

Orientation in a driven lattice gas

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The effect of an electric field on the ordering is studied in a square lattice gas exhibiting anisotropic ground states. Below T_c the particles form parallel chains directed horizontally or vertically. Monte Carlo simulations show that these chains prefer the orientation parallel to the applied field. This phenomenon is analytically investigated by using a simple mean-field approximation and determining the exact solution on a 2×2 lattice. The application of an electric field as a tool for producing an oriented phase is discussed.

I. INTRODUCTION

In partially occupied lattice-gas models the ordered state always has some degeneracy corresponding to the symmetry which is broken at the transition. In the ordered state the particle distribution may become anisotropic in spite of the cubic symmetry of the host lattice. For example, the particles can form parallel chains along one of the crystallographic directions. In this case the ordered states specified by the chain orientation are equivalent. In the presence of an electrical field, however, the equivalence between the principal directions is no longer valid. In a two-dimensional lattice-gas model we have shown that the chains prefer the orientation parallel to the electric field.¹ More precisely, by applying an electric field we can modify the chain direction. Such a technique has already been used successfully to prepare a monodomain Si(001) 2×1 surface by applying a direct current for the wafer annealing.²

This phenomenon is of interest to a large variety of systems. Theoretical investigations suggest anisotropic particle distributions in several two-dimensional lattice-gas models introduced to describe phenomena in monolayers at single crystal surfaces.³⁻⁵ In fact, the lattice gases corresponding to the Ashkin-Teller model⁶⁻⁸ possess all the features necessary for exhibiting the reorientation process. Furthermore, a very similar symmetry breaking is observable in the formation of antiferromagnetic spin density waves along one of the cubic axes in chromium (for a review see the paper by Fawcett⁹).

Driven lattice-gas models have been extensively studied in the last few years. Katz, Lebowitz, and Spohn¹⁰ have investigated the effect of an electric field on the particle distribution in a half-filled system characterized by an attractive nearest neighbor interaction. They found that the system segregates into two phases with interfaces parallel to the field at low temperatures and a large electric field. The electric field induces anisotropic long range order and enhances the critical temperature. Different approaches and mathematical methods have been developed to investigate this system.¹¹ Models with a repulsive nearest neighbor interaction have also been studied by several authors, who found that the critical tem-

perature decreases with increasing field and the transition becomes first order when the field exceeds a threshold value.^{12,13} Observation of the above phenomenon requires sufficiently strong fields whose potential energy difference between two adjacent sites is comparable to the nearest neighbor interaction. In contrast, the reorientation process may be observed at lower fields, particularly in the vicinity of the critical temperature. By this means, our study may be considered as an extension of previous work thereby providing some opportunity for comparison between the nonequilibrium theories and experiments.

Andersen and Mouritsen¹⁴ have recently studied square lattice-gas models driven by a chemical-potential gradient. In principle the chemical-potential gradient can also induce a reorientation process because the equivalence between the principal directions is broken. In this case the particle distribution becomes inhomogeneous and its analysis goes beyond the ability of our present approach which is restricted to homogeneous states. It is worth mentioning that the field-assisted manipulation of adsorbed atoms on a surface by using a scanning tunneling microscope¹⁵ may be considered as a potential tool for the realization of the present phenomenon.

Here, as a continuation of our previous work,¹ we concentrate on the simplest model and we assume a uniform electric field. Although it is not directly applicable to any real system, the choice of this model is reasonable as its static properties and the kinetics of the ordering process have been studied in detail.^{4,5} The ordering under the electric field is investigated by a Monte Carlo (MC) simulation and analytical calculations that include a simple mean-field approximation and an exact solution on a (2×2) lattice. These methods make evident that one of the chain orientations is favored in the presence of an electric field. In addition, using these methods we are able to analyze the efficiency of proposed techniques such as slow cooling or thermalization at constant temperature under an electric field.

II. THE MODEL

We consider a lattice gas on a square lattice with $L \times L = N$ sites under periodic boundary conditions. We

assume repulsive nearest and next-nearest neighbor interactions with equal strength. For simplicity we choose many parameters (i.e., coupling and lattice constants, electric charge, Boltzmann constant) to be unity. Our study is restricted to a fixed number of particles corresponding to a half-filled lattice. The equilibrium properties of this model were studied by Sadiq and Binder.³ The system undergoes an order-disorder phase transition at a critical temperature $T_c \approx 0.525$.⁴ In this system the ground state is fourfold degenerate, in the corresponding states the columns (or rows) are alternately occupied or empty. From these ground states four types of ordered state, A, B, C, D , originate at finite temperature below T_c . Following the notation by Sadiq and Binder³ the appropriate long range order is characterized by dividing the lattice into four sublattices and introducing μ_s ($s = 1, 2, 3, 4$), the average sublattice occupations. For example, in states A and B the chains are vertical, i.e., $\mu_1 = \mu_4 = 0.5 + x$ and $\mu_2 = \mu_3 = 0.5 - x$, where $0 < x < 0.5$ ($-0.5 < x < 0$) for state A (B). Similar parametrization may be introduced for states C and D characterized by horizontal chains: $\mu_1 = \mu_2 = 0.5 + x$ and $\mu_3 = \mu_4 = 0.5 - x$. In the high temperature state E all

the sublattices are occupied with the same probability, i.e., $\mu_1 = \mu_2 = \mu_3 = \mu_4 = 0.5$.

The stochastic dynamics of the system is described by Kawasaki dynamics¹⁶ characterized by single particle jumps to one of the empty nearest neighbor sites. The jump rate is biased by an electric field.¹ Our analysis is restricted to electric fields parallel to one of the principal axes. In the present MC simulations the electric field strength is also limited, $|e_1|, |e_2| < 0.5$.

This system exhibits anisotropic diffusion (and conduction) in the ordered state because the parallel chains indicate the preferred direction for particle motion. The difference between D_{\parallel} and D_{\perp} vanishes at $T = T_c$ and both coefficients become zero at $T = 0$. Judging from our MC simulations $D_{\parallel} - D_{\perp}$ has a maximum at $T \approx 0.51$ where $D_{\parallel}/D_{\perp} \approx 1.7$.

III. MEAN-FIELD APPROXIMATION

The effect of the electric field on the sublattice occupations has already been studied by using a simple mean-field approximation.¹ For later convenience we recall the time dependence of μ_1 :

$$\tau \frac{d\mu_1}{dt} = -\mu_1 \{ (1 - \mu_2) [f(E_{21} - e_1) + f(E_{21} + e_1)] + (1 - \mu_4) [f(E_{41} - e_2) + f(E_{41} + e_2)] \} \\ + (1 - \mu_1) \{ \mu_2 [f(E_{12} - e_1) + f(E_{12} + e_1)] + \mu_4 [f(E_{14} - e_2) + f(E_{14} + e_2)] \}, \quad (1)$$

and the remaining three equations may be derived by cyclic permutation of indices. In these equations

$$f(z) = \frac{1}{1 + \exp(\beta z)} \quad (2)$$

and E_{rs} is the energy difference between the sublattices r and s . In our previous paper¹ E_{rs} is determined by a simple mean-field approximation. In the absence of an electric field this method reproduced the results of a Bragg-Williams approximation. Now, however, the evaluation of E_{rs} is modified by considering the very fact that the jump takes place from an occupied site to an empty one. This modification results in a lower T_c leaving qualitative features unchanged.

The system has a set of stationary solutions. The appropriate solutions may be considered as modified equilibrium states (A, \dots, E). Instead of analyzing all the possible solutions for a given electric field we study only state A under an electric field which is parallel or perpendicular to the chain direction. This simplification is based on the assumption that state A (B) under a vertical field is equivalent to state C (D) in a horizontal field with the same strength, etc. By this means we can avoid a more complicated formulation.

In state A (or B) this assumption yields an implicit expression of the order parameter $x(T)$, viz.,

$$\left(\frac{1 + 2x}{1 - 2x} \right)^2 = \frac{\cosh(\beta e_{\perp}) + \exp(6\beta x)}{\cosh(\beta e_{\perp}) + \exp(-6\beta x)}, \quad (3)$$

which depends on $e_{\perp} = e_{\perp}$, the perpendicular component of the electric field. This equation demonstrates that the temperature dependence of the order parameter depends on the direction of the applied field. For the parallel electric fields the equilibrium states remain unchanged and the appropriate solution is obtained from Eq. (3) for $e_{\perp} = 0$. If the chain orientation is perpendicular to the applied field then the particle distribution [or $x(T)$] is affected by e_{\perp} as plotted in our previous paper.¹ Evidently, if $x(T)$ is an explicit solution of (3) then $-x(T)$ is also a solution, i.e., the states A and B (as well as C and D) remain equivalent to each other. In addition, (3) has a trivial solution ($x = 0$) corresponding to the high temperature state E .

The high temperature state E is expected to transform into one of the ordered states A, B, C , and D when decreasing the temperature. The critical temperature of the continuous order-disorder phase transitions can be determined by the series expansion of Eq. (3) with respect to x . In the limit $x \rightarrow 0$ this manipulation yields the following implicit equation:

$$\frac{3}{2}\beta_c = 1 + \cosh \beta_c e_{\perp}, \quad (4)$$

where $\beta_c = 1/T_c$. In the presence of a vertical field ($e_{\perp} = 0$) the $E \rightarrow A$ phase transition appears at a temperature $T = T_{c1} = \frac{3}{4}$ independently of the value of e_{\parallel} . At the same time, the above equations suggest another critical temperature T_{c2} if the chains are perpendicular to the applied field. According to Eq. (4) T_{c2} decreases

with increasing e_{\perp} and the change is proportional to e_{\perp}^2 . This equation has no real solution if $e_{\perp} > e_{\text{th}} = 0.6717$. Detailed analysis of the above equations has shown that this phase transition becomes first order when the electric field exceeds the threshold value e_{th} . Similar behavior was found by Leung *et al.*¹² and Dickman¹³ in a driven lattice gas characterized by repulsive nearest neighbor interaction.

To summarize, we have two distinct solutions, one of them is certainly preferred to the other. In thermodynamic equilibrium the stable state is selected by the minimum of free energy. In the presence of an electric field, however, we are not able to define an adequate "nonequilibrium free energy" to be minimized. This difficulty may be circumvented by standard linear stability analysis.

IV. LINEAR STABILITY ANALYSIS

Equation (1) allows us to determine the time dependence of the sublattice occupations around the stationary solutions discussed in the previous section. For this purpose the time dependence of the sublattice occupations is written in the following form:

$$\mu_r(t) = \mu_r^{(s)} + \delta\mu_r \exp(\lambda t), \quad (5)$$

where $\mu_r^{(s)}$ is a stationary solution of (1) and $|\delta\mu_r| \ll \mu_r$. In a linear approximation this assumption yields a simple eigenvalue problem, namely,

$$\lambda \delta\mu_r = \sum_{s=1}^4 M_{rs} \delta\mu_s, \quad (6)$$

where M_{rs} is the derivative of the right-hand side of the corresponding element of (1) with respect to μ_s . After some algebraic manipulation one arrives at the following eigenvalues for the stationary state A :

$$\begin{aligned} \lambda_1 &= 0, \\ \lambda_2 &= -2 + 24\beta\left(\frac{1}{4} - x^2\right)f(e_2)f(-e_2), \end{aligned} \quad (7)$$

$$\begin{aligned} \lambda_3 &= -2\left[\left(\frac{1}{2} + x\right)h(6x, e_1) + \left(\frac{1}{2} - x\right)h(-6x, e_1)\right] \\ &\quad + 12\beta\left(\frac{1}{4} + x^2\right)g(6x, e_1), \\ \lambda_4 &= -2 - 2\left[\left(\frac{1}{2} + x\right)h(6x, e_1) + \left(\frac{1}{2} - x\right)h(-6x, e_1)\right], \end{aligned}$$

where

$$h(6x, e_1) = f(6x + e_1) + f(6x - e_1) \quad (8)$$

and

$$\begin{aligned} g(6x, e_1) &= f(6x + e_1)f(-6x - e_1) \\ &\quad + f(6x - e_1)f(-6x + e_1). \end{aligned} \quad (9)$$

In these expressions the value of x is determined by (3).

The first eigenvector $\delta\mu^{(1)} = (1, 1, 1, 1)$ represents a constant perturbation in agreement with the conservation of particle number. It is easy to check that $\lambda_4 < 0$ for arbitrary T , consequently, any perturbations proportional to $\delta\mu^{(4)} = (1, -1, 1, -1)$ decrease rapidly. The remaining two eigenvalues may be positive indicating the

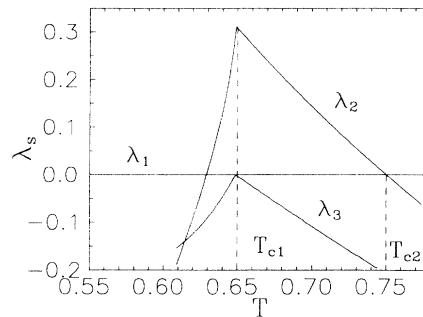


FIG. 1. Temperature dependence of the eigenvalues λ_s for $e_{\perp} = 0.5$.

instability of the given state.

Assuming a vertical electric field ($e_1 = 0, e_2 \neq 0$) in the high temperature state ($x = 0$) $\lambda_2 > 0$ if $T < T_{c2}$ and $\lambda_3 > 0$ if $T < T_{c1}$. Consequently, state E is unstable if $T < T_{c1}$. More precisely, if $T_{c2} < T < T_{c1}$ then $\lambda_2 < 0$ and $\lambda_3 > 0$, therefore any perturbation proportional to the eigenvector $\delta\mu^{(3)} = (1, -1, -1, 1)$ increases exponentially. In this case the particle distribution tends toward state A or B in which the chains are parallel to the applied field. The present result suggests a direct way to produce an ordered state with the desired chain direction. When cooling the system slowly from the disordered state, we can prescribe the chain orientation in the final ordered phase by the application of an electric field. Although λ_2 is also positive if $T < T_{c2}$, λ_3 remains larger than λ_2 . Thus, in the presence of a vertical electric field the present analysis predicts the transformation of state E to states A or B rather than to states C or D .

As expected, in the ordered state all the eigenvalues are negative when the applied field is parallel to the actual chain direction. The effect of the perpendicular field is more complicated. The situation may be visualized by investigating the effect of the horizontal field on state A or B . At low temperatures the eigenvalues are negative. In the close vicinity of T_{c2} , however, λ_2 becomes positive as shown in Fig. 1. The corresponding eigenvector $\delta\mu^{(2)} = (1, 1, -1, -1)$ indicates a rearrangement towards state C or D . In agreement with the subsequent MC simulation these results may be explained by the metastable character of the perpendicular chain orientation which becomes unstable in the close vicinity of the order-disorder phase transition.

V. MONTE CARLO SIMULATIONS

To study the driven lattice gas, MC simulations have been carried out on a square lattice at different electric fields. For details of MC simulations see the review by Binder and Stauffer.¹⁷ Although we produce most of our data with sample sizes 60×60 and 120×120 , we have used different sizes to test the reliability of our data. For practical reasons a MC simulation is restricted to a temperature region in which the diffusion was high enough to reach the equilibrium or steady state within a reasonable run time.

To characterize the “average chain orientation” we introduced an angle $\varphi = \arctan(b_h/b_v)$ where b_h and b_v denote the number of horizontal and vertical bonds. The value of φ vanishes in states A, B and it is 90° in states C, D for $T = 0$. The deviation from $\varphi = 0$ (or 90°) indicates the density of defects characteristic to the states at finite temperatures. This quantity is much less sensitive to the appearance of a mixed state (e.g., polydomain structure of states C and D) compared with the order parameters introduced in the literature.^{3,4} Although we rarely observed the mixed state in our MC simulations, its role becomes more significant when increasing the lattice size.

A. Ordering at fixed temperature

First we studied the instability of the high temperature phase (E) below the critical temperature in a half-filled lattice. Each run was started from a completely disordered state E corresponding to $T = \infty$. The time evolution of φ was monitored at a fixed temperature $T = 0.5$ for various values of the vertical electric field. In these processes the time is measured in units of Monte Carlo steps (MCS) per particle. Figure 2 shows the average behaviors determined from 100 runs for electric fields indicated in the figure caption. In the absence of an electric field, the average φ fluctuates around $\varphi_0 = 45^\circ$ because the chains are oriented horizontally and vertically with the same probability in the final (equilibrium) state. This kind of symmetry is broken when switching a vertical field on.

For low electric fields the chains tend to be oriented vertically rather than horizontally in the final state. Consequently, the average value of φ decreases with the strength of the vertical field. In a few final states we have observed a polydomain structure with a slow spread of vertical domain(s). The linear stability analysis showed that state E definitely tends toward state A or B when the field exceeds a threshold value dependent on temperature as demonstrated by the lowest curve corresponding to $e_2 = 0.25$ in Fig. 2. In other words, for a given electric field there exists a temperature region in which the state E transforms into the state of vertical chains. This

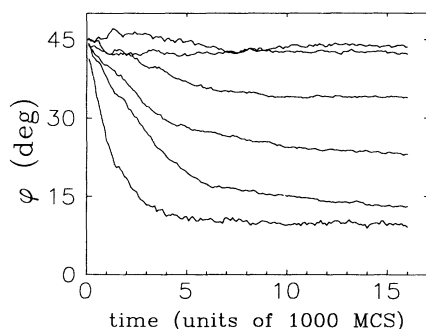


FIG. 2. Average evolution of φ at $T = 0.5$ under different electric fields: $e_2 = 0, 0.05, 0.08, 0.1, 0.13, 0.25$ (from top to bottom). In the initial state the system was completely disordered ($T = \infty$).

fact provides a way to produce an ordered phase with prescribed orientation. The practical application of this method is difficult because in the low field limit the extension of the suitable temperature region is proportional to e_2^2 . This shortcoming inspired us to study the system when it is cooled slowly through the critical temperature under the electric field.

B. Cooling through T_c

In the analogy of the above runs the simulations are started from a disordered state corresponding to the initial temperature ($T_i = 0.55$) above T_c . The temperature is decreased step by step to reach the final temperature $T_f = 0.5$ in time of 16 000 MCS. The time evolutions of the average φ (from 100 runs) are plotted in Fig. 3 for different electric fields. The curves clearly demonstrate the significant effect of the electric field on the particle distribution above the critical temperature. This result confirms the preference of the “vertical clusters” in the critical region above T_c .

Comparing to the previous method, the slow cooling technique seems to be more effective to produce a state with the desired orientation. This advantage is dominant in the low field limit which is important for practical uses. Evidently, the slower the cooling the lower the electric field required to have vertical chains. The numerical analysis of the scaling law, however, goes beyond the scope of the present paper.

C. Reorientation below T_c

In these cases each run was started from a state A following a thermalization of 3000 MCS at a temperature $T < T_c$. We studied the time evolution of the thermalized state when switching on a horizontal or vertical electric field.

The effect of the electric field on the particle distribution depends on the relative direction of the chains. We found that the parallel field causes no significant change

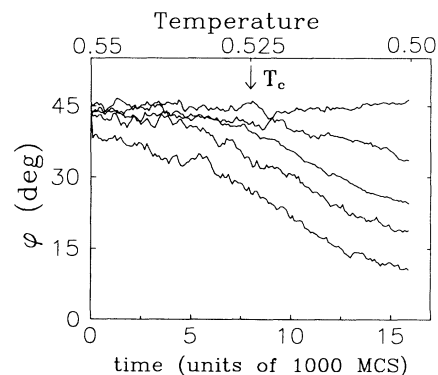


FIG. 3. Time dependence of φ in a slow cooled system under different electric fields: $e_2 = 0, 0.05, 0.08, 0.1, 0.25$ (from top to bottom). The arrow indicates the time when the critical temperature is reached.

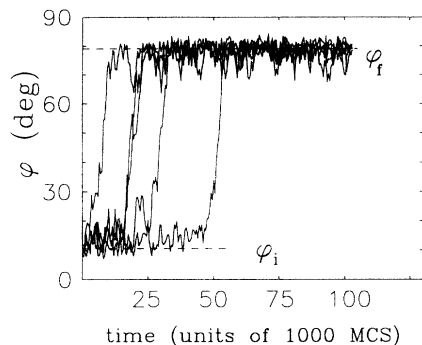


FIG. 4. Time evolution of direction φ in five subsequent simulations for $T = 0.51$, $L = 60$, and $e_{\perp} = 0.1$.

in the particle distribution if $e_{\parallel} < 0.5$. By way of contrast, the application of a perpendicular field results in a complete rearrangement: in the final state the chains are parallel to the electric field. In other words, the initial state A transforms into a steady state C or D . During this process the real time monitoring of the particle distribution demonstrates clearly that the reorientation is analogous to recrystallization including nucleation and growth of the preferred domain(s).

Figure 4 shows some typical time evolutions of φ under the same conditions ($T = 0.51$ and $e_{\perp} = 0.1$). In each curve three regions may be distinguished: the nucleation; the growth of preferred domains; and the stationary state characterized by φ_f , the average value of φ in this final state. In the nucleation interval φ fluctuates around a value close to the initial (or equilibrium) value φ_i . If the electric field is increased the nucleation interval becomes shorter and it disappears above a threshold value. On decreasing the electric field the nucleation interval becomes so long that we are unable to observe the reorientation within the run time. In agreement with the mean-field calculations this behavior may be explained by the metastable character of the states having chains perpendicular to the applied field.

To investigate the rate of reorientation quantitatively we have adopted the definition of relaxation time t_r in-

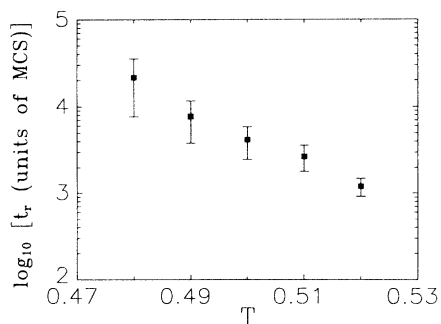


FIG. 5. Reorientation time t_r as a function of temperature for $e_{\perp} = 0.2$. Average values and standard deviations were determined from 100 runs. The solid lines serve to guide the eye.

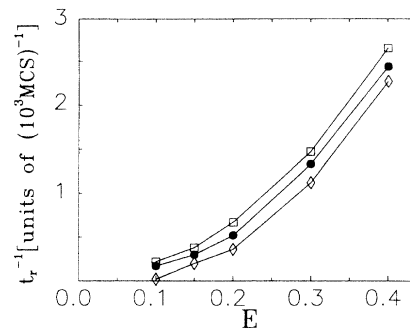


FIG. 6. Rate of reorientation as a function of electric field at fixed temperature $T = 0.51$ for different concentrations: $c = 0.5$ (\diamond); $c = 0.54$ (\bullet); and $c = 0.56$ (\square).

troduced by Binder and Müller-Krumbhaar,¹⁸

$$t_r = \frac{1}{\varphi_f - \varphi_i} \int_0^{t_1} [\varphi_f - \varphi(t)] dt, \quad (10)$$

where φ_i is the equilibrium value of φ in the initial state, φ_f is the stationary value in the final state, and we chose $t_1 \approx 4t_r$ in the MC simulations. The reorientation time decreases with increasing electric field as expected.¹ On the other hand, when the temperature was increased the reorientation process became faster at a fixed value of the electric field as shown in Fig. 5. This effect may be explained by the higher diffusion and by the larger size of the preferred domains in the close vicinity of the critical temperature. In the presence of domains whose size exceeded a critical value the nucleation process is of no importance for the reorientation. Consequently, the metastable states become unstable in the close vicinity of T_c in agreement with the prediction of the mean-field approximation.

In MC simulation the rate of reorientation was characterized by t_r . Its inverse is analogous to λ_2 in the region where $\lambda_2 > 0$. This analogy allows us to make a qualitative comparison between the MC simulation and the stability analysis based on the mean-field approximation. In Fig. 6 the results of MC simulations are plotted at $T/T_c = 0.972$ for three different concentrations. In contrast to the MC simulations the linear stability analysis predicts no reorientation in the metastable region ($\lambda_2 < 0$ if $e_{\perp} < 0.27$). In this region the nucleation mechanism provides a tunnel for the system to reach the stable state.

In order to study the role of nucleation, simulations were performed with extra particles (or holes) added to the system. It was found that when increasing the deviation from the stoichiometric concentration, the nucleation process becomes faster as demonstrated by data (see Fig. 6) for $c = 0.54$ and 0.56 . Similar results were obtained for concentrations $c = 0.46$ and 0.44 in agreement with the particle-hole symmetry.

VI. EXACT SOLUTION ON A 2×2 LATTICE

The exact solutions provide very effective ways of reaching a better understanding. For this purpose the

present model is investigated on a 2×2 lattice with periodic boundary conditions. In this case there exist six particle configurations labeled by $\eta = 1, \dots, 6$ as shown in Fig. 7. The configurations from $\eta = 1$ to 4 may be considered as the ground states A, \dots, D , and configurations 5 and 6 as excited states with the equal energy.

The time dependence of the distribution function $p(\eta, t)$ is determined by a master equation which may be written as

$$\frac{d}{dt}p(\eta, t) = \sum_{\eta'=1}^6 L_{\eta\eta'} p(\eta', t), \quad (11)$$

where the matrix elements are defined by the elementary jumps. Namely,

$$L = \begin{pmatrix} -2a & 0 & 0 & 0 & 2-a & 2-a \\ 0 & -2a & 0 & 0 & 2-a & 2-a \\ 0 & 0 & -2b & 0 & 2-b & 2-b \\ 0 & 0 & 0 & -2b & 2-b & 2-b \\ a & a & b & b & 2a+2b-8 & 2a+2b-8 \\ a & a & b & b & 2a+2b-8 & 2a+2b-8 \end{pmatrix}, \quad (12)$$

where a and b are expressed by the function (2) as

$$a = f(2 + e_1) + f(2 - e_1), \quad (13)$$

$$b = f(2 + e_2) + f(2 - e_2).$$

The solution of (11) may be written in the form

$$p(\eta, t) = \sum_{s=1}^6 c_s p_s(\eta) \exp(\gamma_s t), \quad (14)$$

where γ_s and $p_s(\eta)$ are the eigenvalues and eigenvectors of the matrix L . The coefficients c_s are determined by the initial conditions satisfying the normalization.

Fortunately, the eigenvalues can be evaluated,

$$\begin{aligned} \gamma_1 &= 0, & \gamma_4 &= 2a + 2b - 8, \\ \gamma_2 &= -2a, & \gamma_5 &= -4 + \sqrt{4 + ab - 2a - 2b}, \end{aligned} \quad (15)$$

$$\gamma_3 = -2b, \quad \gamma_6 = -4 - \sqrt{4 + ab - 2a - 2b}.$$

It is easy to check that all the eigenvalues are negative except γ_1 . Consequently, the stationary state corresponding to the first eigenvector is definite, i.e.,

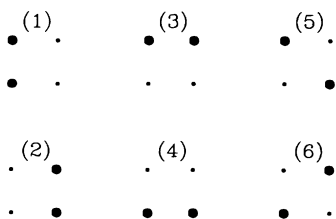


FIG. 7. Configurations on a 2×2 lattice.

$$\begin{aligned} p_1(1) &= p_1(2) = \frac{1}{W} \frac{2-a}{a}, \\ p_1(3) &= p_1(4) = \frac{1}{W} \frac{2-b}{b}, \\ p_1(5) &= p_1(6) = \frac{1}{W}, \end{aligned} \quad (16)$$

where W is the normalization factor. These components of the first eigenvector give the temperature dependence of the probability of each configuration in the stationary state. Figure 8 demonstrates these functions (a) in the equilibrium state and (b) in the presence of a vertical field ($e_1 = 0, e_2 = 0.5$).

The chain configurations ($\eta = 1, \dots, 4$) have the same probability in equilibrium ($a = b$). In this small system the symmetry of the distribution function is not broken because the chain configurations can easily transform to each other via two elementary jumps. The analysis of this finite size effect goes beyond the scope of the present paper. The difference between Figs. 8(a) and 8(b), however, demonstrates clearly the preference of states whose chain direction is parallel to the electric field. More precisely, the probability of configurations 3 and 4, as well as 5 and 6, vanishes at zero temperature. This behavior can be explained by the finding that according to the master equation (11), $2a$ may be identified as the decay rate of states A and B . Similarly, $2b$ describes the decay rate of states C and D . In the presence of a vertical field $a < b$ in which case configurations 1 and 2 are preferred to 3 and 4 as a consequence of their slower decay.

Finally, it is worth mentioning that similar results are obtained when considering the driven lattice gas first studied by Katz *et al.*¹⁰ In this half-filled system, attractive nearest neighbor interaction was assumed, i.e., $J_{NN} = -1$ and $J_{NNN} = 0$. At low temperature the system decomposes into two phases with low and high concentrations. The degeneracy of the ground state is caused by the uncertainty in the position and direction of the

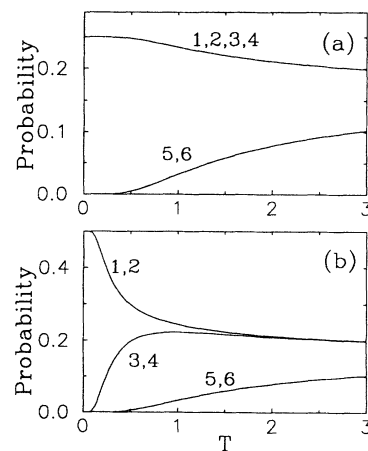


FIG. 8. Temperature dependence of a distribution function for configurations displayed in Fig. 7; (a) in equilibrium, (b) under vertical electric field $e_1 = 0, e_2 = 0.5$.

boundary separating the two phases. In equilibrium the direction of the boundary may be either horizontal or vertical. Under a finite electric field, MC simulations have proved that the phase boundary is parallel to the field in the stationary state. Additional (parallel) phase boundaries were observed under sufficiently high fields. On a 2×2 lattice configurations 1, ..., 4 may be considered as different phase boundaries, therefore the above results offer a hint as to why the boundary lines are parallel to the applied field.

VII. CONCLUSIONS

We have studied the stationary states in a half-filled square lattice-gas model with interactions which support the formation of anisotropic particle distribution. The system is driven by a uniform electric field with a direction parallel to one of the principal axes. Different approaches (MC simulations, mean-field approximation, linear stability analysis, and exact solution on a 2×2 lattice) have been used to investigate the effect of the electric field on the stationary particle distribution. The symmetry causing the fourfold degeneracy of the ground state is broken when the electric field is switched on. In the driven system the states with chains parallel to the field remain stable whereas the other two states (with

perpendicular chains) become metastable or unstable below the critical temperature. Consequently, a reorientation from the vertical chain state to the horizontal one may be induced by the application of a horizontal electric field. This phenomenon is not restricted to the half-filled system; it may be observed in the concentration range exhibiting uniaxial ordering. The reorientation process is analogous to recrystallization. We found that the reorientation time depends strongly on the temperature and strength of field. The application of the electric field may be very useful for the preparation monodomain structures. According to our MC simulations the slow cooling technique seems to be the most effective way to produce a homogeneous phase with a desired orientation. A better understanding of this nonequilibrium process requires the adaptation of more sophisticated techniques as there is only qualitative agreement between the MC simulations and the present analytical calculations.

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¹G. Szabó and A. Szolnoki, Phys. Rev. A **41**, 2235 (1990).

²Y. Enta, S. Suzuki, S. Kono, and T. Sakamoto, Phys. Rev. B **39**, 5524 (1989); H. Kahata and K. Yagi, Jpn. J. Appl. Phys. **28**, L858 (1989); M. Ichikawa and T. Doi, Appl. Phys. Lett. **60**, 1082 (1992).

³A. Sadiq and K. Binder, Surf. Sci. **128**, 350 (1983).

⁴A. Sadiq and K. Binder, Phys. Rev. Lett. **51**, 674 (1983); J. Stat. Phys. **35**, 517 (1984).

⁵H.C. Fogedby and O.G. Mouritsen, Phys. Rev. B **37**, 5962 (1988); K. A. Fichtorn and W. H. Weinberg, Phys. Rev. Lett. **68**, 604 (1992).

⁶J. Ashkin and E. Teller, Phys. Rev. **64**, 178 (1943).

⁷P. Bak, P. Kleban, W.N. Unertl, J. Ochab, G. Akinci, N.C. Bartelt, and T.L. Einstein, Phys. Rev. Lett. **54**, 1539 (1985).

⁸N.C. Bartelt, T.L. Einstein, and L.T. Wille, Phys. Rev. B **40**, 10759 (1989).

⁹E. Fawcett, Rev. Mod. Phys. **60**, 209 (1988).

¹⁰S. Katz, J.L. Lebowitz, and H. Spohn, Phys. Rev. B **28**, 1655 (1983); J. Stat. Phys. **34**, 497 (1984).

¹¹For a review, see B. Schmittman, Int. J. Mod. Phys. B **4**, 2269 (1990).

¹²K.-T. Leung, B. Schmittmann, and R.K.P. Zia, Phys. Rev. Lett. **62**, 1772 (1989).

¹³R. Dickman, Phys. Rev. A **41**, 2192 (1990).

¹⁴J.V. Andersen and O.G. Mouritsen, Phys. Rev. Lett. **65**, 440 (1990); Phys. Scr. T **33**, 141 (1990).

¹⁵J.A. Stroschio and D.M. Eigler, Science **254**, 1319 (1991), and further references therein.

¹⁶K. Kawasaki, Phys. Rev. **145**, 224 (1966).

¹⁷K. Binder and D. Stauffer, in *Applications of Monte Carlo Methods in Statistical Physics*, Topics in Current Physics Vol. 36, edited by K. Binder (Springer-Verlag, Berlin, 1983) p. 1.

¹⁸K. Binder and H. Müller-Krumbhaar, Phys. Rev. B **9**, 2328 (1974).