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Phase transitions in stationary nonequilibrium states of model lattice systems

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We investigated the stationary nonequilibrium states of a lattice gas of interacting particles subject to an external field $\vec{E}$. The dynamics of the system are given by hoppings of particles to nearby empty sites with rates biased for jumps in the direction of $\vec{E}$. This system is often used to model fast ionic conductors. Using computer simulations of a two-dimensional lattice with nearest-neighbor interactions we studied the dependence of the structure function, current, etc., on temperature and $\vec{E}$. We found evidence for a transition line in the temperature-field plane at which the system develops (anisotropic) long-range order. $\vec{E}$ enhances the transition for attractive interactions and represses it for repulsive ones.

I. INTRODUCTION

There is little known about microscopic correlations in stationary nonequilibrium systems. We therefore carried out computer simulations of such a state in a system consisting of a hypercubic lattice in ν dimensions with periodic boundary conditions (torus) containing $N=L^{\nu}$ sites, and cN particles. The microscopic configuration of the system is specified by giving the occupation at all lattice sites, $\underline{C}=\{c_i\}$, $c_i=0,1,\ldots,$ with $\sum_{i=1}^{N} c_i = cN$. The statistical state of the system is described by a probability distribution on the configurations of the system $\mu(\underline{C})$.

The configurations $\underline{C}$ 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 stationary state specified by

$$\mu_{\rm eq}(\underline{C}) = \exp[-\beta U(\underline{C})]/\sum \exp[-\beta U(\underline{C})] \ ,$$

where β is the inverse temperature. The interaction U is assumed for simplicity to involve only nearest-neighbor sites, with periodic boundary conditions,

$$U = -4J \sum c_{\vec{i}} c_{\vec{j}} \ .$$

For $c=0.5$, $\nu=2$, the case we shall study here, the (infinite) system undergoes a phase transition at a critical temperature $T_c \simeq |J|/0.44$.

The field induces a preferential hopping in one direction leading to a stationary nonequilibrium state in which there is a net current. Previous studies of this model, used to describe certain fast ionic conductors,[1,2] have been primarily concerned with the effects of small electric field. We believe this is the first study of the stationary state characteristic for large electric field.

To specify our model more precisely we have to give the transition rates. In the absence of an external electric field these are assumed to satisfy detailed balance, i.e.,

$$W(\underline{C} \to \underline{C}^{\vec{i},\hat{e}})/W(\underline{C}^{\vec{i},\hat{e}} \to \underline{C}) = e^{-\beta \Delta U} \ . \tag{1}$$

Here $\hat{e}$ is a unit lattice vector, $(\vec{i},\hat{e})$ is a bond incident on the site $\vec{i}$ (there are 2ν such bonds), $\underline{C}^{\vec{i},\hat{e}}$ is the configuration obtained from $\underline{C}$ by interchanging occupations at sites $\vec{i}$ and $\vec{i}+\hat{e}$, W is the rate for this transition, β is the inverse temperature, and ΔU is the change in the interaction energy resulting from this exchange. Since ΔU depends only on the $c_{\vec{j}}$'s at sites neighboring the bond $(\vec{i},\hat{e})$ it is generally assumed that $W(\underline{C} \to \underline{C}^{\vec{i},\hat{e}})$ also depends only on the configuration at these sites. This still leaves an enormous choice of rates satisfying (2), Refs. 1–4.

When there is a uniform external electric field $\vec{E}$ on a torus, the stationary, current-carrying, nonequilibrium state will no longer satisfy any global detailed-balance condition. We expect, however, that W_E will satisfy a "local" detailed-balance condition, i.e., one that would be valid if locally the field were the gradiant of an external potential Φ. In that case, $\Delta\Phi$ in the transition $\underline{C} \to \underline{C}^{\vec{i},\hat{e}}$ equals $-(c_{\vec{i}} - c_{\vec{i}+\hat{e}})\hat{e}\cdot q\vec{E}$, where q is the charge. This yields

$$W_E(\underline{C} \to \underline{C}^{\vec{i},\hat{e}})/W_E(\underline{C}^{\vec{i},\hat{e}} \to \underline{C}) = \exp\{-\beta[\Delta U - (c_{\vec{i}} - c_{\vec{i}+\hat{e}})q\hat{e}\cdot\vec{E}]\} \ . \tag{2}$$

Transition rates satisfying (2) (with $W_E \neq 0$) can be proven to have the following two desirable properties[5]: (i) For a finite torus there is a unique stationary state μ_E which is spatially uniform. There is *no* detailed balance in the stationary state except when $E=0$, in which case $\mu_E = \mu_{\rm eq}$. (ii) The Einstein relation $\vec{\sigma} = \chi\vec{D}$ is satisfied, where $\vec{\sigma}$ is the *zero-field* conductivity, χ the equilibrium compressibility, and $\vec{D}$ the bulk diffusion coefficient. Furthermore, the Kubo formula holds in the sense that $\chi\vec{D}$ is given by the space-time integral over the current-current correlation function.

II. COMPUTER SIMULATIONS

We carried out computer simulations on an $L=30$ (or 40) square lattice with periodic boundary conditions at a density $c=0.5$. The values of $K \equiv \beta J$ ranged from -0.5 to 0.5 and that of $q\beta E$, in the y direction, ranged from zero to 50 (effectively infinite). Our transition rates, in units of attempted exchange per bond, were chosen in the manner of Metropolis, with $\Delta\Phi$ added to ΔU,

$$W_E(\underline{C} \to \underline{C}^{\vec{i},\hat{e}}) = \begin{cases} 1, & \text{if } \Delta U - (c_{\vec{i}} - c_{\vec{i}+\hat{e}})\hat{e}\cdot q\vec{E} \geq 0 \ , \\ \exp\{-\beta[\Delta U - (c_{\vec{i}} - c_{\vec{i}+\hat{e}})\hat{e}\cdot q\vec{E}]\} & \text{otherwise} \ . \end{cases} \tag{3}$$

Starting with an "equilibrium" configuration of 450 particles, we turned on the field by implementing (3) and waited long enough, about 15 000 time steps (attempted exchanges per site), for the system to come to a stationary state. We then collected our data as time averages over about 25 000 additional steps. We also averaged over 2–5 runs at each point in the T-E plane.

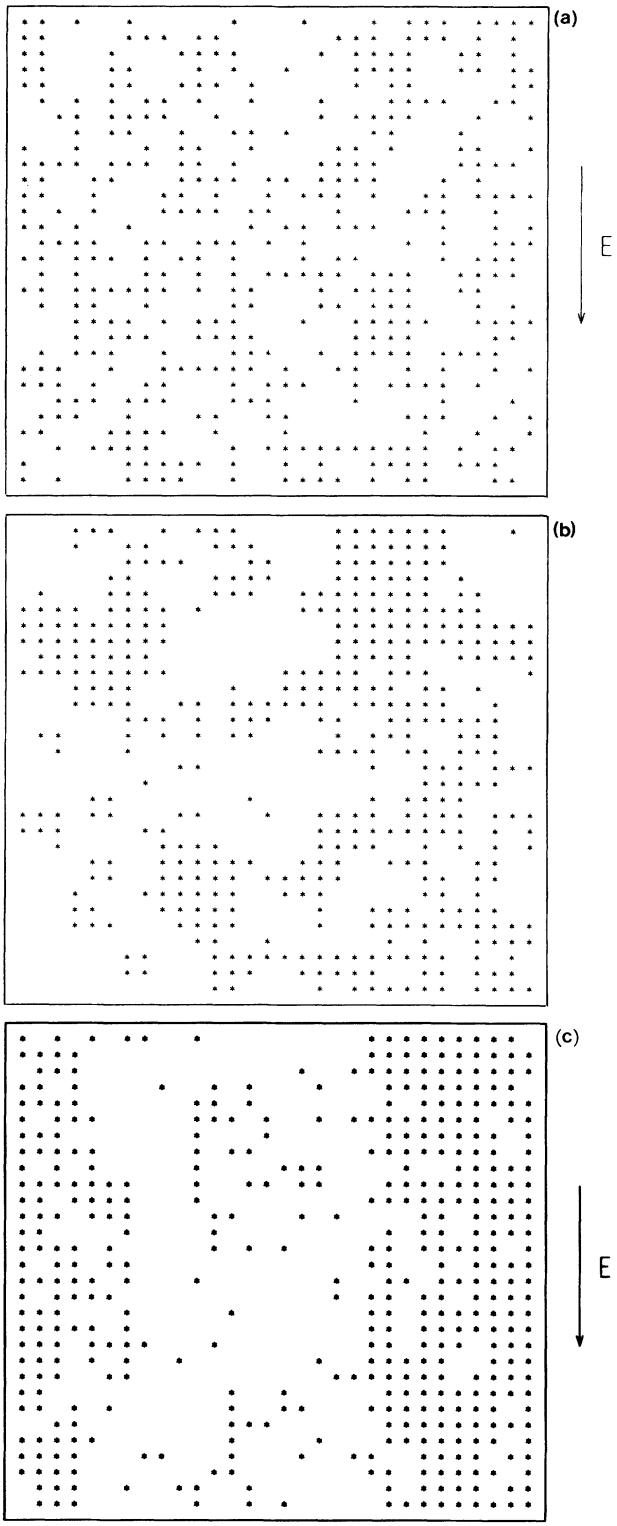

FIG. 1. Typical stationary state configurations at (a) $K=0.2$, $E=10$, (b) $K=0.35$, $E=0$, and (c) $K=0.35$, $E=50$.

RESULTS

We measured a variety of quantities related to the microscopic structure but restrict our attention here to the current $J(E)$ and the structure factor $S(\vec{k})$. $J(E)$ is defined operationally as the total number of jumps in the $+y$ direction minus those in the $-y$ direction during the time of the run divided by the time and by the number of bonds in the y direction. The structure factor $S(\vec{k})$ is the Fourier transform of the pair correlation function,

$$S(\vec{k})=\left\langle \frac{4}{N}\sum\{\exp[i\vec{k}\cdot(\vec{j}-\vec{1})]\}(c_{\vec{j}}c_{\vec{1}}-\tfrac{1}{4})\right\rangle , \tag{4}$$

where $\vec{k}$ is in the first Brillouin zone.

In Fig. 1 we show three typical configurations, corresponding to (a) $K=0.2$, $E=10$, (b) $K=0.35$, $E=0$, and (c) $K=0.35$, $E=50$. We note first that for small K (high temperature) even enormous fields ($E\gtrsim 5$ is effectively the same as $E=\infty$) produce little change in the appearance of typical configurations. They are similar to the equilibrium state $E=0$, being isotropic and disordered. At $K=0.35$, however, the large-E stationary state looks very different from the equilibrium $E=0$ state at that temperature. While the latter, being above the Onsager transition temperature $K=0.44$, is still isotropic with some local order, the former appears to be highly anisotropic and ordered with some columns almost entirely occupied and others entirely empty.

This kind of ordering leads to a drastic reduction in the current and gives a large maximum in $S(\vec{k})$ for $(k_x,k_y)=(2\pi/30,0)$. In order to see whether this really corresponds to the system having undergone a phase transition, we plotted in Fig. 2 the value of the maximum of

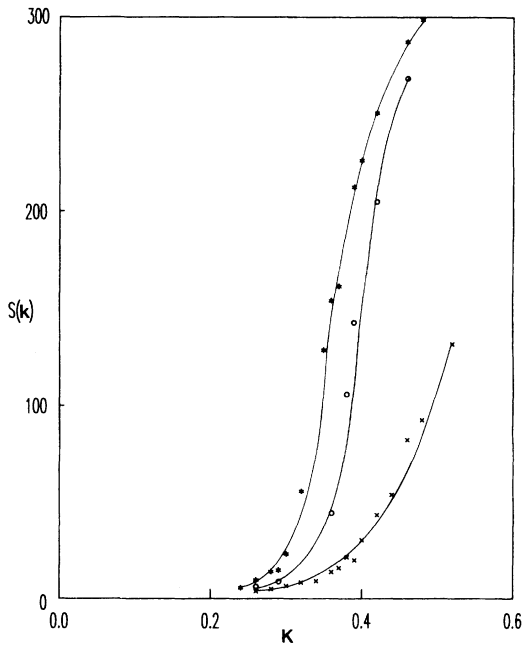

FIG. 2. Structure function $S(\vec{k})$ at the value $k_x=2\pi/30$, $k_y=0$, as a function of $K=\beta J$, for various electric fields. The crosses correspond to $E=0$, the open circles to $E=0.75$, and the asterisks to $E=50$.

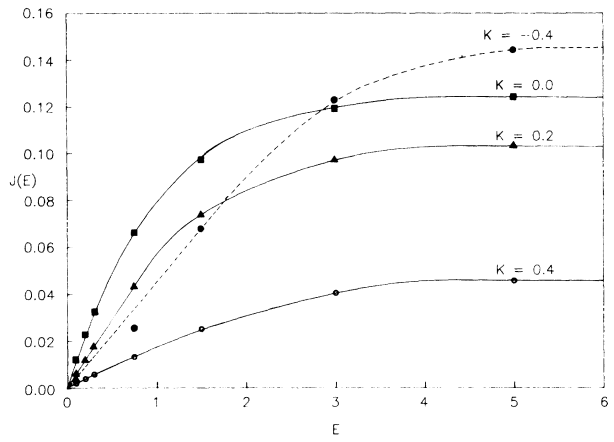

FIG. 3. Current as a function of electric field for various values of K.

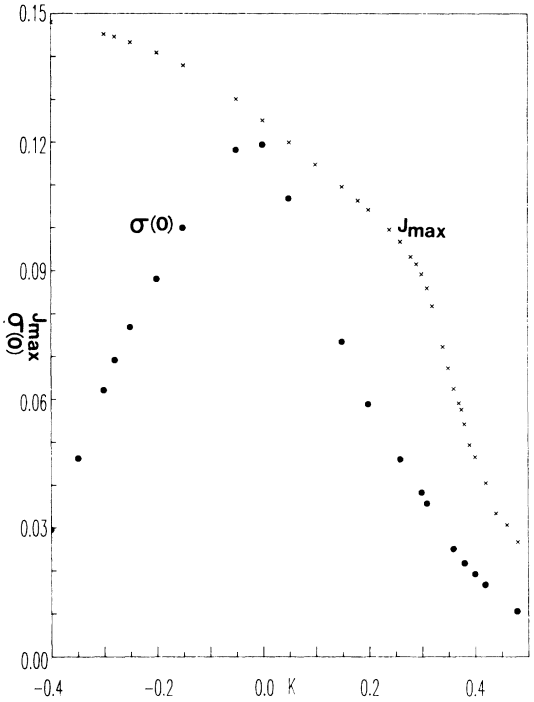

FIG. 4. Crosses represent the saturation current J_{max}. The full circles represent the zero-field conductivity $\sigma(0)$.

$S(\vec{k})$ vs K for the equilibrium state $E=0$ and some current carrying states $E \neq 0$. The sharp increase in $S(\vec{k})$ suggests the existence of a transition at a "critical" $K_c(E)$ which decreases from $K_c(0)=0.44$ (the Onsager value) to $K_c(\infty) \simeq 0.32$. [$K_c(\vec{E})$ may be defined by the maximum value of $S(\vec{k})$, being equal to the value it takes in our system in equilibrium at $K_c(0)$, approximately 50]. The structure of the low-temperature phase depends on E—being hightly anisotropic for large fields.

Figure 3 shows the current as a function of βqE for various values of K. It is seen that $J(E)$ saturates for large fields, $\beta qE \gtrsim 5$. We call $J_{max}(K)$the saturation current. This is plotted in Fig. 4 where we also show the zero-field conductivity $\sigma(0)$. There "appears" to be a break in the slope of $J_{max}(K)$ at $K_c(\infty)$. We also measured the specific heat at constant E. Its peak is shifted to higher temperatures consistent with our data on $S(\vec{k})$. However, the peak is broader than the corresponding one at the equilibrium transition. This makes it hard to determine the critical temperature with accuracy. In particular, we did not try to determine critical exponents.

For repulsive (antiferromagnetic) interactions, $K<0$, the equilibrium state at $E=0$, $K<K_c \simeq -0.44$ has one of the sublattices preferentially occupied. The field E appears to destroy this order. The maximum of the staggered structure function at $E=50$, $K=-0.44$ is of the same magnitude as the maximum at $E=0$, $K=-0.2$. These results are consistent with Fig. 16(b) in the report of work prior to publication, by Murch[1] and the discussion there.

CONCLUDING REMARKS

(i) We are quite confident that our simulations really represent the stationary state. Varying the initial configurations and going to a larger-size lattice (40×40) does not affect the results significantly. Our estimated error for the 30×30 simulations are no larger than the size of the data points on the graph.

(ii) The choice of dynamics *is* important for nonequilibrium behavior.[4] It can drastically affect the stationary states for $E=0$. Thus for $\vec{E}$ directed in the diagonal direction and jumps restricted to nearest-neighbor sets or rates (6) would become *independent* of E when E becomes infinite. This would lead, in that limit, to the unphysical model in which μ_E is the same as μ_{eq} at infinite temperatures.[5]

(iii) We have also carried out simulations and exact theoretical computations for one-dimensional models, the results of which will be published along with further details of the two-dimensional simulations.[5] Simulations in three-dimensional systems are at an early stage (with J. Marro).

(iv) The modification of the transition in our system caused by E should be compared to the effect of a shear flow on the demixing transition in a binary fluid studied in Ref. 6. The flow there, which affects both components equally, causes a lowering of the critical temperature and a change in the critical exponents. As indicated earlier, however, we have not yet made a systematic study of the exponents in our nonequilibrium transition. We plan to study this in the future.

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