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Critical properties of nonequilibrium anisotropic lattice gases [☆]

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Abstract

We discuss the critical behavior of nonequilibrium anisotropic systems, particularly the driven lattice gas and its variants. A large series of available numerical results depict a coherent picture consistent with specific predictions drawn from novel field theory and its renormalization group analysis. © 2000 Elsevier Science B.V. All rights reserved.

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Steady states of many-particle systems that are far from equilibrium, as when a constant flux of matter goes through the system, are common in physics, biology and geology [1,2]. In spite of some formal similarity and superficial resemblance to equilibrium phenomena, the properties of such nonequilibrium steady states are not given by averages over a known probability distribution. Consequently, extending familiar concepts and techniques of statistical physics to these cases is difficult. This is so even for the simplest nontrivial scenario, namely, lattice models that violate detailed balance, which have been attracting considerable interest. As a matter of fact, recent studies have explicitly shown that nonequilibrium steady states are determined by details of the lattice microscopic dynamics, which induces a varied and complex phenomenology and singles out the Ising equilibrium states — which are independent of dynamics — as a particularly simple situation [3]. These difficulties are naturally reflected in our present understanding of the great diversity of *nonequilibrium* phase transitions and

[☆] We dedicate this paper with love to Joel L. Lebowitz who initiated and constantly encouraged our studies in this field.

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critical phenomena in nature. It is to be reported, however, that a class of nonequilibrium anisotropic systems has been intensively studied during more than a decade now, and a coherent picture seems to have emerged lately.

The main system of interest in this paper is the driven lattice gas (DLG), first studied by Lebowitz and collaborators [4,5]. The DLG is the equilibrium, Ising–Yang–Lee lattice gas perturbed by a ‘driving force’ thus resulting in a system which is intrinsically out of equilibrium. More specifically, one assumes both a regular d -dimensional lattice on a torus, i.e., with periodic boundaries, whose sites $\mathbf{x} = 1, \dots, N$ hold occupation variables, $s(\mathbf{x}) = +1$ (‘particle’) or -1 (‘hole’), and a potential energy function $H(\{s(\mathbf{x})\}) = -T^{-1} \sum_{|\mathbf{x}-\mathbf{y}|=1} s(\mathbf{x})s(\mathbf{y})$, where the sum is over nearest-neighbor (NN) sites. The configuration $\{s(\mathbf{x})\}$ evolves in time by (Kawasaki) particle jumps to NN holes. The jumps occur with rate per unit time given by $\omega(\Delta H)$, except for those along a principal lattice axis for which the rate is $\omega(\Delta H + \eta E)$, where $\eta = \pm 1$ for the positive and negative ‘longitudinal’ directions, respectively. Here $E > 0$ represents a constant ‘electric field,’ ω is an arbitrary function, T is the temperature (in units of k_{Boltzman}) of the underlying thermal bath, and ΔH is the change in H after the jump. When the field that biases longitudinal hopping vanishes, one recovers the lattice gas; in the thermodynamic limit, this has a critical point at $\rho \equiv N^{-1} \sum_{\mathbf{x}} s(\mathbf{x}) = \frac{1}{2}$ and $T = T_c(E = 0)$. Otherwise, the system dissipates to the bath the heat generated by the field, and the rate cannot be derived from any potential energy function. Detailed balance does not hold but *locally* (for appropriate choice of ω), though one may still speak of energy and temperature in this ‘perturbed equilibrium’ model. In order to maintain our discussion simple enough, we shall deal below (unless otherwise indicated) with attractive interactions between NN particles, the Metropolis realization $\omega(\lambda) = \min\{1, e^{-\lambda}\}$, an ‘infinite’ field (particles cannot jump backwards), and rectangular $d = 2$ lattices with $\rho = \frac{1}{2}$, i.e., half filled with particles (see Ref. [3] for other interesting cases).

A main observation in Monte Carlo (MC) simulations of the DLG is a continuous (‘second-order’) transition at $T_c(E)$, which monotonically increases with E and saturates at $T_c(E = \infty) \simeq 1.4T_c(E = 0)$. The system exhibits the familiar disordered phase at high T , and two homogeneous phases at low T . Unlike in equilibrium, the condensed phase is strongly anisotropic, forming a single ‘liquid’ strip coexisting with ‘gas’ in the steady state, which holds a net longitudinal current for any non-zero value of E . The observed shift in $T_c(E)$, as well as other qualitative features of this nonequilibrium phase transition are now rather well understood [6,7,3]. The early work left the important question of critical behavior unsettled, however; in fact, this and a natural concern about the existence of nonequilibrium universality classes turned out to be difficult problems [8,9]. Many studies of nonequilibrium critical behavior have focused on the DLG since then; as a matter of fact, the DLG remains as the conceptually simplest system lacking detailed balance which involves strong spatial anisotropies and apparently captures other essential features of nonequilibrium phenomena. There is hope that a full understanding of the DLG will help elucidating more realistic situations.

The first estimate of critical behavior for the DLG suggested rough consistency with the (order-parameter) critical exponent $\beta \simeq \frac{1}{2}$ [5]. This result held little surprise 15

years ago when *classical* exponents were quite familiar from macroscopic descriptions (in which mean-field behavior is implicit) (see for instance Ref. [10]).¹ Furthermore, the pioneering nonequilibrium renormalization-group (RG) prediction [11,12] of a change-over to classical behavior when a binary liquid is set under shear had been reported as confirmed experimentally [13]. (It would be interesting to further examine such agreement, however, in the light of both the results reported below for the DLG, which is a closely related problem, and the fact that a nonequilibrium lattice binary mixture with shear flow indicated $\beta < \frac{1}{2}$ [14].)

Motivated by the fact that the φ^4 theory plus RG techniques produce an excellent description, including dynamics, of the Ising problem [15], more continuum nonequilibrium models that incorporate fluctuations have been developed. In particular, a continuum analog of the DLG, known as the ‘driven diffusive’ system (DDS), was proposed [16–22]. This incursion in the world of symmetries in nonequilibrium phenomena led, for any value of the drive, to the conclusion that the critical behavior is controlled by φ^2 (classical) theory with only an indirect influence of φ^4 . More explicitly, this Langevin model solves *exactly* showing mean-field behavior, including classical critical exponents for any $2 < d < d_c$, $d_c = 5$ (weak logarithmic corrections are predicted for the marginal case $d = 2$). It also ensues the need for two correlation lengths which diverge with distinct exponents, namely, $v_{\parallel} = 1 + \frac{1}{6}(5 - d)$ and $v_{\perp} = \frac{1}{2}$, and *effective isotropy* of the problem. This means that different finite rectangular ($L_{\parallel} \times L_{\perp}$) lattices should be comparable to each other, exhibiting standard finite-size scaling behavior if one fixes the ratio $L_{\parallel}^{v_{\parallel}/v_{\perp}} L_{\perp}^{-1} (= L_{\parallel}^3 L_{\perp}^{-1}$ for $d = 2$). The first MC study of rectangular lattices, including the case $L_{\parallel} \gg L_{\perp} \gg 1$, gave no indication of such behavior, however, and the exponent β was observed to clearly deviate from both $\frac{1}{2}$ and $\frac{1}{8}$, [23] the latter being the Ising value. In fact, excluding an optimistic report, [20,21] none of the several independent MC analysis of the DLG and its variants performed up to date has provided any convincing evidence that the DDS is the continuum version of the DLG [24–29]. On the contrary, the results from such great numerical effort can only be summarized by saying that the DLG does not have classical behavior for $E = \infty$ (the only case which has extensively been analyzed so far). The DDS needs further elaboration before it can be accepted as the appropriate DLG continuum analog.

This is perhaps an example of the many surprises one may be confronted with in nonequilibrium phenomena when expectations are too closely based on the intuition developed from equilibrium situations. In particular, it is not clear-cut yet the role played out of equilibrium by symmetries, including those involved by dynamics. It is true that, lacking a substitute, the DDS should not be questioned based on the available numerical discrepancies only. (In fact, except for the shear flow mentioned above, no related experiment has been performed so far.) However, there is much more than just numerical disagreement. For example, finite-size scaling analysis of MC data indicated

¹ The data backing the report in Ref. [5] clearly showed, for $d = 2, 3$, respectively, that $\beta > \frac{1}{8}, \frac{5}{16}$ (the equilibrium values); it was interpreted as indicating that $\beta \simeq \frac{1}{2}$ according to expectations.

strong surface effects to be naturally associated with the existence of a peculiar, linear liquid–gas interface in the DLG below $T_c(E)$ [24,30]. As a matter of fact, theory has revealed how strongly the interface details influence the DLG steady-state properties [6], which is a rather general fact in nonequilibrium phase transitions [2,10]. This might indicate that the interface rather than the field is relevant for the DLG critical ‘anomaly’. The same is suggested by the behavior of the *layered* DLG [26]. This consists of two DLG planes, one on top of the other, such that particles in different planes never interact — even if they are at NN sites along the transverse direction — but can jump to an NN hole in the other plane. In addition to the nonequilibrium phase transition of the standard DLG, the layered system undergoes a continuous phase transition — *isotropic* liquid in one plane and gas in the other — at $T_c^*(E) < T_c(E)$ for $E < E_c$ (the transition is discontinuous for large E). Near $T_c^*(E < E_c)$, where no anisotropic interface tends to be developed — contrary to the situation at $T_c(E)$ —, one precisely observes Ising exponents, and no dramatic surface effects [30]. (It is also remarkable that the DLG with repulsive interactions undergoes a phase transition with Ising behavior which exhibits no interface nor surface effects.) That is, only the interface (and not the existence of a current) is able to modify the ubiquitous Ising behavior. On the other hand, it is remarkable that short-ranged order parameters including the particle current exhibit a singularity at $T_c(E)$ which is not to be expected under the assumption of classical behavior [3].

The nonclassical behavior of the DLG is also supported by both quantitative and qualitative behavior as observed in its ‘variants’, including: (i) the DLG with broken bonds between NN site pairs oriented parallel to the field [31]; (ii) the DLG with spin flips added to exchanges [32]; (iii) a lattice gas in which longitudinal exchanges occur at random as in contact with a thermal bath at $T \rightarrow \infty$ [33,34]; (iv) the layered DLG mentioned above; and (v) a lattice gas that involves a parameter such that $p=1$ mimics the DLG with $E = \infty$ and $p = \frac{1}{2}$ corresponds to the field pointing at random along either the positive or the negative longitudinal directions [29]. Interestingly enough, this system exhibits precisely the same critical behavior for the two values of p , while the two versions of the DDS to be associated predict $\beta = \frac{1}{2}$ and $\beta < \frac{1}{2}$, respectively [35]. Though the precise relation between these and other ‘DLG variants’ has not yet been established rigorously, it is interesting that their corresponding anisotropies and numerical values for critical exponents loosely suggest that they all might depict the same (nonequilibrium) ‘universality class’ [30,3].

These and related questions could be answered by coarse-graining from the detailed microscopic dynamics. Though this is a difficult task to be fully accomplished at present [36,37], steps in this direction may clarify, for example, the dependence of the (mesoscopic) Langevin coefficients on microscopic parameters. In a recent attempt (DDS2) with this aim, the Langevin equation with specific symmetries is avoided as the starting point, and one proceeds instead from the continuum Markovian model:

$$\frac{\partial P_t(\Phi)}{\partial t} = \sum_{a=1}^d \sum_{\eta=\pm 1} \int d\mathbf{r} [\omega(\Phi^{\eta,\mathbf{r},a} \rightarrow \Phi) P_t(\Phi^{\eta,\mathbf{r},a}) - \omega(\Phi \rightarrow \Phi^{\eta,\mathbf{r},a}) P_t(\Phi)]. \quad (1)$$

Here, $P_t(\Phi)$ is the probability of configuration $\Phi = \{\phi(\mathbf{r}); \mathbf{r} \in R^d\}$ at time t , where the fields $\phi(\mathbf{r}) \in R$ sum up all the original spin variables $s(\mathbf{x})$ within a region of volume Ω around \mathbf{r} , and $\Phi^{\eta, \mathbf{r}, a}$ stands for Φ after changing $\phi(\mathbf{r})$ to $\phi^{\eta, \mathbf{r}, a}(\mathbf{r}) = \phi(\mathbf{r}) + \eta\Omega^{-1}\nabla_a\delta(\mathbf{r} - \mathbf{r}')$, where $\nabla_a = \partial/\partial r_a$, $\mathbf{r} = \{r_a; a = 1, \dots, d\}$. That is, the elementary dynamical rule in this ‘soft spin’ master equation consists in transferring an amount Ω^{-1} of field along $a\eta$.

Let us consider the conceptually simplest case of this equation, which consists in assuming that $\omega(\Phi^{\eta, \mathbf{r}, a} \rightarrow \Phi) = \omega(\Delta H_E^{\eta, \mathbf{r}, a})$ with $\Delta H_E^{\eta, \mathbf{r}, a} = H(\Phi) - H(\Phi^{\eta, \mathbf{r}, a}) + H_E(\Phi \rightarrow \Phi^{\eta, \mathbf{r}, a})$ and

$$H(\Phi) = \Omega \int d\mathbf{r} \left[\frac{1}{2} (\nabla\phi)^2 + \frac{u}{2} \phi^2 + \frac{g}{4!} \phi^4 \right],$$

$$H_E(\Phi \rightarrow \Phi^{\eta, \mathbf{r}, a}) = \eta E \delta_{a,\parallel} \left[1 - \phi(\mathbf{r})^2 + \mathcal{O}(\Omega^{-1}) \right]. \tag{2}$$

There is not rigorous justification from microscopic spin dynamics for these hypotheses – including the assumption that the field parameter has at this level the same properties as in the DLG. In any case, it is to be remarked that local detailed balance holds to order Ω^{-1} , namely, $H_E(\Phi \rightarrow \Phi^{\eta, \mathbf{r}, a}) = -H_E(\Phi^{\eta, \mathbf{r}, a} \rightarrow \Phi)$ as for the original DLG.

Next, a Kramers–Moyal expansion of Eq. (1) using parameter Ω leads to a Fokker–Planck description that can be written as the Langevin equation:

$$\frac{\partial \phi(\mathbf{r})}{\partial \tau} = \sum_{a=1}^d \nabla_a \left[\omega(\lambda_a^E) - \omega(-\lambda_a^E) + \psi_{\tau, a} \sqrt{\omega(\lambda_a^E) + \omega(-\lambda_a^E)} \right], \tag{3}$$

where $\psi_{\tau, a}$ stands for a Gaussian noise and

$$\lambda_a^E = -\nabla_a \frac{\delta H}{\delta \phi} + E \delta_{a,\parallel} (1 - \phi^2). \tag{4}$$

In addition to the obvious symmetry $(E, \phi) \rightarrow (-E, -\phi)$, this involves the basic microscopic structure of the lattice system via the explicit dependence on the elementary rate $\omega(\lambda_a^E)$, which remains unspecified in (3). In fact, model (1)–(2) has already been used to study the critical properties of a number of nonequilibrium lattice systems [38].

The critical behavior of the DDS2 may be investigated from the above simple scenario by standard scaling techniques. In addition to some non-physical cases, one finds up to four critical theories after assuming either isotropic or anisotropic scaling. That is, let (3) be written after scaling as

$$\frac{\partial \phi}{\partial \tau} = \nabla_{\perp} \cdot \mathbf{j}_{\perp} + \nabla_{\parallel} j_{\parallel}. \tag{5}$$

Assuming *isotropic scaling*, namely, after performing the changes (using standard RG notation) $r_{\perp} \rightarrow \mu^{-1}r_{\perp}$, $r_{\parallel} \rightarrow \mu^{-1}r_{\parallel}$, $\tau \rightarrow \mu^{-4}\tau$ and $\phi \rightarrow \mu^{(d-2)/2}\phi$, the following non-trivial fix point theories emerge as $\mu \rightarrow 0$:

- For $E = 0$, the critical behavior of (3) corresponds to the Ising one in ‘model B’, [15] with

$$\mathbf{j}_{\perp} = -\nabla_{\perp} \frac{\delta H}{\delta \phi} + \psi_{\tau, \perp}, \quad j_{\parallel} = -\nabla_{\parallel} \frac{\delta H}{\delta \phi} + \psi_{\tau, \parallel}. \tag{6}$$

- For $0 < E < \infty$, $\mathbf{j} = \mathbf{j}(\Phi, E)$ has a complex structure with many ‘dangerous irrelevant operators’ [38]. The corresponding critical behavior is not known.
- For $E \rightarrow \infty$, one has

$$\mathbf{j}_\perp = -\nabla_\perp \frac{\delta H}{\delta \phi} + \psi_{\tau,\perp}, \quad j_\parallel = \psi_{\tau,\parallel}. \tag{7}$$

That is, longitudinal random interchanges and model B behavior along the transverse directions. This implies a new universality class for which the critical dimension is $d_c = 4$ and (to one-loop order in $\varepsilon = d_c - d$) $\beta = \frac{1}{2} + \mathcal{O}(\varepsilon^2)$ and $\nu = \frac{1}{2} + \frac{\varepsilon}{12} + \mathcal{O}(\varepsilon^2)$, i.e., non-classical critical behavior [39]. It is remarkable that, against the intuition naturally incorporated in the DDS, this (critical) theory does not involve any net longitudinal current, though the starting model (3)–(4) does include a current for any $E > 0$.

Assuming *anisotropic scaling*, $r_\perp \rightarrow \mu^{-1}r_\perp$, $r_\parallel \rightarrow \mu^{-2}r_\parallel$, $\tau \rightarrow \mu^{-4}\tau$ and $\phi \rightarrow \mu^{(d-1)/2}\phi$, one recovers the standard DDS critical theory as $\mu \rightarrow 0$ for any $0 < E < \infty$:

$$\mathbf{j}_\perp = -\nabla_\perp \frac{\delta H_\perp}{\delta \phi} + \psi_{\tau,\perp}, \quad j_\parallel = f_1(E)\nabla_\parallel \phi + f'_1(E)\phi^2, \tag{8}$$

where $H_\perp = \int d\mathbf{r} \frac{1}{2}(\nabla_\perp \phi)^2 + (u/2)\phi^2 + (g/4!)\phi^4$. This case with Galilean symmetry leads to $d_c = 5$ and to $\beta = \frac{1}{2}$ to any order in an ε -expansion. The functions $f_1(E)$ and $f'_1(E)$ go to zero as $E \rightarrow 0, \infty$; as a consequence, model B behavior is not recovered.

Summing up, according to this simple picture, the DLG would depict two different universality classes for $0 < E < \infty$ and $E \rightarrow \infty$, respectively. The latter is not classical. In fact, the absence of a Gallilean symmetry impedes the cancellations characterizing the DDS. One recovers the Ising universality class for $E = 0$. Further consequences of (1) and (3) are presently under study.

Finally, we briefly mention some interesting details concerning the DDS2 critical mechanism as revealed by the structure function. This can be written for any $d > 4$ as

$$S(\mathbf{k}) \propto \frac{F(\mathbf{k}, E)}{u^2 + \mathbf{k}^2}, \tag{9}$$

where $F(\mathbf{k}, E) = 1$ for $E = 0$, and

$$F(\mathbf{k}, E) = \frac{\mathbf{k}_\perp^2 + f_2(E)\mathbf{k}_\parallel^2}{\mathbf{k}_\perp^2 + f'_2(E)\mathbf{k}_\parallel^2} \quad \text{for } 0 < E < \infty, \tag{10}$$

$$F(\mathbf{k}, E) = \frac{2\mathbf{k}_\perp^2 + \mathbf{k}_\parallel^2}{2\mathbf{k}_\perp^2} \quad \text{for } E \rightarrow \infty. \tag{11}$$

Here $f_2(E)$ and $f'_2(E)$ go to zero as $E \rightarrow 0$, while $f_2(E) \rightarrow \frac{1}{2}$ and $f'_2(E) \rightarrow 0$ as $E \rightarrow \infty$. Therefore, one has the length scale $\xi = u^{-1}$ for $E = 0$, and the critical point is then associated to the singular behavior of the structure function as $u \rightarrow 0$, $\xi \rightarrow \infty$; this is the familiar equilibrium situation. For $0 < E < \infty$, (10) reveals long-range (algebraic) correlations at any temperature, which is a main feature of nonequilibrium phenomena [3]. That is, $S(\mathbf{k})$ has a kind of singular behavior even far away from the critical point $u = 0$. This is still dominant, but an extra singularity adds to it. Consequently, the

nonequilibrium critical point does not have a simple characterization as in equilibrium but corresponds to a region in parameter space in which two or more singularities compete. For $E \rightarrow \infty$, $f_2^l(E)$ vanishes so that the longitudinal structure is washed out by the field. The functions involved show dominant terms $\sim e^{-E}$; consequently, the crossover from finite to infinite field is expected to occur for values of E of order of unity.

Note added in proof

The basic continuum model above involves a rate $\omega(\Phi^{n,r,a} \rightarrow \Phi) = \omega(\Delta H_U + \Delta H_S)$ where, respectively, the energetic and entropic contributions to the free-energy change $\Delta H_E^{n,r,a}$ are shown explicitly. Trying to understand further the consequences of (1), we very recently considered a situation in which the rate factorizes $\omega(\Phi^{n,r,a} \rightarrow \Phi) = \omega(\Delta H_U)\omega(\Delta H_S)$ and the field enters in ΔH_U . This study strongly confirmed the relevance of microscopic dynamics in this class of nonequilibrium models. In fact, even though such a modification can in a sense be simply interpreted as endowing the DDS2 with a mass, the resulting Langevin equation (to be denoted ADS) exhibits novel interesting behavior [40]. The ADS, which also depicts two different classes, for finite and infinite E , respectively, in addition to solve a criticism in Ref. [41] – i.e., the one concerning structure factors above criticality in the DDS2, which is sensible [40] –, predicts for $E \rightarrow \infty$ (under the assumption of anisotropic scaling) that $\nu \simeq 0.63$, $\beta \simeq \frac{1}{2}\nu$, $\nu_\perp = \nu$, $\nu_\parallel = \nu(1 + \Delta)$ and $\Delta \simeq 1$ for $d = 2$ ($d_c = 3$). These values for ν and β and the result $\nu_\perp \simeq 2\nu_\parallel$ are all in perfect agreement with MC observations [3]. While such agreement may confirm that using rectangular lattices is not essential to obtain good MC estimates for the critical properties of the DLG, the ADS also suggests that looking for *standard* finite-size scaling one should fix the lattice sides to $L_\parallel^2 L_\perp^{-1}$ rather than to $L_\parallel^3 L_\perp^{-1}$. This might explain why Refs. [27,28], for instance, failed to obtain good data collapse below T_c ($E = \infty$).

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