Generalized mean-field study of a driven lattice gas

György Szabó and Attila Szolnoki
Research Institute for Materials Science, H-1525 Budapest, P.O.Box 49, Hungary
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A generalized mean-field analysis has been performed to study the ordering process in a half-filled square lattice-gas model with repulsive nearest-neighbor interaction under the influence of a uniform electric field. We have determined the configuration probabilities on two-, four-, five-, and six-point clusters, excluding the possibility of sublattice ordering. The agreement between the results of six-point approximations and Monte Carlo simulations confirms the absence of phase transition for sufficiently strong fields.

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I. INTRODUCTION

The driven lattice-gas models have been extensively investigated in order to understand the effect of electric field on the ordering processes (for a review see [1]). These models were introduced as a generalization of the traditional lattice-gas models taking into account the effect of a uniform driving (electric or gravitational) field on the particle jumps [2]. More precisely, besides the nearest-neighbor interactions the particle jumps are affected by a driving field E. In the absence of driving field these systems undergo a well-known phase transition. The external field induces a material transport through the system, modifies the ordering processes, and generates long-range correlations. In this area most of the research activity has been concentrated on the system with attractive interaction.

In this work our attention is focused to the half-filled, two-dimensional lattice gas with repulsive nearest-neighbor interaction. Here we follow the notation given in a previous paper [3]. The equilibrium ($E = 0$) system exhibits a phase transition (at the Néel temperature, T_N) belonging to the Ising universality class. According to renormalization-group [4] and mean-field [5] analyses the sublattice ordering remains continuous for weak driving fields while T_N decreases with E. The sublattice ordering becomes first order above a threshold field and vanishes for $E > 2$ (in units defined later). The mean-field analysis has demonstrated clearly that both the field dependence of critical temperature and the value of threshold field are affected by the choice of jump rate. For example, the threshold field is about 1 or 1.5 when using Metropolis or Kawasaki rates, respectively. Some features of the predicted phase transitions were checked by Monte Carlo (MC) simulations performed on lattices whose sizes were smaller than 60×60 [1,4]. These system sizes, however, are proved to be too small to exhibit the relevant behavior.

Using MC simulations in a previous work we have shown that instead of the homogeneous ordered state a self-organizing polydomain state will be stable at low temperatures for sufficiently large system sizes [3]. Several authors have observed a nucleation process that destroys the monodomain state into a polydomain one [3,6]. This means that the monodomain structure is unstable in the thermodynamic limit. The above phenomena are explained as a consequence of the enhanced particle transport along the domain boundaries leading to interfacial instability. More precisely, a simple phenomenological model was able to describe both the interfacial instability [3] and the existence of a critical nucleon size that depends on field strength.

The translation symmetry is not broken in the polydomain structure at low temperatures, therefore this state is considered as an analytical continuation of the high-temperature one. This fact inspired us to reinvestigate the earlier mean-field analysis based on the hypothetical stability of the symmetry-breaking ordered state at low temperatures. Now we will suppose that the translation invariant state is stable for arbitrary temperatures.

The dynamical mean-field technique was used by Dickman to evaluate the average sublattice occupations and the probability of all the possible configurations on neighboring sites oriented horizontally and vertically [5]. The time-consuming extension of this method for larger clusters is straightforward. These extended methods proved to be very successful for the one-dimensional systems, particularly for a driven lattice gas [7] and stochastic cellular automata [8].

In this work the above model is studied with determining the configuration probabilities on two-, four-, five-, and six-point clusters. Details of such a calculation are given in previous papers [5,7–11], therefore now we concentrate on the discussion of this series of calculations. Within this approach the appearance of polydomain structure is indicated by the strengthening of short-range order, i.e., the configurations corresponding to the ordered particle distributions become dominant on the given cluster.

The output of mean-field calculation is easily comparable with the results of MC simulations. Systematic MC simulations on sufficiently large systems were performed only for $E = 0.4$. Now we have carried out simulations for larger fields. The present MC results confirm our previous conclusions and support the predictions of six-point approximations for sufficiently large fields when the typ-

ical domains are not significantly larger than the cluster used in our six-point approximation.

II. THE METHOD

In the driven lattice-gas model the interacting particles are distributed on the sites of a square lattice imposing periodic boundary conditions. The particle distribution is described by a set of occupation variables n_i taking the values 1 or 0 if a particle is present or absent at site i. In the half-filled ($c = 1/2$) system the particles can jump to one of the empty nearest-neighbor sites with a probability depending on the energy difference between the final and initial positions as formulated in Ref. [3]. To avoid the difficulties that come from the nonanalytic feature of the Metropolis rate we used the Kawasaki rate. Following the traditions the strength of the repulsive nearest-neighbor pair interaction is chosen to be unity. The strength of vertical electric field is measured in such a unit expressing the potential-energy variation for a jump along the field. Choosing $k_B = 1$ the temperature is measured in units of coupling constant. For horizontal jumps the driving field does not modify the jump rates corresponding to detailed balance.

At the level of k-point approximation the translation invariant stationary particle distribution is characterized by the quantity $p_k(n_1, \ldots, n_k)$, which describes the probability of a given $(n_1, \ldots, n_k)$ configuration on a compact cluster of k sites. These quantities satisfy consistency conditions related to translation invariance [7,8] and other symmetry relations [1]. The approach involves finding a hierarchy of equations of motion for these configuration probabilities. The set of these equations is solved numerically in the stationary state.

Using this technique we have determined the configuration probabilities at different levels. In the two-point (pair) approximation the configuration probabilities are evaluated on two neighboring sites oriented horizontally and vertically. Due to the consistency conditions these quantities are described by introducing only two parameters in the half-filled system. For the four-point approximation we need six parameters to characterize the probability of each possible configurations on a 2×2 cluster. In the five-point cluster the central site is surrounded by its nearest neighbors. Finally, different six-point approximations are performed using rectangular clusters of both 2×3 and 3×2 sites. In these latter cases we had to determine 16 and 18 independent parameters. In the present work larger clusters are not investigated because the number of parameters increases rapidly with the cluster size.

To check these results we have carried out MC simulations with varying the temperatures T for $E = 1$, 1.5, 2, 3, and 4. In these simulations the system size is chosen to be much larger than the typical domain size observable when displaying the particle distribution. Namely, the simulations are performed on rectangular boxes with sizes of 256×512 and 180×180 for $E = 1$ and stronger fields, respectively. In each case we have confirmed that the chessboardlike initial configuration transforms into a high-temperature (or polydomain) state after some thermalization. Unfortunately, the relaxation time becomes extremely long for low temperatures. In this situation the simulation of relaxation process may be accelerated by either generating several point defects (Frenkel pairs) in the initial ordered state or using the algorithm described by Sadiq [12]. These simulations justified undoubtedly our basic assumption, namely, the absence of sublattice ordering (long-range order) in the stationary state.

In principle, using MC simulations all the cluster configuration probabilities are easily checkable with a desired accuracy. For simplicity, however, our comparison will be restricted to the values of $p_{\|}(1,0)$ and $p_{\perp}(1,0)$ denoting the probability of $(1,0)$ configurations on neighboring sites oriented parallel or perpendicular to the field. These quantities express the short-range order and the difference between the horizontal and vertical pairs reflects the violation of x-y symmetry. Furthermore, their sum is directly related to the average internal energy.

III. RESULTS

In order to illuminate the predictions of the k-point approximations we report the results in order from $k = 2$ to 6. In the two-point approximation our results agree with those found by Dickman at high temperatures [5]. Figure 1 illustrates the quantities $p_{\|}(1,0)$ and $p_{\perp}(1,0)$ as a function of temperature for some typical values of E. Henceforth the subscript will be omitted if it is possible.

In the absence of driving field the parallel and perpendicular directions are equivalent and $p(1,0) = p(0,1) \to 1/2$ if $T \to 0$. This limit represents a completely ordered (chessboard) structure. For low temperatures an estimation may be given for characterizing the extension of ordered domains along the principal directions. Namely, the probability of finding ordered structure on x subsequent sites is proportional $\exp(-x/\xi)$ where $\xi = -1/\ln[2p(1,0)]$ defines a characteristic length. In

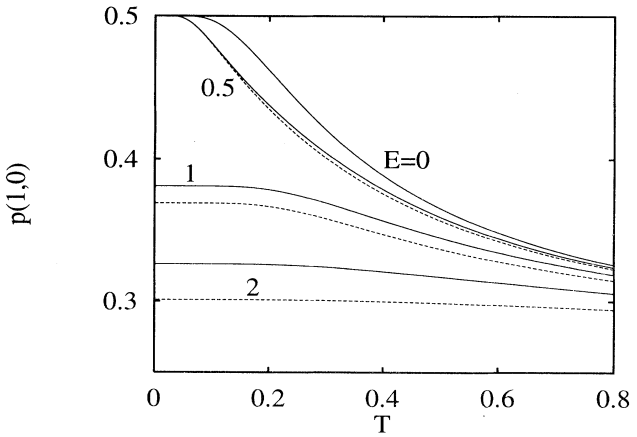

FIG. 1. Temperature dependence of the probability of $(1,0)$ configurations on two neighboring sites positioned parallel (solid line) and perpendicular (dashed line) to the driving field whose strength is indicated by the figures.

this sense, the present calculation suggest a polydomain structure with "typical domain sizes" increasing when the temperature is decreased ($\xi \to \infty$ if $T \to 0$).

For low fields the ordering process is slightly modified. The appearance of large domains is predicted at lower temperature and the ordered regions are elongated along the field. For the fields $E < 1$ the characteristic lengths (ξ) diverge along both directions in the limit $T \to 0$. For stronger fields, however, the formation of large domains is suppressed and the difference between $p_{\|}(1,0)$ and $p_{\perp}(1,0)$ becomes more striking.

From the results of four-point approximation (see Fig. 2) a significantly different picture may be concluded. In the high-field limit this approximation confirms qualitatively the previous results. The violation of x-y symmetry is also recognizable. In spite of our naive expectation we have not found a stable solution satisfying translation invariance at low temperatures for fields $E < 2$. In these cases the numerical solution of the time-dependent equations indicates that the system develops toward the chessboardlike distribution. In the close vicinity of the perfectly ordered state, however, the rounding errors forced the computation to stop. These observations may be interpreted as arguments to support the sublattice ordering. Contrary to the early results this approximation predicts an increase of Néel temperature at low fields. There is another indication making the reliability of the four-point approximation questionable. Namely, the probabilities of the one- and some two-particle configurations coincide for $E = 0$, while the symmetry relations allow them to be different.

To resolve the discrepancy between the suggestions of two- and four-point approximations we have extended the mean-field analysis taking larger clusters into consideration. The results of five-point approximation are plotted in Fig. 3. For low fields the results suggest continuous transition in qualitative agreement with the prediction of two-point approximation. Now the formation of large domains appears at higher temperatures. This calculation predicts first-order transition within a range of electric field as demonstrated by a typical curve ($E = 1$) in Fig. 3. If $E > 1.2$ then the five-point approximation supports that the system remains disordered in the zero-field limit.

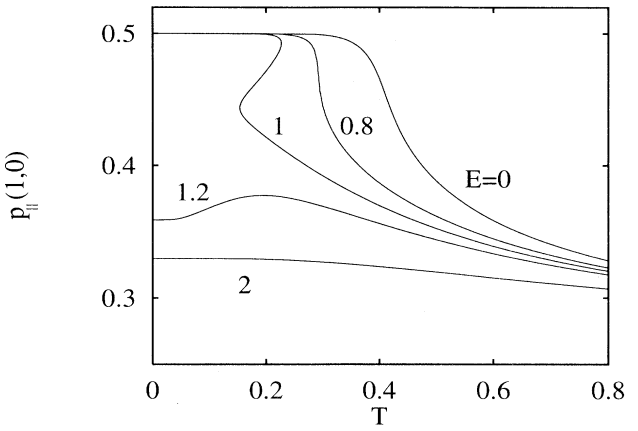

FIG. 3. Configuration probability $p(1,0)$ vs temperature for different fields in the five-point approximation.

Similar set of curves have been obtained when repeating this calculation at the levels of (2×3)- and (3×2)-point approximations. The quantitative agreement with MC data is satisfactory if $E \geq 1.5$ as demonstrated in Fig. 4.

Notice that the MC simulations confirm the absence of phase transitions at the given fields, contrary to early predictions mentioned in the Introduction. In these cases the correlation lengths in both directions (defined above) remain finite in the limit $T \to 0$. For example, decreasing the temperature $\xi_{\|}$ goes to 3.6 if $E = 1.5$. This value of ξ is close to 3, which is the longitudinal size of the cluster providing the best agreement.

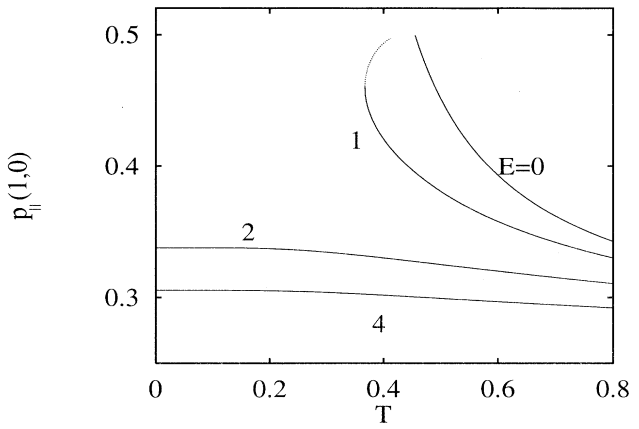

FIG. 2. Probability of (1,0) configuration along the drive as suggested by the four-point approximations for different fields as indicated. Dotted line represents unstable solution.

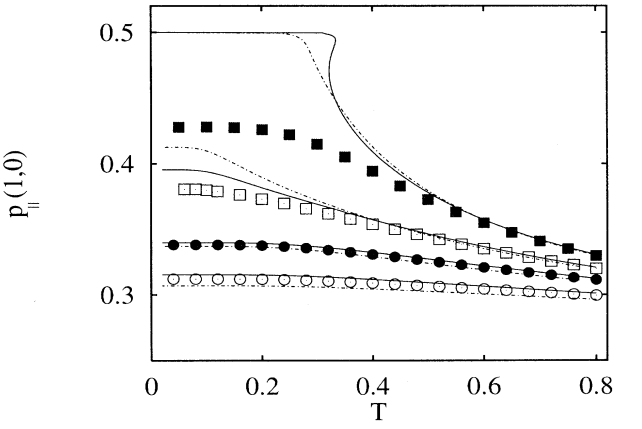

FIG. 4. Comparison of $p(1,0)$ results of (2×3)- (solid lines) and (3×2)-point (dashed lines) approximations with MC data for driving fields $E = 1$, 1.5, 2, and 3 (from top to bottom).

For weaker fields the MC simulations suggest longer correlation lengths in the zero-temperature limit. For example, $\xi_{||} = 6.4$ and $\xi_{\perp} = 5.5$ if $E = 1$ and $T = 0$. In this case the "typical domain" is significantly larger than the clusters used in the present approximations. These "typical domains" (as well as the enhanced material transport along the interfaces maintaining this structure) appear clearly when visualizing the particle distribution during the MC simulations. The complicated structure and pattern formation mechanism cannot be taken into account correctly by such a small cluster. We believe that this is the reason why we have found substantial differences between the predictions of the generalized mean-field analysis and the results of MC simulations for $E = 1$ and lower fields in the low-temperature region.

Obviously, choosing larger and larger clusters, one can increase the accuracy of the present method and shift the boundary of validity toward lower fields and temperatures. Unfortunately, the efficiency of this strategy is questionable because the number of parameters to be determined numerically increases exponentially with the number of lattice points within the cluster.

Beside the x and y directions this technique distinguishes the forward and backward directions in the presence of driving field. As discussed in previous papers [7,11] the difference between the forward and backward directions cannot appear explicitly at the level of pair approximation due to the strong restrictions of consistency conditions. At higher levels, however, differences can appear between the probabilities of two distinct configurations considered as reflections with respect to the transverse symmetry axis of the cluster. In the four-point approximation this type of symmetry breaking may be described by a parameter that is an odd function of E. At the same time we need four parameters to characterize this symmetry breaking on the 2×3 cluster. In general we can say that this forward-backward symmetry breaking is a weak effect. The corresponding parameters vanish both in the absence of driving field and in the disordered (high temperature and/or high field) state.

IV. CONCLUSIONS

The mean-field analysis of the half-filled two-dimensional driven lattice-gas model with repulsive interaction has been revised and extended to the four-, five-, and six-point approximations. In the present investigations we have taken into consideration the results of Monte Carlo simulations. Varying the temperature at some fixed driving fields these simulations have justified the absence of sublattice ordering. That means that in the low-temperature stationary state one can observe a self-organizing polydomain structure. In other words, instead of the long-range order (typical in equilibrium systems) now we can find only short-range order. For such particle distributions the translation invariance of the system is not broken. As a consequence the mean-field analysis may be simplified because the low-temperature (self-organizing polydomain) structure can be considered as an analytical continuation of the high-temperature state.

The mean-field analyses have been performed at different levels. As expected the best agreement with MC data is found when using the largest clusters (2×3 and 3×2) on which the configuration probabilities are evaluated numerically. For driving fields $E = 1.5$, 2, and 3 the six-point approximations give an adequate description of the effect of the driving field on the ordering process. In these cases the typical area of ordered regions is small even at zero temperature. More precisely, it does not exceed the area of cluster we used.

The size difference between the ordered domains and the 2×3 cluster becomes more significant at lower fields because the typical transverse size increases as $1/E$ [3]. In this situation the predictions of the six-point approximations are no longer valid because it cannot take into account the effect of enhanced interfacial material transport responsible for the self-organizing domain structure. Since the capability of the present mean-field analysis is limited we need other approaches to have a more complete description of this nonequilibrium state.

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