(T_{c}^{IKLS} = 3.20 \pm 0.01\). So, \(T_{c}^{IKLS} \approx 1.41T_{c}\), where \(T_{c}\) is the Onsager temperature of the \(d = 2\) Ising model. Notice that this value is fully consistent with previous estimations \[13\] Data collapsing of the raw data already observed for different lattice sizes supports the ansatz of Eq. (6), and this result confirms the assumption, also implicit in Eq. (6), that for the case of FDC the only relevant length of the lattice is that parallel to the drive along which the precursors of the striped patterns start to develop. The best fit of the data shown in Figure 1(a) gives \(c_{2} = 0.114 \pm 0.005\). Notice that all the critical exponents evaluated in this work are listed in Table I.

\[
\begin{align*}
T_{c}^{IKLS} & = 3.20 \pm 0.01, \\
T_{c}^{IRKLS} & \approx 1.41T_{c}, \\
T_{c}^{OKLS} & = 3.16 \pm 0.02,
\end{align*}
\]

Figure 1(b) allows the comparison of data obtained for the four different models studied. A perfect overlap of the data corresponding to the IKLS, the IRKLS \(T_{c}^{IKLS} = 3.16 \pm 0.02\) and the OKLS \(T_{c}^{OKLS} = 3.16 \pm 0.02\) is found, leading to almost the same exponent \(c_{2}\), as shown in Table I. Data of the FKL\(S\) model \(T_{c}^{FKLS} = 2.78 \pm 0.015, E = 0.5\) exhibit a crossover from a very early behavior with appreciable curvature to a latter regime \((t \geq 10^{5})\) where the slope of the other cases is recovered (within error bars, see Table I).

Furthermore, taking the logarithmic derivative of \(OP\) given by Eq. (6) at criticality, one has \[13\]
\[
\partial \ln OP(t, \tau) |_{\tau = 0} \propto t^{c_{\parallel}}, c_{\parallel} = \frac{1}{\nu_{||} z}. \tag{7}
\]

The best fits of the data give the values of the exponents \(c_{\parallel}\) listed in Table I.

Starting from GSC’s, we propose that the standard scaling behavior of \(OP\) can be generalized as \[13\]

\[
OP(t, \tau, L_{x}, L_{y}) = b^{-\beta/\nu_{z}} OP^{**}(b^{-\gamma} t, b^{1/\nu_{z}} \tau, b^{-\nu_{||} /\nu_{z}} L_{y}, b^{-1} L_{x}), \tag{8}
\]

where \(OP^{**}\) is a scaling function. Taking \(b \approx t^{1/2}\) in Eq. (8) at criticality \((\tau = 0)\), it follows that:

\[
OP(t) \propto t^{-\beta/\nu_{z}}. \tag{9}
\]

Also taking the derivative of Eq. (8) with respect to \(\tau\) it follows that

\[
\partial OP(t, \tau)|_{\tau = 0} \propto t^{c_{||}}, c_{\parallel} = \frac{1}{\nu_{||} z} - \frac{\beta}{\nu_{z}}. \tag{10}
\]

Figure 2(a) shows log-log plots of \(OP(t) vs t\) for the IKLS model obtained for \(T = 3.200\). Notice that starting from a GSC, the power law decay of the OP as described by Eq. (9) is obtained after a long time, e.g. for \(t \geq 10^{5}\) in Figure 2(a). A detailed view of this behavior is shown in Figure 2(b) for the four cases studied. Also, fitting these curves using Eq. (9) the slopes given by \(\beta/\nu_{z}\) can be obtained, as listed in Table I.

It should be noticed that tiny downward and upward deviations from linearity are observed for temperatures slightly out of criticality (not shown here). However, using GSC, this method for the location of \(T_{c}\) is roughly twice less sensitive than that used starting with FDC. So, our second (independent) estimation of the critical temperature is \(T_{c}^{IKLS} = 3.20 \pm 0.02\). This value is fully consistent with our previous estimation made starting from FDC, as expected for second-order transitions. The same behavior is observed in the other cases studied. Data collapsing of the raw data as observed in Figure 2(a) supports the assumption, implicit in the proposed scaling ansatz \((\text{Eqs. (8-9)})\), that starting from a GSC the only relevant length of the lattice is that perpendicular to the drive along which a diffusion-like process causes relaxation to the NESS. Our results confirm that the dynamics does not reveal the anisotropy of the system through the shape of the lattice \(S = L_{y}^{\nu_{||}/\nu_{||}}/L_{x}\), in contrast to the scaling treatment of data obtained under NESS conditions \[10,11,17\]. Instead, the anisotropy enters through the different correlation length exponents used in the scaling relationships, i.e., \text{Eqs. (6) and (9)}.

Log-log plots of the derivative of Eq. (8) (not shown here) support the scaling ansatz of Eq. (10) and allow the evaluation of \(c_{\parallel}\), as listed in Table I.

Combining the exponents \(\beta/\nu_{z}\) and \(c_{\parallel}\) obtained starting with GSC it is possible to evaluate \(\beta\). Also, using those exponents, as well as \(c_{2}\) and \(c_{\parallel}\) as evaluated starting from FDC, it is possible to calculate \(\nu_{z}\), \(\nu_{||}\) and \(z\) (see Table I). Furthermore, for anisotropic systems such as the KLS model, the following modified hyperscaling relation is expected to hold \[17\]:

\[

\nu_{||} + (d - 1)\nu_{z} - 2\beta = \gamma. \tag{11}
\]

where \(\gamma\) is the exponent of the susceptibility. So, using the numerically evaluated exponents, our estimations of \(\gamma\) made with the aid of Eq. (11) are also listed in Table I.
FIG. 2. Log-log plots of the order parameter vs $t$ as obtained starting with GSC. a) Results corresponding to the IKLS model using lattices of different sizes as shown in the figure. b) Results obtained for the different models studied as identified in the figure. Data obtained using lattices of size $L_x = 480$, $L_y = 240$, except for the FKLS model with $L_x = 960$, $L_y = 60$.

Based on the results summarized in Table I, it is concluded that: i) All critical exponents can be obtained self-consistently within the dynamics framework. In contrast to previous numerical estimations performed under NESS conditions, the values of the exponents are not biased by any assumption on the shape of the lattice used. ii) All the evaluated exponents are consistent with Eq.(2), and the predictions of Eq.(1) are far outside our error bars. iii) Since two models with macroscopic current (IKLS, FKLS) and another two without it (IRKLS, IOKLS), have the same critical exponents, it follows that such current is not relevant neither to determine the universality class nor for the emergence of the anisotropy. iv) The short-time dynamics of the studied non-equilibrium systems exhibits universal critical behavior, as already observed in equilibrium systems.

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| MODEL | $T_c$ | $c_2(\ast)$ | $c_3(\ast)$ | $\beta/\nu \gamma$ | $c_{\perp}(\ast)$ | $\beta(\ast)$ | $\nu_{||}(\ast)$ | $z(\ast)$ | $\gamma$ |
|-------|------|-------------|-------------|-------------------|-----------------|-----------|----------------|--------|-------|
| IKLS  | 3.200(10) | 0.114(5) | 0.406(10) | 0.254(15) | 0.16(15) | 0.330(30) | 0.644(40) | 1.221(40) | 2.016(40) | 1.21(11) |
| FKLS  | 2.780(15) | 0.108(5) | 0.409(10) | 0.245(15) | 0.487(15) | 0.335(30) | 0.668(40) | 1.198(40) | 2.041(40) | 1.20(11) |
| IRKLS | 3.160(20) | 0.115(5) | 0.421(10) | 0.228(15) | 0.506(15) | 0.311(30) | 0.671(40) | 1.168(40) | 2.033(40) | 1.22(11) |
| IOKLS | 3.160(20) | 0.116(5) | 0.424(10) | 0.235(15) | 0.505(15) | 0.281(30) | 0.635(40) | 1.110(40) | 2.126(40) | 1.18(11) |
| Eq. (1) | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ |
| Eq. (2) | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ | $\approx$ |

TABLE I. List of critical temperatures and exponents. The symbols ($\ast$), (+) and ($\ast$+) stand for exponents obtained using data corresponding to FDC and GSC, and combinations of both, respectively. The predictions of both Eq. (1) and Eq. (2), up to the first term of the $\epsilon$ expansion, are also listed. The results of the oscillatory models are less sensitive to tiny changes of $T$, causing the exponents to be less accurate than in the other cases. Notice that $z$ is renormalized with respect to the perpendicular direction.