

Correlations induced by transport in one-dimensional lattice gas

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Using dynamical mean-field theory, we study the two-, three- and four-point correlations in a one-dimensional lattice gas driven by a uniform electric field. In the zero-temperature limit, the ordering is precluded when the electric field exceeds a critical value. The electric field results in a breaking of reflection symmetry in the four-point configurations.

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I. INTRODUCTION

Nonequilibrium phenomena have extensively been studied in lattice-gas models driven by electric fields (for a recent review see the paper by Schmittman [1]). These investigations are concentrated on two-dimensional systems with first-neighbor interactions. The critical temperature of the order-disorder transition increases (decreases) with the field for attractive (repulsive) interactions [2, 3]. For repulsive interaction the ordering is suppressed when the electric field exceeds a threshold value [3, 4, 6, 7]. Very recently Hwang, Schmittman, and Zia [5] have found that the three-point correlation becomes nontrivial in a driven two-dimensional lattice gas.

In a one-dimensional system the situation is different because the critical temperature is zero. In early papers the particle transport was studied within the framework of linear approximation [8–10]. In a comparison with two-dimensional systems Katz, Lebowitz, and Spohn [3] briefly considered both the particle transport and the structure function in such a system by Monte Carlo simulation.

In the present paper we have adopted the dynamical mean-field approximation used by Dickman [6, 7] for investigating the nonequilibrium phase transition in two-dimensional systems. In a one-dimensional lattice gas, this method becomes very simple and the analytical result reproduces the exact pair-correlation function [11] in the absence of an electric field. In comparison with Monte Carlo data we have found, however, a small difference (a few percent) in the presence of an electric field. This defect inspired us to extend the dynamical pair approximation. The four-point approximation is capable of describing reflection symmetry breaking in configuration of particles located on four adjacent sites. More precisely, we have found that the probabilities of the configurations (0010) and (0100) are not equivalent in the presence of the electric field. Similar reflection symmetry breaking is prohibited by the translation invariance for the two- and three-point configurations as detailed in the subsequent section. In Sec. III the model is studied at the level of dynamical pair approximation. The results of the three- and four-point approximations are presented in Sec. IV. In numerical analyses including Monte Carlo simulations

we restrict ourselves to repulsive nearest-neighbor interaction in a half-filled lattice.

II. FORMALISM

We study a one-dimensional lattice-gas model described by the usual Hamiltonian

$$H = J \sum_i n_i n_{i+1}, \quad (1)$$

where J is the nearest-neighbor interaction and $n_i = 0$ if site i is empty and $n_i = 1$ if occupied. The stochastic dynamics of the system is described by Kawasaki dynamics [12] characterized by single-particle jumps to one of the nearest-neighbor sites. The jump rate $\Gamma(i \rightarrow i \pm 1)$ from site i to $i \pm 1$ is affected by a uniform electric field E at a temperature T , namely,

$$\Gamma(i \rightarrow i \pm 1) = \frac{1}{1 + \exp[\beta(\Delta H \mp E)]}, \quad (2)$$

where ΔH is the energy difference between the final and initial states and $\beta = 1/T$.

Assuming translation invariance the probability of a given k -point configuration (n_1, \dots, n_k) on subsequent sites $(i + 1, i + 2, \dots, i + k)$ of the lattice is denoted by $p_k(n_1, \dots, n_k)$. These quantities are normalized,

$$\sum_{n_1, \dots, n_k} p_k(n_1, \dots, n_k) = 1 \quad (3)$$

and they satisfy the following conditions:

$$p_k(n_1, \dots, n_k) = \sum_{n_{k+1}} p_{k+1}(n_1, \dots, n_k, n_{k+1}), \quad (4)$$

$$p_k(n_1, \dots, n_k) = \sum_{n_0} p_{k+1}(n_0, n_1, \dots, n_k).$$

It is evident that on a single lattice point

$$p_1(0) = 1 - c, \quad p_1(1) = c, \quad (5)$$

where c is the average particle concentration. According to the above equations the probability of the two-point configurations may be given as

$$\begin{aligned}
p_2(0,0) &= (1-c)^2 + z, \\
p_2(0,1) &= p_2(1,0) = c(1-c) - z, \\
p_2(1,1) &= c^2 + z,
\end{aligned} \tag{6}$$

where z is the pair correlation function. It is emphasized that we need only one additional parameter (z) to express the above probabilities for a fixed concentration. Following this strategy at higher level, Eqs. (3) and (4) may also be satisfied by suitable parametrization of the configuration probabilities. For this purpose we suggest an iterative way if $k > 1$:

$$\begin{aligned}
p_{k+1}(n_1, \dots, n_{k+1}) &= \frac{p_k(n_1, \dots, n_k)p_k(n_2, \dots, n_{k+1})}{p_{k-1}(n_2, \dots, n_k)} \\
&\quad + \eta_k(n_1, \dots, n_{k+1}).
\end{aligned} \tag{7}$$

In this notation $\eta_k(n_1, \dots, n_k)$ indicates an extra correlation that goes beyond the prediction of a mean-field theory of lower level. The possible values of these correlations, however, are strongly constrained by Eqs. (3) and (4). For the three-point configuration these quantities are expressed by introducing two additional variables, v_1 and v_2 :

$$\begin{aligned}
\eta_3(0,0,0) &= \eta_3(1,0,1) = -\eta_3(0,0,1) \\
&= -\eta_3(1,0,0) = v_1, \\
\eta_3(0,1,0) &= \eta_3(1,1,1) = -\eta_3(0,1,1) \\
&= -\eta_3(1,1,0) = v_2.
\end{aligned} \tag{8}$$

No reflection symmetry breaking can be observed in the two- and three-point configurations because $p_2(1,0) = p_2(0,1)$, $p_3(1,0,0) = p_3(0,0,1)$, and $p_3(1,1,0) = p_3(0,1,1)$. These equalities may be considered as special cases of a more general relation derived from Eqs. (4);

$$p_k(0, \dots, 0, 1) = p_k(1, 0, \dots, 0), \tag{9}$$

$$p_k(1, \dots, 1, 0) = p_k(0, 1, \dots, 1),$$

where the dots represent empty (occupied) sites in the first (second) expression.

With the four-point configurations, however, some reflection symmetry breaking is allowed because

$$\begin{aligned}
\eta_4(0,0,0,0) &= \eta_4(1,0,0,1) = -\eta_4(0,0,0,1) \\
&= -\eta_4(1,0,0,0) = w_1, \\
\eta_4(0,0,1,0) &= \eta_4(1,0,1,1) = -\eta_4(0,0,1,1) \\
&= -\eta_4(1,0,1,0) = w_2, \\
\eta_4(0,1,0,0) &= \eta_4(1,1,0,1) = -\eta_4(1,1,0,0) \\
&= -\eta_4(0,1,0,1) = w_3, \\
\eta_4(0,1,1,0) &= \eta_4(1,1,1,1) = -\eta_4(0,1,1,1) \\
&= -\eta_4(1,1,1,0) = w_4;
\end{aligned} \tag{10}$$

consequently the probability $p_4(0,0,1,0)$ may differ from $p_4(0,1,0,0)$. This type of reflection symmetry breaking is characterized by

$$\Psi = w_2 - w_3 \tag{11}$$

because there are three additional pairs of four-point configurations which exhibit reflection symmetry breaking with the same measure. In equilibrium (no electric field) $\Psi = 0$.

In the half-filled system ($c = \frac{1}{2}$) the particle-hole symmetry reduces the number of free parameters. In this particular case $v_1 = v_2$ and $w_1 = w_4$.

III. DYNAMICAL PAIR APPROXIMATION

The dynamical mean-field theory can be carried out at different levels (for details see the papers by Dickman [6, 7] and further references therein). In the dynamical pair approximation we assume that $\eta_k(n_1, \dots, n_k) = 0$ if $k > 2$. In other words, the probability of a given k -point configuration is determined by the pair distributions as

$$p_k(n_1, \dots, n_k) = p_2(n_1, n_2) \prod_{j=2}^{k-1} \frac{p_2(n_j, n_{j+1})}{p_1(n_j)}. \tag{12}$$

Consequently, we have only one parameter (z) to be evaluated for a fixed concentration.

The elementary jumps give gain and loss contributions to the probability of a given pair configuration. The rate of such a process is the product of the jump probability given by Eq. (2) and the probability of the four-point configuration, which includes the pair and its neighbors affecting the jump. In the stationary state the time derivative of $p_2(n_1, n_2)$ vanishes for any configuration. Summarizing all the contributions for $p_2(0,0)$ (or any other) one obeys the following result:

$$p_2(1,0) = \frac{-1 + \sqrt{1 + 4c(1-c)(B-1)}}{2(B-1)}, \tag{13}$$

where

$$B = \frac{\exp(-\beta J) + \cosh(\beta E)}{\exp(\beta J) + \cosh(\beta E)}. \tag{14}$$

In the absence of an electric field ($E = 0$) these expressions reproduce the exact result obtained by the transfer matrix technique (see, for example, the book by Baxter [11]). In the presence of an electric field, however, we should use Monte Carlo simulations to check the accuracy of the above approach.

The Monte Carlo simulations were carried out on a half-filled ($c = \frac{1}{2}$) lattice of 4096 sites with periodic boundary conditions. In the standard simulations we restricted ourselves to repulsive interaction ($J = 1$). The runs were performed at different temperatures and electric fields. The particle current and probabilities of two-, three-, and four-point configurations were calculated by averaging over 100 000 Monte Carlo steps per site in each run.

A comparison between the pair approximation and the

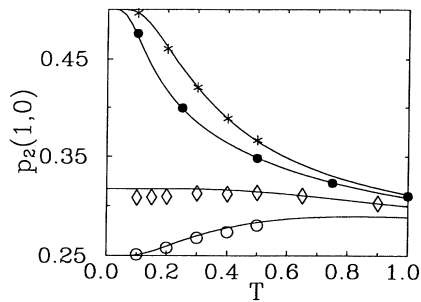


FIG. 1. Probability of (1,0) pair configuration as a function of temperature. Monte Carlo data are shown for different electric fields: $E = 0$ (*); $E = 0.5$ (•); $E = 1$ (◊); $E = 1.5$ (○). Solid lines represent the results of dynamical pair approximation.

Monte Carlo simulation is demonstrated in Fig. 1 where the solid lines are obtained from Eqs. (13) and (14). In this figure the statistical error of the Monte Carlo simulations is comparable to the line thickness. The difference between the results of these methods, having a maximum at $E \approx 1$, is less than three percent.

The results clearly show that the system goes to an ordered state with decreasing temperature if $E < 1$. No ordering can appear at zero temperature when the electric field is strong enough to overcome the strength of interaction, i.e., $E > |J|$ (these statements remain valid for attractive interaction too). Similar behavior was observed in a two-dimensional lattice gas with repulsive first-neighbor interaction for sufficiently strong fields [4, 7].

In the knowledge of distribution functions we can easily determine the particle current as well as the dc conductivity. The temperature and concentration dependence of dc conductivity agree with the previous results [8–10]. For $c = \frac{1}{2}$ the ordering process prevents the particle jumps; therefore particle transport decreases with temperature if $E < |J|$. In contrast to this, particle current I goes to a saturation value I_s when decreasing the temperature for $E > |J|$. Persistent current is an appropriate characteristic of this nonequilibrium state. This phenomenon is displayed in Fig. 2. In this figure

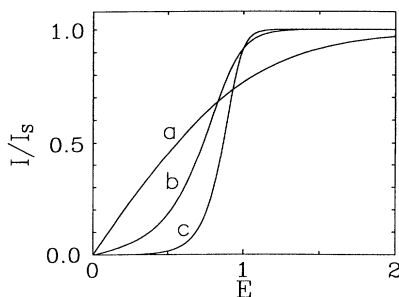


FIG. 2. Electric-field dependence of particle current related to the saturation value for different temperatures: (a) $T = 0.05$; (b) $T = 0.2$; (c) $T = 0.5$.

the Monte Carlo data are omitted because of their small deviations from the results of pair approximation.

IV. THREE- AND FOUR-POINT APPROXIMATION

In the three-point approximation the probability of any particle configuration is given by three parameters, z , v_1 , and v_2 . At this level of the dynamical mean-field theory, however, one finds that $v_1 = v_2 = 0$. In other words, the three-point approximation cannot go beyond the pair approximation detailed above. It is emphasized that v_1 and v_2 do not vanish at the higher level of the dynamical mean-field theory as sketched below.

In the four-point approximation it is assumed that $\eta_k(n_1, \dots, n_k) = 0$ for $k > 4$. In this case the probability of the configurations is characterized by seven parameters. On the analogy of pair (and three-point) approximation these quantities are determined by a set of equations from the time derivative of the probability for those configurations which are linearly independent.

It is easy to check that a comparison between the time derivatives of $p_3(0, 0, 0)$ and $p_4(0, 0, 0, 0)$ as well as $p_3(1, 1, 1)$ and $p_4(1, 1, 1, 1)$ gives

$$w_1 = w_4 = 0 \quad (15)$$

independently of c and E . The remaining quantities (z, v_1, v_2, w_2, w_3) are evaluated numerically. In the present work we simplified the numerical analysis by restricting ourselves to a half-filled system providing $v_1 = v_2$.

In the four-point approximation the temperature dependence of the pair correlation z agrees reasonably well with those results obtained from the dynamical pair approximation. The agreement with the Monte Carlo data, however, became much better. More precisely, the numerical results reproduce the Monte Carlo data within the statistical error (less than 10^{-3}) except for a narrow region of the electric field ($E \approx 1$) where the deviation is less than one percent. These results confirm the general conclusions drawn on the basis of pair approximation.

In agreement with expectations the extra correlations v_1, w_2, w_3 vanish for $E = 0$. Furthermore, these quantities also vanish in the limit $T \rightarrow 0$ except for the value of the electric field $E = 1$. This latter fact refers to a critical behavior when the electric field exceeds the critical value ($E = 1$) in the zero-temperature limit. Obviously, for a more accurate description in this critical region we need to extend the dynamical mean-field approximation to a higher level. In the high-temperature limit no correlations can be observed.

The most striking result of the present work is the reflection symmetry breaking generated by the electric field. This phenomenon is illustrated in Fig. 3 where the solid line is derived from the four-point approximation. The size of the data symbols is characteristic of the statistical error of the Monte Carlo simulation. This figure clearly shows that Ψ is an odd function of electric field for a fixed temperature. According to our numerical analysis $\Psi \propto E^3$ in the low-field limit. This relationship suggests

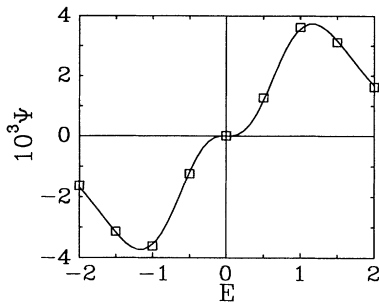


FIG. 3. Reflection symmetry breaking induced by electric field for a fixed temperature $T = 0.5$. Solid line is predicted by the four-point approximation, squares represent Monte Carlo data.

a simple way of determining the direction of particle current from the particle distribution at a given moment.

V. CONCLUSIONS

We have studied the two-, three-, and four-point correlations in a half-filled one-dimensional lattice gas driven by a uniform electric field. In this system there is a competition between the first-neighbor interaction and the electric field. The first-neighbor interaction forces the system to form an ordered structure in the zero-temperature limit at the same time the biased hopping mechanism prevents the survival of any local order. As a result of this competition the ordering process is pre-

vented by the electric field if its magnitude exceeds the strength of the first-neighbor interaction. The lower the temperature the sharper the order-disorder transition when increasing the electric field ($E \approx 1$). In the (nonequilibrium) disordered phase a saturation particle current remains present in the limit $T \rightarrow 0$.

Despite its simplicity, dynamical pair approximation gives a satisfactory description of the phenomenon mentioned above. Due to the absence of extra correlations this approach reproduces the exact results for $E = 0$. In the low-temperature limit the extra three- and four-point correlations we have studied are proportional to E^2 or E^3 . This is the reason that the pair approximation describes correctly the concentration and temperature dependence of the dc conductivity.

In equilibrium, the right- and left-hand directions are equivalent. This equivalence, however, is no longer valid in the presence of an electric field. It is found that the electric field induces extra correlations including reflection symmetry breaking which may be observed in the probabilities of four-point configurations. In the knowledge of the stationary particle distribution this reflection symmetry breaking allows us to determine the direction of particle current. The measure of these extra correlations, however, is very weak except in the close vicinity of the order-disorder transition at low temperatures.

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- [1] B. Schmittman, *Int. J. Mod. Phys. B* **4**, 2269 (1990).
 - [2] S. Katz, J. L. Lebowitz, and H. Spohn, *Phys. Rev. B* **28**, 1655 (1983).
 - [3] S. Katz, J. L. Lebowitz, and H. Spohn, *J. Stat. Phys.* **34**, 497 (1984).
 - [4] K.-T. Leung, B. Schmittman, and R. K. P. Zia, *Phys. Rev. Lett.* **62**, 1772 (1989).
 - [5] K. Hwang, B. Schmittman, and R. K. P. Zia, *Phys. Rev. Lett.* **67**, 326 (1991).
 - [6] R. Dickman, *Phys. Rev. A* **38**, 2588 (1988).
 - [7] R. Dickman, *Phys. Rev. A* **41**, 2192 (1990).
 - [8] W. Dieterich, I. Peschel, and W. R. Schneider, *Commun. Phys.* **2**, 175 (1977).
 - [9] J. C. Kimball and L. W. Adams, *Phys. Rev. B* **18**, 5851 (1978).
 - [10] H. Singer and I. Peschel, *Z. Phys. B* **39**, 333 (1980).
 - [11] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, London, 1982).
 - [12] K. Kawasaki, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 2.