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Nonequilibrium Phase Transition in Stochastic Lattice Gases: Simulation of a Three-Dimensional System[1]

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We report results of computer simulations of a three-dimensional lattice gas of interacting particles subject to a uniform external field E. The dynamics of the system is given by hoppings of particles to nearby empty sites with rates biased for jumps in the direction of E. As for the two-dimensional system we find that here too there exists a critical temperature, $T_c(E)$ such that for $T < T_c(E)$ the systems orders in a very anisotropic phase with striplike typical configurations parallel to the field. $T_c(E)$ increases with E but substantially less strongly than in two dimensions. There is a break in the slope of the saturation current at $T_c(E)$. Our data are consistent with the critical exponent β being mean field.

KEY WORDS: Steady states; stochastic lattice gases; Ising model under electric field; superionic conductors.

1. INTRODUCTION

The equilibrium properties of macroscopic systems can be obtained as averages over suitable Gibbs ensembles. Among the most interesting features of such systems, where macroscopic size plays an essential role, is the occurrence of phase transitions. The qualitative understanding and quantitative calculation of such phenomena from first principles is one of the great triumphs of Gibbsian statistical mechanics. It would clearly be very desirable to have a similarly powerful formalism also for nonequilibrium systems. This is unfortunately not the case at present even for the simplest

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models. It therefore appears useful to find out information about the nature of possible phase transitions in nonequilibrium systems through computer simulations. This note describes the result of such a study. It is an extension of the work described in detail in Refs. 1 and 2, where we studied the steady state of a stochastic lattice gas in two dimensions subject to a uniform external field E. The model is defined as follows. We consider a hypercubic lattice in d dimensions with periodic boundary conditions containing $N = L^d$ sites and ρN particles. The microscopic configuration of the system is specified by giving the occupation at all lattice sites, $\eta = \{\eta_i\}$ with $\eta_i = 0, 1$ corresponding to site i empty or occupied and with $\sum_i \eta_i = \rho N$. The statistical state of the system is described by a probability distribution $P(\eta)$ on the configurations of the system.

The configurations η evolve according to a stochastic hopping dynamics. In the absence of an electric field, this is the familiar kinetic lattice gas or Ising model with Kawasaki-type dynamics which leads to an equilibrium state specified by

$$P_{\mathrm{eq}}(\eta) = \exp[-H(\eta)/k_B T] \Big/ \sum_\eta \exp[-H(\eta)/k_B T]$$

where T is the temperature and k_B Boltzmann's constant. The interaction energy H is assumed for simplicity to involve only nearest-neighbor sites, with periodic boundary conditions,

$$H(\eta) = -4J \sum_{|i-j|=1} \eta_i \eta_j$$

We consider only attractive interactions, $J > 0$. For $\rho = 0.5$ and $d = 3$, the case we shall study here, the (infinite) system with $E = 0$ undergoes a phase transition at a critical temperature $k_B T_c \cong 4.5J$.

The field E induces a preferential hopping in the field direction leading to a nonequilibrium steady state with a uniform density and a net current. If we follow the Monte Carlo prescription of Metropolis *et al.*,[3] the bias is most naturally introduced by adding to the potential energy difference, ΔH, the work done by the electric field in a jump. This yields the rates for an exchange of the occupations at sites i and $i + e$ in the configuration η as

$$c(i, i+e, \eta) = \begin{cases} 1, & \text{if } \Delta H - (\eta_i - \eta_{i+e})\, e \cdot qE \leqslant 0 \\ \exp[-(\Delta H - (\eta_i - \eta_{i+e})\, e \cdot qE)/k_B T], & \text{otherwise} \end{cases} \tag{1.1}$$

Here e is a unit vector in the lattice, $|e| = 1$, and $q(<0)$ is the charge. Only nearest-neighbor jumps occur.

In two dimensions all properties studied depend monotonically on the strength of the field and the temperature dependence turned out to be the more interesting one. Therefore we study here only the case of a strong field, $E \to \infty$, and the temperature is the only parameter to be varied. The E field is directed along the positive z axis ($d = 3$). Then for $E = \infty$ (1.1) simply means that jumps in the $+z$ direction are always performed, jumps in the $-z$ direction are forbidden, whereas jumps in the x–y planes are governed by the usual equilibrium Monte Carlo rates *à la* Metropolis with no electric field, i.e.

$$c(i, i + e_z) = 1, \qquad c(i, i - e_z) = 0$$

$$c(i, i + e) = \begin{cases} 1, & \text{if} \quad \Delta H \leqslant 0 \\ \exp[-\Delta H/k_B T], & \text{if} \quad \Delta H > 0, \quad e_\alpha = \pm e_x, \pm e_y \end{cases} \tag{1.2}$$

where $e_{x(y,z)}$ are the unit vectors along the positive $x(y, z)$ axis.

We argued in Ref. 2 that of the multitude of possible rates the physically acceptable ones should satisfy *locally* detailed balance and should be a function of the energy difference, the work done by the field included. The rate (1.1) satisfies these conditions and provides many exchanges per unit time. We refer to Ref. 2 for a more detailed discussion of these points.

2. COMPUTER SIMULATION

We carried out computer simulations on a simple cubic lattice of sides $L = 30$, with periodic boundary conditions, at density 0.5. The field E was set equal to ∞ and the temperature ranged from $0.6T_c$ to $2T_c$ (T_c always refers to the critical temperature at equilibrium.). Starting with a random configuration of 13,500 particles we implemented (1.1) and waited long enough, on the order of 10^4 Monte Carlo time steps, until a steady state is reached. (A time steps equals to 13,500 attempted exchanges.)

In two dimensions (with $E = \infty$) we found that at a temperature of roughly $1.3T_c$ the system undergoes a phase transition in which the system segregates in dense fluid phase and a vapor phase. Unlike in thermal equilibrium the fluid–vapor system is strongly anisotropic with typical configurations being striplike in the direction of the field. This basic physical phenomenon persists in three dimensions. Below the transition temperature strips form along the z axis. In the x–y planes there is no preferred direction. Therefore cross sections of typical configurations orthogonal to the field look roughly like a typical cluster in equilibrium at the corresponding temperature.

To be more quantitative we display in Fig. 1 histograms for the occupation number of columns along the z direction at $T/T_c = 0.6, 0.9, 1.0$, and 1.5. Because $\rho = 0.5$ the graphs are symmetric around $n = 15$ and therefore only one half is shown. From these histograms we conclude that

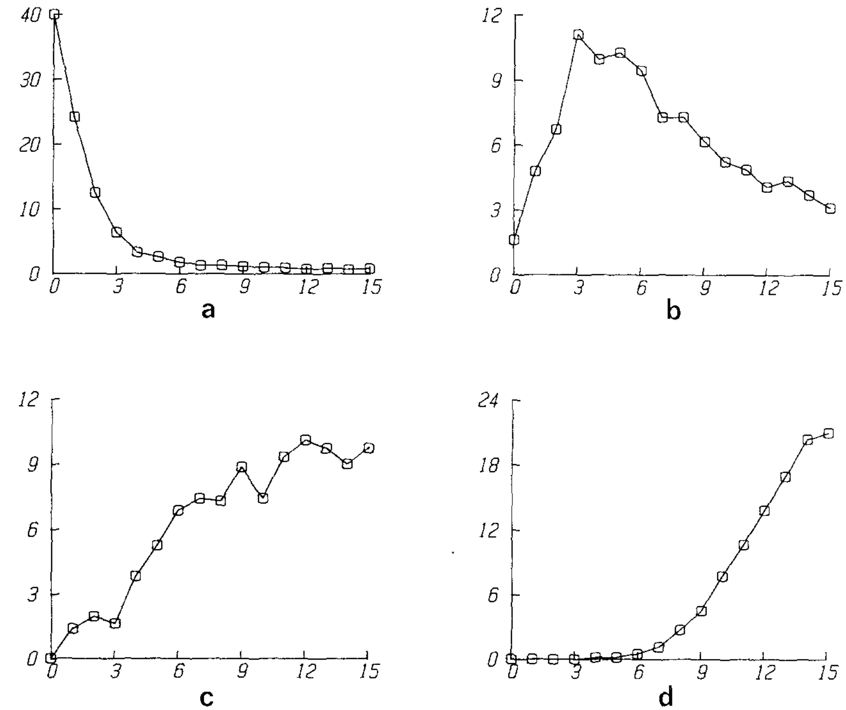

Fig. 1. Histograms for the occupation number of columns along the field direction at $T/T_c = 0.6$(a), 0.9(b), 1.0(c), and 1.5(d) and saturation field. The vertical axes represent the percentage of particles in the system being located in columns along the field direction each having $n = 0, 1, 2, \ldots$. The horizontal axis is for n. Because of symmetry when $\rho = 1/2$ (the case of interest here) columns with n occupied sites and $(30 - n)$ vacants are considered equivalent to columns with n vacants and $(30 - n)$ occupied sites; therefore only $n \leqslant 15$ is shown. Because such symmetry does not exist for $n = 15$, contributions for $n = 15$ were doubled in compiling the histograms.

ordering sets in around T_c. The low-temperature histograms are characteristic for striplike configurations. For example, at $0.6T_c$ more than 3/4 of the columns contain either $0, 1, 2$ or $28, 29, 30$ particles which is distinctively different from thermal equilibrium at $0.6T_c$. Our interpretation is further confirmed by the structure function $S(k_x, k_y, k_z = 0)$ for the same values of temperature; cf. Table I.

The natural-order parameter is the difference in density between the particle-rich and particle-poor phases. If we define the vertical and horizontal "magnetization squared" as

$$M_v^2 = \frac{1}{L^2} \sum_{x,y=1}^{L} \left[\frac{1}{L} \sum_{z=1}^{L} (2\eta_{x,y,z} - 1) \right]^2 \tag{2.1}$$

Table I. Structure Function $S(k_x, k_y, k_z = 0)$ at the Same Temperatures as the Histograms of Fig. 1

(a) $T = 1.5T_c$

$\frac{30}{2\pi}k_y$ \ $\frac{30}{2\pi}k_x$	0	1	2	3	4
0	0	9	4	5	4
1	5	4	3	3	3
2	6	3	3	4	2
3	3	3	4	2	2
4	2	3	3	3	3

(b) $T = T_c$

$\frac{30}{2\pi}k_y$ \ $\frac{30}{2\pi}k_x$	0	1	2	3	4
0	0	8	32	23	4
1	168	141	58	32	8
2	189	14	72	21	7
3	16	22	7	5	5
4	10	12	7	5	6

(c) $T = 0.9T_c$

$\frac{30}{2\pi}k_y$ \ $\frac{30}{2\pi}k_x$	0	1	2	3	4
0	0	38	168	69	16
1	29	666	263	30	8
2	2592	35	4	13	4
3	55	12	12	10	11
4	10	5	2	3	4

(d) $T = 0.6T_c$

$\frac{30}{2\pi}k_y$ \ $\frac{30}{2\pi}k_x$	0	1	2	3	4
0	0	880	36	19	13
1	275	1655	121	31	14
2	391	31	62	29	13
3	102	5	14	7	7
4	12	18	4	4	4

[a] The meaning of $k_z = 0$ is to count the number of particles in each column and to compute then the structure function of the resulting two-dimensional density profile. For $k_x, k_y \geqslant 5(2\pi/30)$ $S(\mathbf{k})$ exhibits no particular structure. Therefore we display only $k_x, k_y = 0, 1, 2, 3, 4$ $(2\pi/30)$.

and

$$M_h^2 = \frac{1}{L} \sum_{z=1}^{L} \left[\frac{1}{L^2} \sum_{x,y=1}^{L} (2\eta_{x,y,z} - 1) \right]^2 \tag{2.2}$$

then the order parameter may be defined by

$$\Delta\rho = (M_v^2 - M_h^2)^{1/2} \tag{2.3}$$

If the alignment was perfect, then $\Delta\rho = 1$, while in the isotropic case (e.g., at infinite temperature) $\Delta\rho = 0$. $\Delta\rho$ is given in Fig. 2.

According to the mean-field-type theory of van Beijeren and Schulman[3] the critical temperature at $E = \infty$ and density 1/2 increases with dimension but the relative change $[T_c(E = \infty) - T_{c,m}]/T_{c,m}$, where $T_{c,m}$ is the mean field critical temperature, decreases with increasing dimension. Our results show that this prediction is qualitatively correct.

To locate the critical temperature it is convenient to have a bulk quantity which is singular at T_c. In our model the average current seems to serve this purpose. Because it is obtained by averaging over all bonds parallel to the z axis its fluctuations are small. Van Beijeren and Schulman predict that the current at $E = \infty$ stays constant all the way to $T_c(\infty)$ and then drops roughly linearly. We plot in Fig. 3 the saturation current $j(T)$

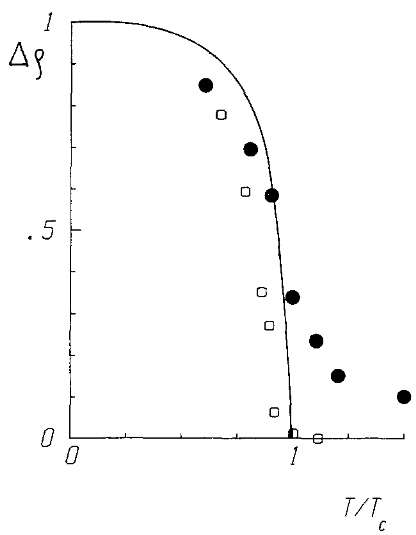

Fig. 2. Order parameter $\Delta\rho$ versus T/T_c at saturation field. The open circles are included for comparison and represent Binder's Monte Carlo results[5] for a simulation of the three-dimensional Ising model on a $12 \times 12 \times 12$ lattice. The full curve is the spontaneous magnetization for the infinite system as obtained from series expansions.

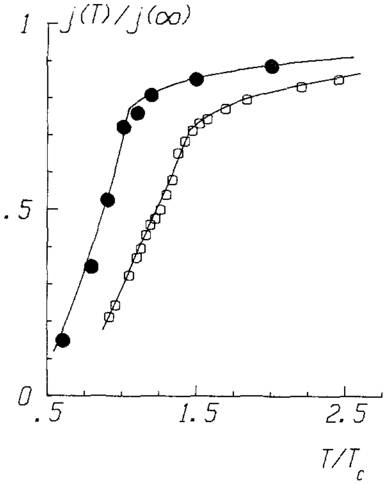

Fig. 3. Average saturation current ($E = \infty$) versus T/T_c normalized by the average current at infinite temperature. The full circles represent the results for three dimensions. For the sake of comparison we also include the two-dimensional result (open circles).

normalized by its value at infinite temperature. There seems to be a break in its slope around T_c consistent with the information from the histograms. For comparison we also included the data of the two-dimensional system. The break at $1.3T_c$ is quite pronounced. This value for $T_c(\infty)$ agrees with the value for $T_c(\infty)$ obtained from the maximum of the specific heat and from a Monte Carlo renormalization group analysis.[5]

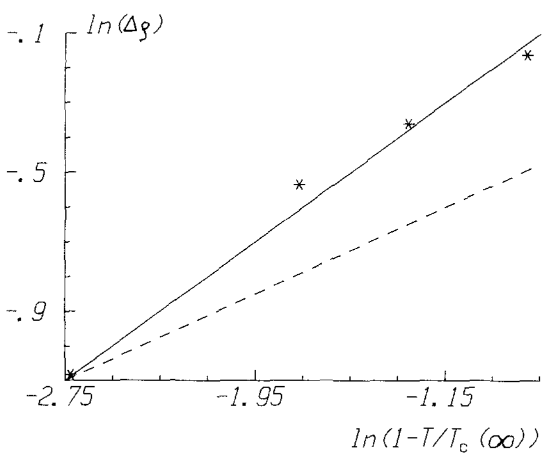

Fig. 4. $\log(\Delta\rho)$ with $\Delta\rho$ from Fig. 2 versus $\log(1 - T/T_c(\infty))$ with $T_c(\infty) = 1.07T_c$ from Fig. 3. The straight line has slope 1/2 and, as comparison, the broken line has the Ising slope 5/16.

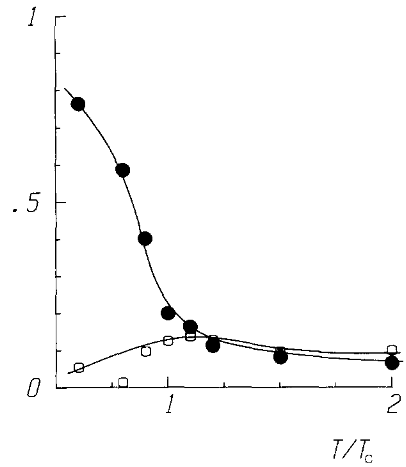

Fig. 5. Truncated nearest-neighbor correlation functions in the direction parallel to the field (full circles) and orthogonal to the field (open circles) versus T/T_c at $E = \infty$.

From the break in the slope of the saturation current we estimate $T_c(\infty) \cong 1.07T_c$. We use this value in a double logarithmic plot of $\Delta\rho$ versus $[T_c(\infty) - T]/T_c(\infty)$; cf. Fig. 4. The slope of this curve defines the critical exponent β. Our data are consistent with the mean field value $\beta = 1/2$ but seen to rule out the Ising $\beta = 5/16$. This conclusion depends on the choice of $T_c(\infty)$. But we would have to go to $T_c(\infty) = T_c$ to obtain consistency with the Ising β. While this is certainly possible the numerics are more consistent with mean field behavior.

We also studied the nearest-neighbor correlations; cf. Fig. 5. Since below $T_c(\infty)$ the density in a column differs from 0.5, we truncate by the square of the average density in each column. The electric field suppresses any correlations in the field direction. In fact, in one dimension there would be no correlations at all. The horizontal nearest-neighbor correlations build up short-range order as one lowers the temperature.

3. CONCLUSIONS

The main purpose of our simulation was to find out whether the phase transition found for a two-dimensional lattice gas subject to a constant external electric field persists in three dimensions. This is certainly the case. Qualitatively the transition in $d = 2$ and 3 look alike. The shift in the critical temperature follows the prediction of van Beijeren and Schulman. We do not have enough data to pin down the precise nature of the transition. But our data are consistent with $T_c(\infty) = 1.07T_c$ and $\beta = 1/2$. For a binary liquid

Kawasaki and Onuki[6] predicted a change over to mean field behavior when the fluid is set under shear. Beysens and Gbadamassi[7] confirmed this experimentally. Our simulation points in the same direction, but whether the critical behavior of a stochastic lattice gas in a constant external electric field is mean-field-like remains as an intriguing open question.

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