Non-equilibrium phase transition in a two-temperature lattice gas

Attila Szolnoki

Research Institute for Materials Science, H-1525 Budapest, POB 49, Hungary

A two-temperature lattice gas model with repulsive nearest-neighbour interactions is studied using Monte Carlo simulations and dynamical mean-field approximation. The evolution of the two-dimensional, half-filled system is described by an anisotropic Kawasaki dynamics assuming that the hopping of particles along the principal directions is governed by two heat baths at different temperatures $T_x$ and $T_y$. The system undergoes an order-disorder phase transition as $T_x$ ($T_y$) is varied for sufficiently low fixed $T_y$ ($T_x$). The non-equilibrium phase transition remains continuous and the critical behaviour belongs to the Ising universality class. The measure of violation of the fluctuation-dissipation theorem can be controlled by the value of the fixed temperature. We have found an exponential decay of spatial correlations above the critical region in contrast to the two-temperature model with attractive interactions.

05.50.+q, 05.70.Ln, 64.60.Cn

I. INTRODUCTION

The study of driven diffusive lattice gas model, which served a convenient tool to produce stationary non-equilibrium state, revealed a lot of new phenomena compared to the corresponding equilibrium properties [1]. Such a phenomenon is the emergence of a novel non-equilibrium fixed point of critical behaviour in the case of attractive interactions or the surprising feature of the fluctuations of internal energy [2]. In this model an external uniform electric field is applied to induce a preferential hopping in one direction leading to a permanent particle transport in the stationary state [3]. Unfortunately, it is rather difficult to realise the model in laboratory because the driving field cannot be derived as the gradient of an electrostatic potential.

This problem can be avoided if we use an alternating field instead of the uniform one, which also enlarges the probability of jumps along specified lattice directions without resulting in a non-zero average particle current. Similar effect can be obtained in a two-temperature model where the hopping of particles along the principal directions is governed by two heat baths at different temperatures $T_x$ and $T_y$. Now the flow of energy between the heat baths drives the system into a non-equilibrium stationary state. The non-equilibrium phase diagrams have already been studied in two-dimensions in the case of attractive interactions [3] and for nearest- and next-nearest neighbour repulsive interactions [8]. Common feature of the two diagrams is the existence of an ordered phase even at $T_x = \infty$, if $T_y$ is low enough. Similar behaviour is observed when the uniform electric field drives the systems into non-equilibrium states. Here the ordered phases also exist at infinite $E$ if the temperature is low enough [4]. Completely different behaviour is found for nearest-neighbour repulsive interactions where the field induced interfacial transport prevents the long-range ordering [4]. Although similar effect cannot be expected for the corresponding two-temperature model because of the zero macroscopic current, still the stability of the ordered phase is doubtful [6].

In this paper we determine the phase diagram of a two dimensional two-temperature model with nearest-neighbour repulsive interactions. For this purpose we perform dynamical mean-field analysis to calculate the phase transition points. These results are supported by Monte Carlo simulations. We also study how the non-equilibrium conditions influence the critical behaviour of the system. This problem is especially exciting because similar non-equilibrium perturbation results in a critical behaviour different from its equilibrium counterpart in some models where the global current vanishes [4,5]. The finite-size scaling of the MC data indicates that the present model falls into the universality class of the equilibrium Ising model in agreement with a theoretical prediction [2].

The next section is devoted to the violation of fluctuation-dissipation theorem (FDT) which is generally one of the benchmarks of non-equilibrium phenomena. The breakdown of this theorem results in a difference between the specific heats defined as the temperature derivative of the average energy on the one hand and derived from the fluctuations of energy on the other hand. For example, in the uniformly driven model with attractive interaction the field suppresses the fluctuations and the difference is relevant [3]. Using both ways we calculate the specific heat for our model and show that the rate of the violation of FDT can be influenced by the variation of the fixed temperature.

A wide variety of non-equilibrium systems exhibit "generic scale invariance", namely, long-range spatial correlations for arbitrary parameter values. An example of such a system is the two-temperature model with attractive interactions where a power law decay of pair correlation function is observed for all temperatures above criticality [4]. We also examine the two-point correlations of our model and find short-range correlations at high temperatures.
II. THE MODEL

Consider a two-dimensional lattice gas on a square lattice with $L \times L = N$ sites under periodic boundary conditions. The occupation variables $n_i = 0$ or $1$ (if the lattice site is empty or occupied) and we assume half-filled occupation ($\sum_i n_i = N/2$). The Hamiltonian is given by

$$H = -J \sum_{(i,j)} n_i n_j$$

(1)

where the summation is over nearest-neighbour pairs and $J = -1$. Kawasaki exchange dynamics is assumed [14], namely the particles can jump to one of the empty nearest-neighbour sites. Anisotropic hopping rates are used for directions $\alpha = x$ or $y$:

$$g_\alpha(\Delta H) = \frac{1}{1+\exp(\Delta H/T_\alpha)}$$

(2)

where $\Delta H$ is the energy difference between the final and initial configurations. The lattice constant and the Boltzmann constant are chosen to be unity as usual.

In the case of $T_x = T_y$, the above model is equivalent to the celebrated kinetic Ising model which undergoes a continuous phase transition at $T_N = 0.567$. Below $T_N$ the system orders into a checkerboard-like pattern. If the lattice is divided into two interpenetrating sublattices ($A$ and $B$) then particles prefer staying in one of these sublattices. Hence the difference between the two averaged sublattice occupations is the global order parameter: $m = |\rho_A - \rho_B|$, where $\rho_A$ denotes the averaged occupation of sublattice $A$. A suitable local order parameter is the staggered magnetization at site $j$: $\phi_j = (-1)^j(2n_j - 1)$. It is important to note that $\phi$ is not conserved resulting in an important effect on the spatial correlations at high temperatures.

When $T_x$ and $T_y$ are different the energy flows permanently from the heat bath of higher temperature to the lower one through the system and maintains a stationary non-equilibrium state. In other two-temperature model the previous studies set one of the temperatures (e.g. $T_y$) to be infinite, which reduced the number of control parameter to one [14] and the phase transition was studied as a function of $T_x$. Now we cannot use this simplification because the long-range ordered phase is expected to be unstable when one of the temperature is too high (the explanation of this expectation will be given in the next section). Therefore we keep $T_y$ at a constant (finite) value when we vary $T_x$ to find the order-disorder transition point. Naturally similar behaviour would be obtained by exchanging the roles of the two temperatures.

III. PHASE TRANSITION AND CRITICAL BEHAVIOUR

The study of non-equilibrium phase diagram by dynamical mean-field approach proved to be useful in many instances [14]. In this approach we determine the stationary solution of the equations describing the time evolution of configuration probabilities. At the level of $k$-point approximation, these probabilities are given by probabilities of the possible configurations on $k$-point clusters. We refer to [14] for further details of this method.

First we use the two-point level, consequently correlations larger than two lattice constants are neglected. In spite of this simplification, the simple approximation predicts the relevant features of the phase diagram well as shown in Fig. 2. Namely, the ordered phase becomes unstable even at $T_y = 0$ if $T_x$ is high enough. This behaviour may be understood qualitatively because the nearest-neighbours of the occupied lattice sites are empty in the ordered phase. Therefore the high temperature can influence the jumps and particles may leave the preferred sublattice. The phase transition remains continuous at any value of $T_y$. Evidently, the quantitative predictions of this approximation are far from the correct values (e.g. $T_c^{2P}(T_x = T_y) = 0.72$, $T_c^{2P}(T_y = 0) = 1.18$).

To obtain more accurate data, we apply four-point approximation. Here we have to solve a system of eight coupled nonlinear equations numerically. The results (e.g. $T_c^{4P}(T_x = T_y) = 0.60, T_c^{4P}(T_y = 0) = 0.76$) are already comparable to the data of Monte Carlo simulation as shown in Fig. 2. (The simulation data $T_c^{MC}(T_x = T_y) = 0.56$ and $T_c^{MC}(T_y = 0) = 0.74$). The phase transition is continuous even at $T_y = 0$, therefore the order parameter decreases gradually when $T_x$ tends to the the transition point as Fig. 2 shows. Naturally, we have the same function when $T_x = 0$ and $T_y$ is varied. As a consequence the system becomes not perfectly ordered when we cool it “horizontally” to $T_x = 0$ axis on the phase diagram at a fixed nonzero value of $T_y$. Namely, the order parameter saturates to a value less than 1 when $T_x \to 0$. The visualisation of particle distributions during the MC simulation shows that there are still some defects in the ordered homogenous phase even at $T_x = 0$ because some particles do not stay in the preferred sublattice in consequence of the nonzero value of $T_y$. 

2
The MC simulations were performed on a square lattice \((L_x = L_y = L)\) where system sizes ranged from \(L = 20\) to \(150\). At given \((T_x, T_y)\) temperatures following a thermalization of \(2,000 - 40,000\) MC steps, the time interval between two independent measurements ranged from 5 MCS for \(L = 20\) systems to \(100\) MCS for \(L = 100\) systems. Increasing \(T_x\), the whole procedure was repeated. To preclude the possibility of first-order transition, especially at low \(T_y\), we repeated the measurement starting from high \(T_x\) and decreasing \(T_x\), but we have not detected hysteresis in the order parameter function. It is worth mentioning that the anisotropic dynamics does not result in anisotropy, namely the pair correlation functions to the \(x\) and \(y\) directions are identical within the limit of accuracy.

We turn now to study the critical behaviour of the model. For the previously studied two-temperature models the non-equilibrium behaviours differ from the equilibrium counterparts. In case of attractive interaction instead of the equilibrium Ising universality class, the anisotropic finite-size scaling resulted in new exponents \(\beta = 0.33\) and \(\nu = 0.60\). The other model with repulsive nearest- and next-nearest neighbour interactions leaves the equilibrium universality class of the x-y model with cubic anisotropy and is described by the Ising exponents. Common features of these models are that the degenerate ground states violate the x-y symmetry of the systems. For example in case of the attractive interaction the particles condense into a strip oriented either horizontally or vertically in the ordered phase. In the other previously studied model with repulsive interactions the particles form alternately occupied and empty columns (or rows). The fact that the anisotropic dynamics breaks the x-y symmetry and reduces the number of the stable groundstates may result in a new non-equilibrium behaviour. In contrast to these models, in the present model the checkerboard-like groundstate does not break the x-y symmetry, therefore the non-equilibrium perturbation does not reduce the number of the possible groundstates.

As a consequence of the previous argument our conjecture is that the critical behaviour of the non-equilibrium model may be described by Ising exponents. This expectation agrees with the prediction of the field theoretic renormalisation group analysis.

Although the dynamical mean-field approach provides a correct phase diagram, it is not applicable to describe critical behaviour. To study the critical behaviour we have performed a finite size scaling of MC data where the usual scaling form of the order parameter was used:

\[
m(L, T_x) = L^{-\beta/\nu} \overline{m(\tau_x L^{1/\nu})}.
\]  \(3\)

Here \(\tau_x\) denotes the reduced horizontal temperature deviation from the critical temperature. Notice that \(T_y\) is constant. Using \(\beta = 1/8\) and \(\nu = 1\) in the scaling form, we have got nice data collapse at \(T_y = 0\) as Fig. shows. Similar excellent data collapses were found when we repeated the finite-size scaling at \(T_y = 0.33\) and \(0.64\). The Ising universality exponents are believed to hold along the entire line of phase transitions.

IV. NON-EQUILIBRIUM FLUCTUATIONS

The character of the phase diagram makes possible to study the phase transition in a wide range of \(T_y\). The non-equilibrium phase transitions are generally accompanied by the violation of the FDT. It results in difference between the specific heats defined as the derivative of energy with respect to the temperature \((C_D = \partial E / \partial T)\) and derived from the fluctuations in the energy \((C_F = \langle (E^2) - \langle E \rangle^2 \rangle / kT^2\) where \(\langle \rangle\) stands for averaging over time). To check this \(C_D\) and \(C_F\) are compared at different fixed values of \(T_y\) when we cross the phase transition line by increasing \(T_x\). In this case the correct definition of the two quantities are:

\[
C_D = \frac{\partial E}{\partial T_x} \bigg|_{T_y} \quad \text{and} \quad C_F = \frac{\langle (E^2) - \langle E \rangle^2 \rangle}{kT_x^2}.
\]  \(4\)

At \(T_y = 0\) the fluctuations are suppressed by the low temperature, therefore \(C_F\) is smaller than \(C_D\) even at the phase transition point. Increasing \(T_y\), larger fluctuations can appear, which decrease the difference between \(C_D\) and \(C_F\). At a special value of \(T_y = 0.33\), the specific heats, which are calculated different ways, collapse. Further increasing \(T_y\), the fluctuations become larger and \(C_F\) exceeds \(C_D\). Figure indicates, how strongly the difference depends on \(T_y\). Thus we can control the rate of violation of FDT by changing \(T_y\), moreover, FDT seems to be valid at a special value of \(T_y\). It is easy to detect that the \(C_F\) curve is not symmetrical around the transition point \((T_c)\) when \(T_y = 0.64\). This feature may be understood qualitatively. When \(T_x\) is increased at fixed value of \(T_y\) near \(0.64\), the system is close to the phase transition line in the sub-critical region \((T_x < T_c)\). While in the super-critical region \((T_x > T_c)\) the system is further away from the critical line. Therefore the fluctuations are enhanced in the \(T_x < T_c\) region comparing to the \(T_x > T_c\) region.

Though the data are obtained from small systems, similar behaviour can be observed for larger systems. This fact is illustrated in Fig. where the specific heats are plotted for different system sizes at the above mentioned special
value of $T_y$. It is worth mentioning that in the corresponding uniformly driven diffusive model the sharpening of the specific heat is not a monotonic function of the system size $[1]$. The reason of this unusual behaviour is that the self-organising domain structure, which characterises the thermodynamic limit, can only appear when the system sizes is large enough. We expect traditional size dependence of specific heat in the two-temperature model because the reflection symmetric dynamics does not cause enhanced interfacial transport here. Although the peaks of the specific heats are more moderate than in the equilibrium case, the intensity of the peaks increases with lattice size suggesting a divergence in the thermodynamic limit as Fig. 2 shows.

Finally, we consider the spatial correlations above the phase transition point. Long-range correlations are so often observed in non-equilibrium systems that the exponential decay of spatial correlations seems to be exception. It is believed that in the non-equilibrium steady-state the spatially anisotropic conserved dynamics produces such long-range correlations $[3, 4]$. In agreement with this argument both simulations $[3]$ and perturbative approaches $[13]$ found power law decay of correlations at high temperatures in different two-temperature models. In our model the order parameter, which is the 'staggered' density, obeys no conservation law therefore the theory predicts exponentially decaying correlations. However, the question comes up whether the validity or the violation of FDT may influence the spatial correlations somehow at high temperatures in the present model.

To measure the equal time pair-correlation function

$$G(r) = \langle \phi(0) \phi(r) \rangle,$$  \hspace{1cm} (5)

where $\phi$ is the local order parameter, we chose the system size to be considerably larger than the correlation length. Thus we have chosen $L$ ranged from 50 to 100 when we measured $G(r)$ at $T_y = 0.33$ for three different $T_x$ which are above the transition point ($T_x = 1.2T_c, 1.3T_c$, and $1.4T_c$). In every case $G(r)$ converged to zero. We have plotted log $G(r)$ vs. $r$ in Fig. 4 to demonstrate the exponential decay of correlations. Obviously the negative slopes become smaller when $T_x$ decreases resulting in larger correlation lengths. Similar behaviours were found for other values of $T_y$.

V. CONCLUSION

The phase transition and critical behaviour of a two-temperature model with repulsive nearest-neighbour interactions were studied by dynamical mean-field approximation and Monte Carlo simulations. According to both approaches, the system undergoes a phase transition if one of the temperatures is high enough. The phase transition is continuous even at zero fixed temperature and the critical behaviour is not affected by the non-equilibrium perturbation. This result agrees with the earlier theoretical expectations.

The present model gives an example that FDT can be valid or violate in case of the same non-equilibrium model at different values of the control parameter. The Monte Carlo data of the pair correlation function resulted exponential decay in the high temperature regime, which is in agreement with the theoretical prediction since the order parameter is not conserved. We found that the nature of spatial correlations are independent of the violation FDT.

VI. ACKNOWLEDGEMENTS

The author thank G. Szabó for his critical reading of the manuscript. He is grateful to Profs. Ole G. Mouritsen and Martin J. Zuckermann for helpful comments. It is pleasure to thank the hospitality of the Technical University of Denmark where this work was started. This research was supported by the Hungarian National Research Fund (OTKA) under Grant No. F-19560.

[1] For a review, see B. Schmittmann and R. K. P. Zia 1995 Phase Transition and Critical Phenomena vol 17 eds C. Domb and J. L. Lebowitz (Academic, New York)
[2] H. K. Janssen and B. Schmittmann 1986 Z. Phys. B 64 503
[3] J. L. Vallés and J. Marro 1987 J. Stat. Phys. 49 89
[4] S. Katz, J. L. Lebowitz, and H. Spohn 1984 J. Stat. Phys. 34 497
[5] P. L. Garrido, J. L. Lebowitz, C. Maes, and H. Spohn 1990 Phys. Rev. A 42 1954
FIG. 1. Phase diagram predicted by two-point (dashed line) and four-point (solid line) dynamical mean-field approximations. Filled boxes indicate the results of Monte Carlo simulation.

FIG. 2. Order parameter as a function of $T_x$ suggested by four-point approximation at $T_y = 0$.
FIG. 3. Finite size scaling plots of MC data for the order parameter at $T_y = 0$. System sizes are $L = 20 (\times), 30 (\Box), 50 (\triangle)$, and 100 (•). The slopes of the inserted lines are $1/8$ and $-7/8$.

FIG. 4. MC data for specific heats at different values of $T_y (0.64 (\times), 0.46 (\triangle), 0.33 (\Box)$, and 0 (•)). Solid lines represent the specific heat calculated from the energy fluctuation. The system sizes are $20 \times 20$. 

6
FIG. 5. Specific heats calculated both ways at $T_y = 0.33$ for different system sizes $L = 20 (\bullet)$, 30 (○), 50 (+), and 100 (□). The error bars of $C_D$ are indicated.

FIG. 6. Pair correlation functions at different $T_x$ above the critical region when $T_y = 0.33$ for all cases. $T_x = 1.2 T_c (\triangle)$, $1.3 T_c (\bullet)$, and $1.4 T_c (\square)$. 