

## Brief Reports

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### Coupled-chain approximation for driven lattice-gas models

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A coupled-chain approximation is presented for lattice-gas models driven by an external electric field. The method is used to study a square lattice gas exhibiting anisotropic ground states consisting of alternately occupied and empty rows or columns. This approximation suggests a small decrease in  $T_c$  when increasing the electric field and the continuous phase transition becomes first order.

The chain mean-field approximation was derived to explain the magnetic behavior of chainlike materials.<sup>1,2</sup> In coupled-chain arrays the problem was reduced to that of a single Ising chain in an effective field determined self-consistently by the neighboring ones. The resulting one-dimensional problem is exactly solvable.<sup>3</sup> This method has been successfully adapted for lattice-gas models to study oxygen ordering in the family of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  compounds.<sup>4</sup> The above papers<sup>1,2,4</sup> are restricted to equilibrium systems. Very recently, however, the nonequilibrium phenomena have attracted considerable interest since their analysis goes beyond the ability of traditional statistical physics based on Gibbs ensembles. Such stationary states far from thermal equilibrium may be easily generated by the application of a driving force producing a persistent material transport.

The effect of an external field on segregation was first studied by Katz, Lebowitz, and Spohn<sup>5</sup> in a square lattice gas with attractive nearest-neighbor interaction. The stochastic dynamics of the system is characterized by single-particle jumps to one of the adjacent empty sites and the jump rate is affected by an electric field parallel to one of the principal axes. In this system the phase boundaries become parallel to the applied field and the critical temperature increases with its strength. Detailed analyses (for a review see the paper by Schmittman<sup>6</sup>) have shown that the field results in anisotropic correlations despite the cubic symmetry of the host lattice.

The stationary state of the above driven system was exactly determined by van Beijeren and Schulman<sup>7</sup> in the limit of an infinite ratio of jump rates parallel and perpendicular to the field direction. Furthermore, they assumed the driving force to be infinitely strong. In this particular case the jumps against the field are forbidden and all the correlations along the field are destroyed. In this treatment the problem is reduced to  $d - 1$  spatial dimensions and the master equation governs the particle exchanges between neighboring chains. This method was generalized by Krug *et al.*<sup>8</sup> by taking the density

fluctuations into account. These treatments predicted mean-field-like critical behavior with a small increase of transition temperature  $T_c$ .

The above approximations are restricted to fields of infinite strength. For finite driving fields, however, the interaction between the particles results in such correlations which influence the phase transitions significantly. We studied these correlations in a one-dimensional system in a previous paper.<sup>9</sup> The ordering process is precluded when the electric field exceeds the threshold value related to the interaction. The forward and backward directions may be distinguished as a consequence of persistent material transport. We showed that the prediction of a dynamical pair approximation agrees reasonably well with the results of Monte Carlo simulations. More precisely, this method reproduces the exact result in the absence of an external field. This is why the one-dimensional dynamical pair approximation is considered as a basis for extending the above methods to finite fields.

In this paper we concentrate on a driven lattice gas with repulsive interactions of equal strength between the first and second neighbors ( $J_1 = J_2 = J = 1$ ) on a half-filled square lattice. In the fourfold degenerate ground state the rows (or columns) are alternately occupied or empty.<sup>10</sup> In previous papers the equilibrium properties<sup>10</sup> as well as the domain growth dynamics<sup>10,11</sup> are studied in detail. This system exhibits intrinsically the anisotropic jump behavior assumed as a condition by van Beijeren and Schulman<sup>7</sup> in their approximation. Due to the anisotropic particle distribution the longitudinal diffusion constant and conductivity are larger than the transversal ones.<sup>12</sup> In the presence of an external field the equivalence between the horizontal and vertical directions is no longer valid. Monte Carlo simulations and a four-sublattice mean-field analysis are carried out to investigate the stability of the different states when the driving field is switched on.<sup>12</sup> The states in which the chains are perpendicular to the field become metastable or unstable depending on the temperature

and field strength. In the stable stationary state the chains are oriented along the field. Consequently, this system is an excellent candidate for demonstrating the capability of the present coupled-chain approximation for driven systems.

The dynamical pair approximation is the lowest level of the dynamical mean-field theory suggested by Dickman<sup>13</sup> for investigating the driven systems mentioned above. Within this approximation the probability of a given  $k$ -point configuration on neighboring sites is described as a product of two-point distribution functions. In a one-dimensional system the results of the dynamical pair approximation are evaluated analytically.<sup>9</sup> In the stationary state under electric field  $E$  the probability of the (1, 0) pair configuration is

$$p_2(1, 0) = \frac{-1 + \sqrt{1 + 4c(1-c)(B-1)}}{2(B-1)}, \quad (1)$$

where

$$B = \frac{\exp(-\beta J) + \cosh(\beta E)}{\exp(\beta J) + \cosh(\beta E)}, \quad (2)$$

$c$  is the concentration, and  $T = 1/\beta$  is the temperature. The probability of other pair configurations is determined by sum rules as detailed in Ref. 9.

According to the four-sublattice mean-field approximation<sup>12</sup> the continuous transition from the disordered state to the stable one is in no way affected by the driving field. This prediction was not confirmed by the Monte Carlo simulations because the electric field induced excess defects and resulted in a small decrease of  $T_c$  for  $E < 0.5$ . This shortcoming of the four-sublattice mean-field approximation inspired us to develop a more sophisticated technique described as follows.

The ordered state of the two-dimensional lattice gas may be described as a set of parallel chains with average concentration  $c_0 + x(T)$  and  $c_0 - x(T)$  alternately. The traditional chain mean-field approximation connects these chains with each other via an average chemical potential. In the driven systems, however, the concept of chemical potential is not applicable because of the lack of a consistent theory. This difficulty may be circumvented if we formulate the condition of steady state.

The transversal jumps increase and decrease the concentration in the chains concerned. The rate of such an elementary process is the product of the jump rate and the probability of the 12-point configuration, which includes the pair and its neighbors affecting the jump. Here we assume that the relation between the neighboring chain configurations is completely determined by the alternate concentrations. In the stationary state the sum of the contributions over all the possible configurations vanishes. This manipulation gives an implicit equation for  $x(T)$  which can be solved numerically. Henceforth, the numerical solution is restricted to the half-filled lattice ( $c_0 = 0.5$ ).

This approximation suggests the phase transition to be continuous if the driving field does not exceed a threshold value, i.e.,  $E < E_{th} = 0.90$ . In thermal equilibrium  $T_c(E = 0) = 0.4716$  and the transition temperature decreases with the field as shown by the solid curve in Fig. 1.

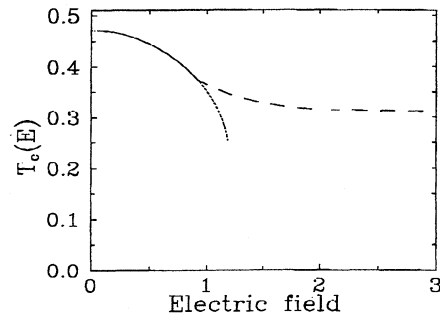


FIG. 1. Critical temperature vs external field; solid and dashed lines represent second- and first-order phase transitions. The dotted line represents the analytical continuation of the second-order phase transition.

The variation of  $T_c$  is proportional to  $E^2$  in the low field limit. The analytical continuation of this second-order phase transition is denoted by a dotted curve in Fig. 1. This curve indicates that a hysteresis may appear in a limited region as was discussed by Dickman.<sup>14</sup> It is worth mentioning that previous Monte Carlo simulations suggest a slightly higher transition temperature ( $T_c^{MC} = 0.525$ ) in equilibrium.<sup>10,11</sup>

If the driving field exceeds the threshold value then the ordering process is first order and the transition temperature tends to a constant value [ $T_c(E = \infty) = 0.3114$ ] as plotted in Fig. 1. The transition temperature is  $0.80T_c(E = 0)$  at the tricritical point ( $E = E_{th}$ ).

The existence of a tricritical point has already been suggested by Leung *et al.*<sup>15</sup> and Dickman<sup>13</sup> in a square lattice gas with a repulsive first-neighbor interaction. In this system an ordered (chessboard-like) phase appears below a critical temperature. The phase transition remains continuous only for weak driving fields, and  $T_c$  decreases with the field strength. For a larger field the transition becomes first order and disappears above a threshold value. In other words, this type of ordered structure is destroyed by the strong electric field.

In the present model, however, the transition temperature remains finite in the strong field limit, i.e., the chain structure oriented along the field is stable for arbitrary strength. At the same time, the ordered states with perpendicular chains are completely destroyed by the strong fields. In the low temperature limit the stable states become completely ordered and the particle jumps are blocked along the occupied chains therefore the driving field cannot affect this type of ordered state.

Preliminary Monte Carlo simulations confirm the small decrease of the critical temperature. Rigorous Monte Carlo simulations require long runs because of the enhanced fluctuations induced by the driving field. This analysis is in progress.

It is worth mentioning that the present model has been studied by following the method (dynamical pair approximation) suggested by Dickman.<sup>13,14</sup> Unfortunately, this method as well as the equilibrium pair approximation predict a first-order phase transition for this model. The failure of the dynamical pair approximation is particularly interesting because our chain approximation may be

considered as a simplified dynamical pair approximation. More precisely, in our approximation the configurations in neighboring chains of alternate density are independent of each other whereas the dynamical pair approximation takes the transversal correlations explicitly into consideration.

In summary, we have described a simple coupled-chain approximation for studying driven lattice gases. This method is based on the analytical solution of the one-dimensional driven lattice gas in a dynamical pair approximation. The capability of this approximation is demonstrated by applying it to a two-dimensional lattice gas in which the particles form parallel chains along the applied field. In this system the particles prefer the

longitudinal jumps to the transversal ones and the difference results in a time scale separation of longitudinal and transversal relaxation rates. This feature seems to be very advantageous for this very simple approximation. According to the coupled-chain approximation the ordering temperature decreases with the field strength and tends to a constant value. Furthermore, the continuous phase transition becomes first order when the driving field exceeds a threshold value. These suggestions agree reasonably well with the results of preliminary Monte Carlo simulations.

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