Physics Letters A 172 (1992) 29–33
North-Holland

PHYSICS LETTERS A

Lattice gas near two dimensions

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Received 30 June 1992; accepted for publication 24 September 1992
Communicated by A.R. Bishop

We report theoretical and computer studies of steady states in a particle-conserving lattice gas near 2D. The system comprises two equal parallel square lattice planes; any particle can hop between them, and there is attraction only between particles on nearest neighbor sites within the same plane. Surprisingly enough, we find an equilibrium critical point *for each particle density*, and two different phase transitions (one of them is discontinuous while the other is similar to a nonclassical one in several nonequilibrium systems) when a large driving constant field is applied.

The nature of a phase transition is known to depend essentially on the dimension D and symmetries characterizing a system. We present here a (quasi) 2D lattice gas model in which an additional degree of freedom (the particles can hop to other planes) induces the existence of novel phase transitions. Namely, equilibrium and nonequilibrium phase transitions can occur (the latter, in the presence of a driving field) which have no counterpart in the familiar cases lacking that peculiarity. Furthermore, our system admits various nontrivial generalizations.

Let us denote by λ the standard lattice gas [1,2] on a square (e.g.) lattice which we shall imagine either infinite or with periodic boundary conditions. The configurational energy is $H(\sigma) = -4J\sum'_{x,y} \sigma_x\sigma_y$, where $J>0$, $\sigma=\{\sigma_x;\ x\in\mathbb{Z}^2,\ \sigma_x=0,\ 1\}$, and the sum is over pairs of NN lattice sites. Thus, $\rho\equiv|\lambda|^{-1}\sum_x\sigma_x$ is a density, $|\lambda|$ stands for the *volume*, and $N\equiv\rho|\lambda|$. In the infinite-volume limit, λ is known to undergo a continuous phase transition for $\rho=\frac{1}{2}$ at a temperature $T_C\approx 2.269$ ($J/k_B\equiv 1$), while the phase transition is of first order at temperature $T_T(\rho)$ for $\rho\neq\frac{1}{2}$; e.g., $T_T(\rho=0.1)\approx 0.964T_C$ and $T_T(\rho=0.2)\approx 0.996T_C$, and $T_T(\rho=\frac{1}{2})=T_C$.

Consider the system $\Lambda\equiv\lambda_1\cup\lambda_2$, $\lambda_1\cap\lambda_2=\emptyset$, of *volume* $|\Lambda|=2|\lambda|$, whose configurations have energy $H_\Lambda(\sigma)=H(\sigma^1)+H(\sigma^2)$, where $\sigma^i=\{\sigma_x;\ x\in\lambda_i\}$, $i=1,2$. That is, Λ consists of two twin square lattices, *one on top of the other*, such that any site has five NN, with one of them in the other plane. There is no restriction on the possible configurations of Λ, e.g., any given particle has access to any of the two lattices. Note, however, that any two particles interact only when they are located at NN sites such that both belong either to λ_1 or to λ_2, i.e., all bonds between the planes are broken.

Next, consider a Markovian kinetic version of Λ. The probability of any configuration at time t, $P_E(\sigma;t)$, is governed by the master equation [3]

$$\frac{\partial P_E(\sigma;t)}{\partial t} = \sum_{x,y}{}' \left[c_E(\sigma^{xy};x,y)P_E(\sigma^{xy};t) - c_E(\sigma;x,y)P_E(\sigma;t)\right],$$

where σ^{xy} represents σ with the occupation variables at NN sites x and y interchanged, and $c_E(\sigma;x,y)$ is the transition probability per unit time for that interchange given σ. Thus, the kinetics consists of stochastic jumps of particles to NN empty sites, including jumps from one plane to the other. This process is driven by a heat bath at temperature T and, eventually, also by an external *electric* field E, which is constant in both space and time and points along one of the principal lattice directions. This is implemented by

$$c_E(\sigma; x, y) = f[\beta H(\sigma^{xy}) - \beta H(\sigma) - E\cdot(x-y)(\sigma_x - \sigma_y)] ,$$

where β is the inverse temperature and $f(X) = e^{-X} f(-X)$, $f(0)=1$, and $f(X)\to 0$ as $X\to\infty$. For $E=0$, $c_E(\sigma; x, y)$ satisfies a detailed balance which guarantees that the master equation goes asymptotically to canonical equilibrium states. For $E\to\infty$ (the only field case which we examine here), $c_E(\sigma; x, y)$ introduces a preferential hopping in the field direction, and the steady state is a nonequilibrium one. In fact: (a) E is not the gradient of a potential, so that the electric energy cannot be included in the Hamiltonian; (b) $c_E(\sigma; x, y)$ only satisfies a detailed balance condition locally; and (c) a net steady dissipative current sets in for periodic boundary conditions. Let us denote by Λ_∞ the nonequilibrium system; it is a nontrivial variation of the standard driven diffusive system (DDS); the latter has been used before to study nonequilibrium steady states and critical phenomena and also to model fast (solid) ionic conductors [3,4].

The study of Λ_∞ may help to answer two interesting questions concerning both equilibrium and nonequilibrium phase transitions: (i) The influence on macroscopic behavior of the extra degree of freedom in Λ. In particular, one would like to know the nature of the expected phase transitions in Λ, and their relation to the familiar ones in λ. (ii) In spite of much recent effort, the issue of the universality class to which the DDS and some related nonequilibrium systems belong is controversial, and Λ_∞ may perhaps undergo a sharp, well-defined phase transition which is related to the one in the DDS. We have studied these questions and some related ones by various methods: analysis of the exact partition function for Λ, (MC) computer simulations of both Λ and Λ_∞, and by a field theoretic approach. We describe the main results obtained in this Letter. The details, including a kinetic mean-field theory, a finite-size scaling analysis of MC data, and the study of some natural generalizations of our model (e.g., J has a different sign for each lattice, and $n>2$ lattices, each having a different D, are placed side by side) will be reported elsewhere.

Neglecting terms of order $|\Lambda|^{-1/2}$ or smaller, the steepest descent method allows us to write the canonical partition function of Λ after some algebra,

$$Z_\Lambda \approx \exp[-\beta|\Lambda| g(\beta, \boldsymbol{\rho}^*)] . \qquad (1)$$

Here, $g(\beta, \boldsymbol{\rho}) = p_1 g^0(\beta, \rho_1) + p_2 g^0(\beta, (\rho - p_1\rho_1)/p_2)$, $\boldsymbol{\rho} = (\rho_1, \rho_2)$, $p_i \equiv |\lambda_i|\,|\Lambda|^{-1}$ $(=\frac{1}{2})$, $g^0(\beta, \rho_i)$ represents the free-energy density describing λ with given density ρ_i, and $\boldsymbol{\rho}^* = (\rho_1^*, \rho_2^*)$ is a function of β, ρ, p_1 and p_2 which is defined as the solution of $\partial g^0/\partial\rho_1|_{\rho_1=\rho_1^*} = \partial g^0/\partial\rho_2|_{\rho_2=(\rho-p_1\rho_1)/p_2}$. Thus, $g(\beta, \boldsymbol{\rho}^*)$ which characterizes Λ may have a much richer unstable behavior than $g^0(\beta, \rho^*)$: perhaps surprisingly, the properties of Λ and λ are not simply related. The only expected result which is necessarily implied by (1) is, on the one hand, that both systems have identical high-T (homogeneous) thermodynamics. This follows (e.g.) by noticing that the case of an even distribution of particles between the planes is a solution $\boldsymbol{\rho}^*$, i.e., $\rho_i^* = \rho$, which makes successively $g(\beta, \boldsymbol{\rho}^*) = p_1 g^0(\beta, \rho_1) + p_2 g^0(\beta, \rho_2) = g^0(\beta, \rho)$. On the other hand, global stability (i.e., $g(\beta, \boldsymbol{\rho})$ is an absolute minimum at $\boldsymbol{\rho} = \boldsymbol{\rho}^*$) implies that the critical point in λ for $\rho_i = \frac{1}{2}$ occurs in Λ for $\rho = \rho_i = \frac{1}{2}$ at T_C also; in particular, λ and Λ have the same critical exponents *when* $\rho = \frac{1}{2}$ (see below for $\rho < \frac{1}{2}$). Further interesting consequences may be obtained from (1) by considering sub-systems λ whose function $g^0(\beta, \rho)$ is known, e.g., the 1D lattice gas or a lattice gas under a mean-field hypothesis, but that is not our aim here. Instead, we report now some observations from a series of computer experiments on Λ and Λ_∞, as defined above, and try to relate them to some theory.

Λ and Λ_∞ have been studied by the standard MC algorithm, i.e., with $f(X) = \min\{1, e^{-X}\}$, for $\rho \leqslant \frac{1}{2}$ and $|\Lambda| = 2|\lambda| \leqslant 2\times 128^2$. While the particles distribute evenly between the planes at high enough T (as predicted above), both systems segregate for $T < T^*$ into a particle-rich (*liquid*) phase in one of the planes and a particle-poor (*gas*) phase in the other; cf. figs. 1a, 1b. For Λ, each phase seems isotropic and *macroscopically* homogeneous. Thus, we have studied the order parameter $\Delta\rho(T) \equiv |\rho_1(T) - \rho_2(T)|$, where $\rho_i(T)$ is the actual density in plane i at T; cf. fig. 2a. It confirms how the data for $\rho = \frac{1}{2}$ agree with the Onsager solution, apart from the expected finite size effects. We also find $|E_1 - E_2| = 0$ for $\rho = \frac{1}{2}$, where $E_i = |\lambda|^{-1}\eta_i^{+-}$ and η_i^{+-} is the stationary mean number of particle–hole pairs in plane i, as expected. For

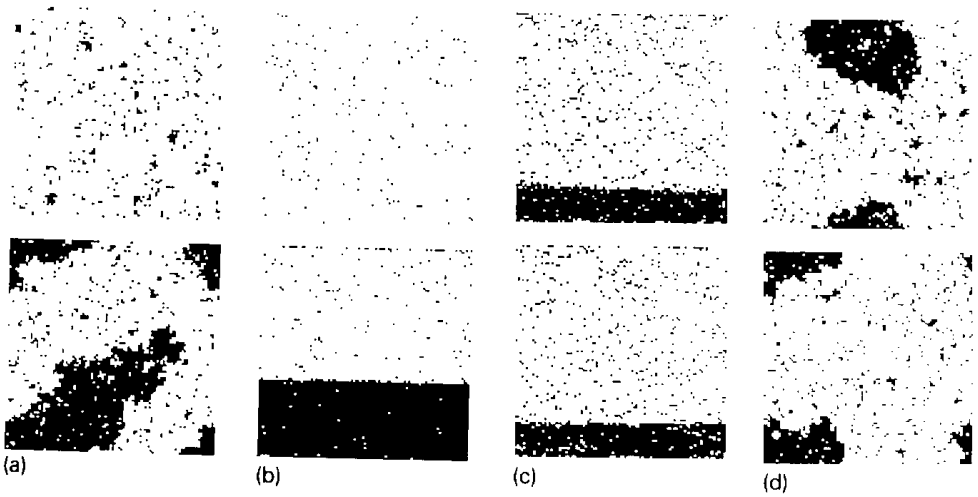

Fig. 1. Low-temperature typical stationary configurations in each plane for $\rho=0.2$: (a) for Λ when $T<T^*(\rho)$, (b) for Λ_∞ when $T<T^*_\infty(\rho)$, (c) for Λ_∞ when $T^*_\infty(\rho)<T<T_\infty(\rho)$, (d) same as (a), but a transient state. (A horizontal field exists in (b) and (c).)

$\rho<\frac{1}{2}$, the segregation in Λ is qualitatively similar, i.e., it occurs in one of the planes and *it is of second order* (we find no evidence of any discontinuity), and $T^*(\rho)$ decreases with ρ. Namely, we estimate $T^*(\rho=\frac{1}{2})\approx T_C$ (as predicted above), $T^*(\rho=0.2)\approx 0.97T_C$ and $T^*(\rho=0.1)\approx 0.93T_C$; the latter two are in contradistinction with the values of $T_T(\rho)$ for λ mentioned above. Summing up, the segregation in Λ of a liquid phase into one of the planes seems to differ essentially from the familiar first- order phase transition in λ; this is confirmed theoretically below.

The nonequilibrium phase transitions occurring in Λ_∞ are also most interesting; we would like, in particular, to relate the behaviors of Λ_∞ and of the standard 2D DDS [4]. Perhaps surprisingly, the MC data reveal two different phase transitions in Λ_∞ as T is decreased from $T=\infty$ (cf. figs. 1b, 1c). First, the liquid phase segregates itself highly anisotropically below $T_\infty(\rho)$; i.e., two approximately equal strips form along the field direction, one on top of the other (cf. fig. 1c). This is continuous for $\rho=\frac{1}{2}$ and of first order when $\rho<\frac{1}{2}$ (at least for $\rho\ll\frac{1}{2}$); we find $T_\infty(\rho=\frac{1}{2})\approx 1.3T_C$ and $T_\infty(\rho=0.2)\approx 1.14T_C$. One may describe this phase transition by the morphological order parameter $m=\frac{1}{2}(m_1+m_2)$, where

$$m_i=|\langle M^2_h\rangle-\langle M^2_v\rangle|^{1/2} \text{ and}$$

$$M^2_{h(v)}=|\lambda|^{-3/2}\sum_{h(v)}\left(\sum_{v(h)}(1-2\sigma_x)\right)^2$$

(h/v indicate summation along the two directions) on each plane; cf. fig. 2b. The critical behavior $m\sim|T-T_\infty(\rho=\frac{1}{2})|^b$ is a specific question here. Previous MC experiments indicated $b\approx\frac{1}{4}$ for several 2D nonequilibrium conservative lattice systems involving anisotropies. Namely, the standard DDS [4], the cases in which kinetics is speeded up by involving also a relatively small amount of creation–annihilation processes [5] or in which exchanges along one of the lattice axes are performed completely at random with no field [6], and a model with broken bonds between site pairs oriented parallel to $\boldsymbol{E}$ [7]. Against that convergence of numerical results, a field theoretic argument has been claimed to predict $b=\frac{1}{2}$ *with possible logarithmic corrections* [8] for the DDS with $E=$const (while a similar argument when E is random predicts $b\approx\frac{1}{4}$ also [9]). Our data, which excludes the case $b=\frac{1}{2}$ and deviates clearly from the Onsager equilibrium value, suggest instead $b\approx\frac{1}{4}$; cf.

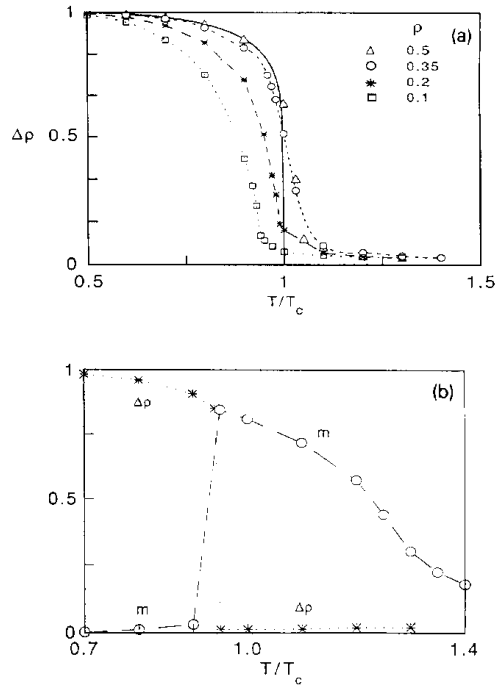

Fig. 2. Temperature variation of the order parameters: (a) for Λ and different values of ρ, as indicated; the solid line represents the Onsager solution; (b) for Λ_∞ when $\rho=\frac{1}{2}$.

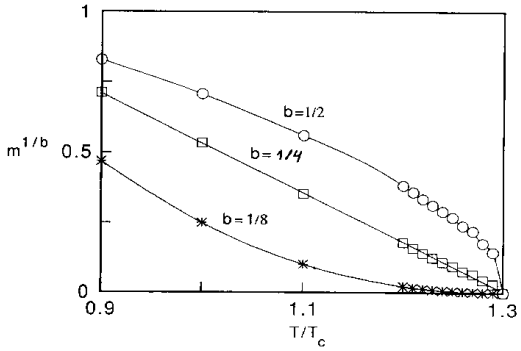

Fig. 3. Plots of $m^{1/b}$ versus T under different hypotheses, as indicated, for Λ_∞ obtained as an extrapolation $|\Lambda|\to\infty$.

some evidence in fig. 3 concerning an empirical extrapolation to $|\Lambda|\to\infty$. Furthermore, we find a phase transition in Λ_∞ which is revealed by $\Delta\rho(T)$; cf. fig. 2b. That is, $\Delta\rho$ increases sharply (as in a first-order phase transition for any ρ) at $T^*_\infty(\rho)$; e.g., $T^*_\infty(\rho=\frac{1}{2})\approx 0.95T_C$ and $T^*_\infty(\rho=0.2)\approx 0.88T_C$. As illustrated in fig. 1b, a liquid phase which exhibits a strong anisotropy induced by the field segregates in only one of the planes below $T^*_\infty(\rho)$.

The system Λ may be analyzed by a field-theoretic approach of the Ginzburg–Landau type [2] that incorporates all facts reported above which then allows a conclusion about critical properties. λ_i may be described by the functional $g\{\phi_i\}=\frac{1}{2}(\nabla\phi_i)^2+\frac{1}{2}r\phi_i^2+u\phi_i^4$ in terms of the *fields* at each plane, $\phi_i=\phi_i(\boldsymbol{x})$. Then,

$$Z_\Lambda=\int \mathrm{D}\phi_1\,\mathrm{D}\phi_2\exp\Big(-\int \mathrm{d}\boldsymbol{x}\,(g\{\phi_1\}+g\{\phi_2\})\Big)$$

$$\times\,\delta\Big(\int_{|\Lambda|}\mathrm{d}\boldsymbol{x}\,(\phi_1+\phi_2),\,|\Lambda|\Phi\Big),$$

where $\Phi=1-2\rho$. Let us write $\phi_1(\boldsymbol{x})=\psi+\Theta(\boldsymbol{x})$ and $\phi_2(\boldsymbol{x})=\psi-\Theta(\boldsymbol{x})$. More precisely, one is thinking about homogeneous solutions (i.e., $\rho\approx\frac{1}{2}$) in which the spatial variations within each plane are smooth enough, as compared to the field variations at each site between the two planes, to write $\psi(\boldsymbol{x})\approx\psi=\text{const}$. One thus finds after substitution that Z_Λ is governed by $\frac{1}{2}(\nabla\Theta)^2+\frac{1}{2}r_{\text{eff}}\Theta^2+u\Theta^4$ with $r_{\text{eff}}=r+12u\psi^2$. Since the eigenvalues of a matrix are invariant under changes of basis, standard renormalization group arguments [2] then lead to the existence for Λ of a critical point, whose associated critical exponents are the ones characterizing a ϕ^4 theory, *for each value of* ρ, thus generalizing the result above for $\rho=\frac{1}{2}$. Also, a perturbative treatment suggests $T^*(\rho)=T_C-12u(1-2\rho)^2$ from $r^*=12u(\Phi+\int \mathrm{d}q\,q^{-2})$ obtained in the *one-loop* approximation. This is in rough agreement with the MC values reported above for $T^*(\rho)$ and, in particular, it implies $T^*(\rho=\frac{1}{2})=T_C$ as concluded exactly after eq. (1). This is puzzling because preliminary MC data for Λ seem to suggest that the order parameter critical exponent b increases with decreasing ρ from $b\approx\frac{1}{8}$ for $\rho=\frac{1}{2}$. Would that be the case, there would follow both: (1) Λ illustrates a rather uncommon situation in statistical

mechanics of critical phenomena which is to be understood, and (2) our field-theoretic argument above is not valid except for $\rho = \frac{1}{2}$ (in which case the argument is rigorous). We are presently running larger systems as a first step trying to settle this issue.

Finally, we mention that Λ sometimes exhibits states in which the low-T segregation occurs in both planes, as in fig. 1d. While the general rule seems to be that such states decay with time into states with the liquid phase in only one of the planes (in fact, the configuration in fig. 1a occurred after the one in fig. 1d), they did not evolve like that at all in some of our MC experiments. One may convince oneself that both kinds of states are characterized by the same bulk free-energy density in the infinite-volume limit, but states such as those in fig. 1d have an extra surface energy which justifies our MC observation that the other ones are the real stable ones. On the contrary, the same comment does not apply to the states of Λ_∞ in figs. 1b and 1c, respectively, which are both stable states but corresponding to different temperatures.

We acknowledge leading remarks by J.L. Lebowitz, a critical reading of the manuscript by J.F. Fernández, some graphics software by H. la Roche, and financial support from the DGICYT (PB88-0487) and Junta de Andalucía (PAI) of Spain, and from the Comisión de las Comunidades Europeas (CI1.0409).

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