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

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Abstract. A two-temperature lattice gas model with repulsive nearest-neighbour interactions is studied using Monte Carlo simulations and dynamical mean-field approximations. 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.

1. Introduction

The study of the driven diffusive lattice gas model, which served as a convenient tool to produce a stationary non-equilibrium state, revealed a lot of new phenomena compared with 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, 3]. 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 [4]. Unfortunately, it is rather difficult to realize the model in the 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. A 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 [5, 6]. 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 [7] and for nearest-, and next-nearest-neighbour repulsive interactions [8]. A 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, 9]. Completely different behaviour is found for nearest-neighbour repulsive interactions where the field-induced interfacial transport prevents the long-range ordering [10]. Although a 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 [1].

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 a dynamical mean-field analysis to calculate the phase transition points. These results are supported by Monte Carlo (MC) 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 [11, 8]. The finite-size scaling of the MC data indicates that this model falls into the universality class of the equilibrium Ising model in agreement with a theoretical prediction [12].

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. For example, in the uniformly driven model with attractive interaction the field suppresses the fluctuations and the difference is relevant [1, 3, 13]. Using both methods 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 [6]. We also examine the two-point correlations of our model and find short-range correlations at high temperatures.

2. 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

$$H = -J \sum_{(i,j)} n_i n_j \quad (1)$$

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

$$g_\alpha(\Delta H) = \frac{1}{1 + \exp(\Delta H/T_\alpha)} \quad (2)$$

where ΔH 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 well known 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 the particles prefer to stay 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 ρ_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 ϕ 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 to the one with lower temperature, through the system and maintains a stationary non-equilibrium state. In other two-temperature models the previous studies set one of the temperatures (e.g. T_y) to be infinite, which reduced the number of control parameter to one [6, 15] 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.

3. Phase transition and critical behaviour

The study of non-equilibrium phase diagrams by the dynamical mean-field approach has proved to be useful in many instances [8, 16]. Using this approach we determine the stationary solution of the equations describing the time evolution of configuration probabilities. At the level of a k -point approximation, these probabilities are given by probabilities of the possible configurations on k -point clusters. We refer to [16] 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 figure 1. 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 a 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 with the data of MC simulations as shown in figure 1. (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 transition point as figure 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 non-zero value of T_y . Namely, the order parameter saturates to a value less than 1 when $T_x \rightarrow 0$. The visualization 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 non-zero value of T_y .

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 2000–40 000 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

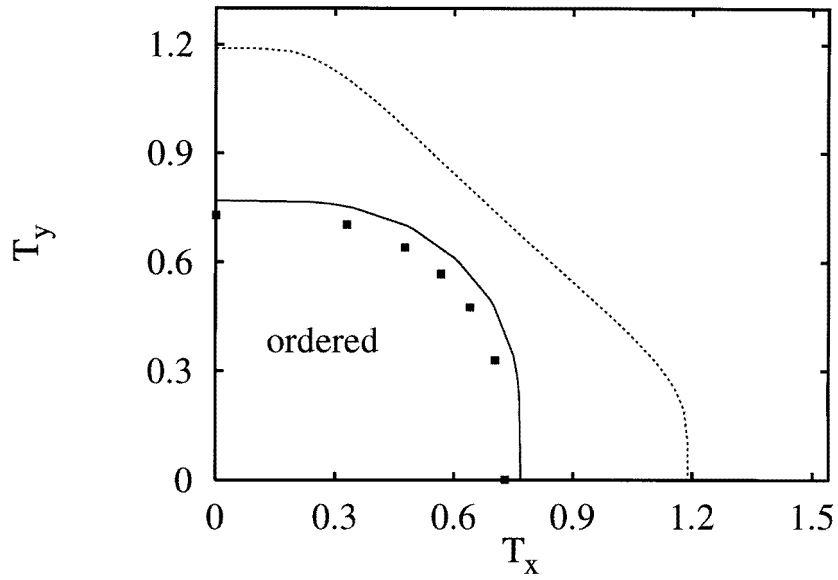


Figure 1. Phase diagram predicted by two-point (broken curve) and four-point (full curve) dynamical mean-field approximations. Full squares indicate the results of Monte Carlo simulation.

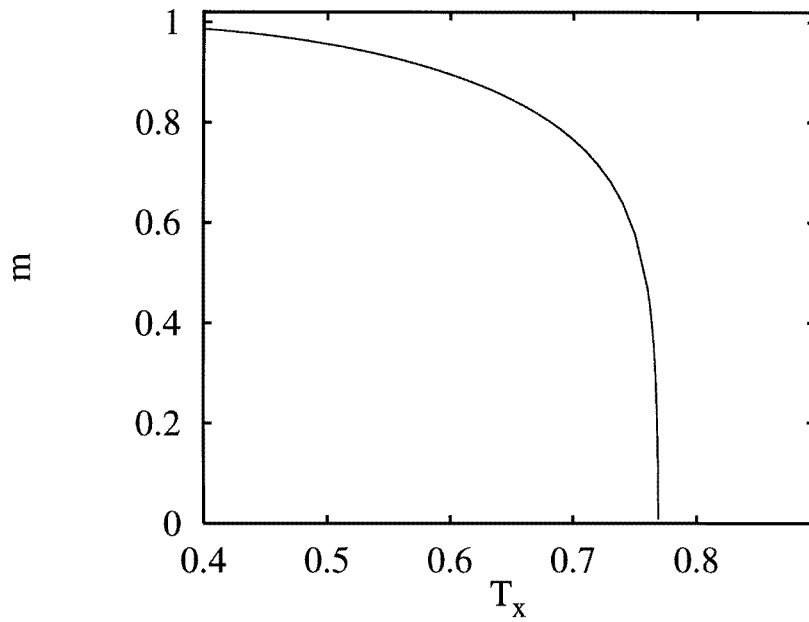


Figure 2. Order parameter as a function of T_x suggested by a four-point approximation at $T_y = 0$.

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 their equilibrium counterparts. In the case of attractive interaction instead of the equilibrium Ising universality class, the anisotropic finite-size scaling resulted in new exponents $\beta = 0.33$ and $\nu = 0.60$ [15]. 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 [8]. Common features of these models are that the degenerate ground states violate the x - y symmetry of the systems. For example in the 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 stable ground states may result in a new non-equilibrium behaviour. In contrast to these models, in this model the checkerboard-like ground state does not break the x - y symmetry, therefore the non-equilibrium perturbation does not reduce the number of the possible ground states.

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 renormalization group analysis [1, 12].

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:

$$m(L, T_x) = L^{-\beta/\nu} \bar{m}(\tau_x L^{1/\nu}). \quad (3)$$

Here τ_x denotes the reduced horizontal temperature deviation from the critical temperature. Notice that T_y is constant. Using $\beta = \frac{1}{8}$ and $\nu = 1$ in the scaling form, we have good data collapse at $T_y = 0$ as figure 3 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.

4. Non-equilibrium fluctuations

The character of the phase diagram makes it possible to study the phase transition in a wide range of T_y . The non-equilibrium phase transitions are generally accompanied by violation of the FDT. It results in differences 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 ($C_F = (\langle E^2 \rangle - \langle E \rangle^2) / kT^2$, 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:

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

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. Increasing T_y further, the fluctuations become larger and C_F exceeds C_D . Figure 4 indicates, how strongly the difference depends on T_y . Thus we can control the rate of violation of FDT by changing T_y ,

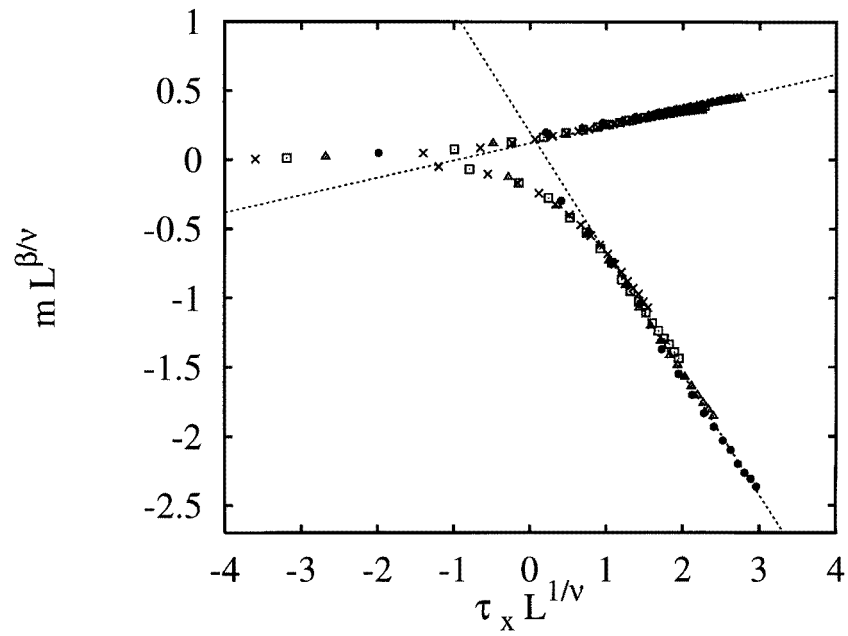


Figure 3. Finite-size scaling plots of MC data for the order parameter at $T_y = 0$. System sizes are $L = 20$ (\times), 30 (\square), 50 (\triangle), and 100 (\bullet). The slopes of the inserted lines are $\frac{1}{8}$ and $-\frac{7}{8}$.

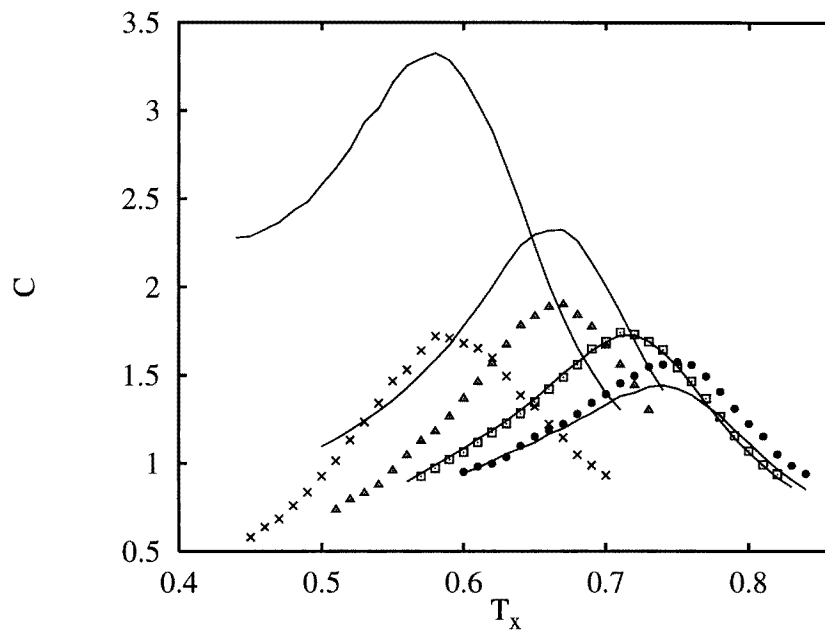


Figure 4. MC data for specific heats at different values of T_y (0.64 (\times), 0.46 (\triangle), 0.33 (\square), and 0 (\bullet)). Full curves represent the specific heat calculated from the energy fluctuation. The system sizes are 20×20 .

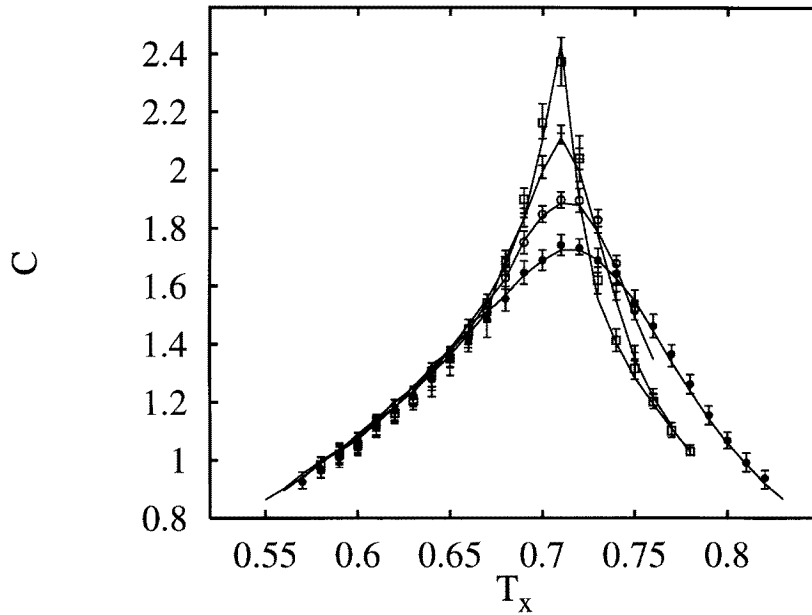


Figure 5. Specific heats calculated both ways at $T_y = 0.33$ for different system sizes $L = 20$ (\bullet), 30 (\circ), 50 ($+$), and 100 (\square). The error bars of C_D are indicated.

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, with a 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 supercritical 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 compared with 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 figure 5 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 [17]. The reason for this unusual behaviour is that the self-organizing domain structure, which characterizes the thermodynamic limit, can only appear when the system size 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 figure 5 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 an exception. It is believed that in the non-equilibrium steady state the spatially anisotropic conserved dynamics produces such long-range correlations [18, 5]. In agreement with this argument both simulations [6] and perturbative approaches [19] 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

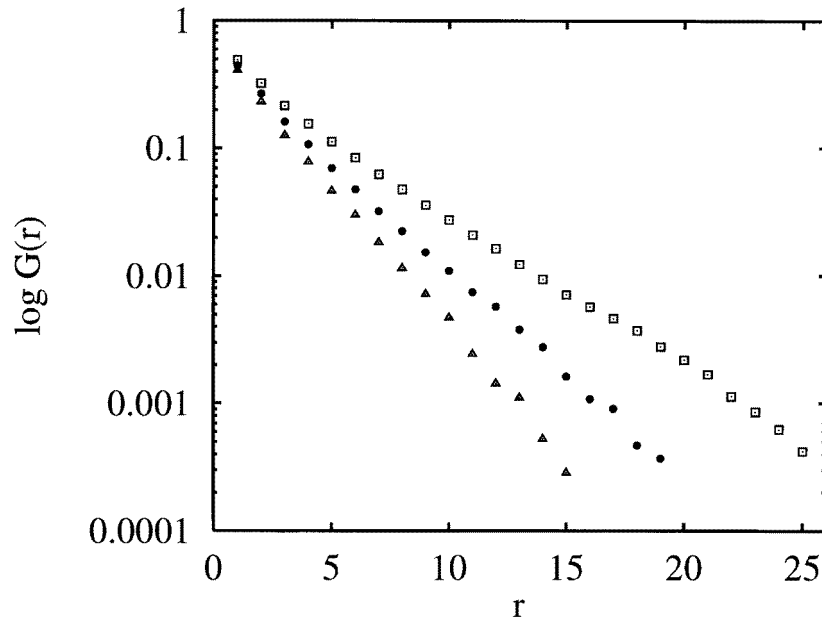


Figure 6. Pair correlation functions at different T_x above the critical region when $T_y = 0.33$ for all cases. $T_x = 1.2T_c$ (Δ), $1.3T_c$ (\bullet), and $1.4T_c$ (\square).

correlations. However, the question arises, whether the validity or the violation of FDT may influence the spatial correlations somehow at high temperatures in this model.

To measure the equal time pair-correlation function

$$G(r) = \langle \phi(0)\phi(r) \rangle \quad (5)$$

where ϕ 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 the transition points above ($T_x = 1.2T_c$, $1.3T_c$, and $1.4T_c$). In every case $G(r)$ converged to zero. We have plotted $\log G(r)$ versus r in figure 6 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 .

5. 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 MC 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.

This model gives an example that FDT can be valid or violated in the case of the same non-equilibrium model at different values of the control parameter. The MC data of the pair-correlation function resulted in 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.

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