

Non-equilibrium critical dynamics of pure and diluted 2D XY -model

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Abstract. Comprehensive study of the ageing and the violation of the fluctuation-dissipation theorem in a pure and diluted two-dimensional XY -model were carried out. Two-dimensional XY -model tend to a particular type of phase transition is called a phase transition *Berezinskii-Kosterlitz-Thouless* associated with the change of the correlation properties of the system.

1. Introduction

In the past few years, systems with slow dynamics have attracted considerable theoretical and experimental interest [1–3]. Ageing phenomena are observed during this everlasting non-equilibrium evolution. This is due to the predicted and observed ageing at a slow evolution of non-equilibrium systems and violations of the fluctuation-dissipation theorem [1, 4]. Known examples of such systems with abnormal slow dynamics are complex disordered systems like glasses: dipole, metal and spin glasses [5–7]. However, these features of the non-equilibrium behaviour, as shown by analytical and numerical studies [8], can also be observed in systems near the critical temperature as critical dynamics of such systems is characterized an abnormally large relaxation times. The two-dimensional XY -model demonstrates abnormal slow dynamics, but the main distinguishing feature of the 2D XY -model is that it shows an anomalous behaviour is not only close to the temperature phase transition *Berezinskii-Kosterlitz-Thouless* T_{BKT} , but $T < T_{\text{BKT}}$ [9, 10]. Ageing is a phenomenon of growth of the relaxation time system with the increase of the *age* of the material ie older samples respond more slowly [1, 4, 11]. The *age* of the system t_w or also waiting time, being the time elapsed since the preparation of the system. An important aspect of ageing systems is that the equilibrium fluctuationdissipation theorem (FDT) does not hold.

Relevance of the study of two-dimensional XY -model due to the extensive a number of physical systems whose behaviour can be described by this model. There are examples of such systems: monolayer magnetic films of transition metals such as Co and Ni, on a nonmagnetic substrate, such as Cu [12]; an important class of planar magnetics [12, 13]; two-dimensional crystals [13]; superconducting thin films [13]; two-dimensional Bose liquid films of superfluid He [10, 13]; Josephson junction array and the array of SFS contacts [13, 14].

Most real-world systems contain structural defects that can have a significant influence on the critical behaviour of the system. According to the Harris criterion [15] the presence of structural defects can be significant if critical exponent of the heat capacity α is positive. Thus, it is predicted that the presence of structural defects does not affect to two-dimensional XY -model behaviour near the critical temperature T_{BKT} . However, in low-temperature phase for



$T < T_{\text{BKT}}$, as shown by analytical and numerical study of the equilibrium properties of the model [16–18], the presence of defects lead to changing of the equilibrium characteristics for the correlation features and their concentration dependence. However, the dynamics of structurally disordered XY -dimensional model was still not investigated carefully.

In this paper the non-equilibrium critical dynamics of pure and diluted $2D$ XY -model were investigated by Monte Carlo methods in whole low-temperatures *Berezinskii-Kosterlitz-Thouless* phase.

2. Model and methods

The XY -model is a example of the general lattice models with n -component parameter, with $n = 2$. Phase transition in such systems associated with the changing of the asymptotic behaviour of the correlation functions from an exponential decay in high-temperature phase to power decay in low-temperature phase.

The two-dimensional XY model is defined by the Hamiltonian [9]:

$$H = -J \sum_{\langle i,j \rangle}^N \vec{S}_i \vec{S}_j \quad (1)$$

where $J > 0$ is the exchange integral, \vec{S}_i - classical planar spin, associated with the i -th node of two-dimensional lattice, $N = L^2$.

The Hamiltonian for disordered model has the form:

$$H = -J \sum_{\langle i,j \rangle}^N p_i p_j \vec{S}_i \vec{S}_j \quad (2)$$

where p_i are random variables: $p_i = 1$, if the i -th node is the spin, and $p_i = 0$, if the i -th node is a non-magnetic atom.

Dynamics of the two-dimensional XY -model is provided by two contributions: the spin waves and topological excitations such as vortex and antivortex (Fig. 1).

In this paper, for the study of non-equilibrium critical behaviour of two-dimensional XY -model was used Metropolis algorithm [19]. The dynamics of one-spin-flips Metropolis corresponds to dissipative processes which described by dynamic model A in Halperin-Hohenberg classification [20])

$$\frac{\partial \phi(x, t)}{\partial t} = -\Gamma_0 \frac{\delta H}{\delta \phi(x, t)} + \xi(x, t), \quad (3)$$

where ϕ – order parameter, Γ_0 – kinetic factor, $\xi(x, t)$ – gaussian random force. The dynamic correlation functions are determined by the solution of this equation.

3. Ageing effects

The ageing effects in non-equilibrium critical relaxation of $2D$ XY -model were studied from low-temperature initial state with $T = 0$, $m_0 = 1$ and from high-temperature initial state with $T \gg T_{\text{BKT}}$, $m_0 \ll 1$. The values of ageing times were chosen $t_w = 100, 500$ and 1000 MCS/s. The initial state with $m_0 \ll 1$ is prepared by the dynamic evolution of the system from $T_0 = 3.0 \gg T_{\text{BKT}}$. The value of initial magnetization was $m_0 = 0.001$ with accuracy $\Delta m_0 = 0.01 m_0$.

The time dependencies of autocorrelation function were presented in Fig. 2. The data clearly demonstrates presence of two scaling regimes with power dependence of autocorrelation function:

$$A(t, t_w) = \left\langle \frac{1}{N} \sum_i \vec{S}_i(t) \vec{S}_i(t_w) \right\rangle - \left\langle \frac{1}{N} \sum_i \vec{S}_i(t) \right\rangle \left\langle \frac{1}{N} \sum_i \vec{S}_i(t_w) \right\rangle. \quad (4)$$

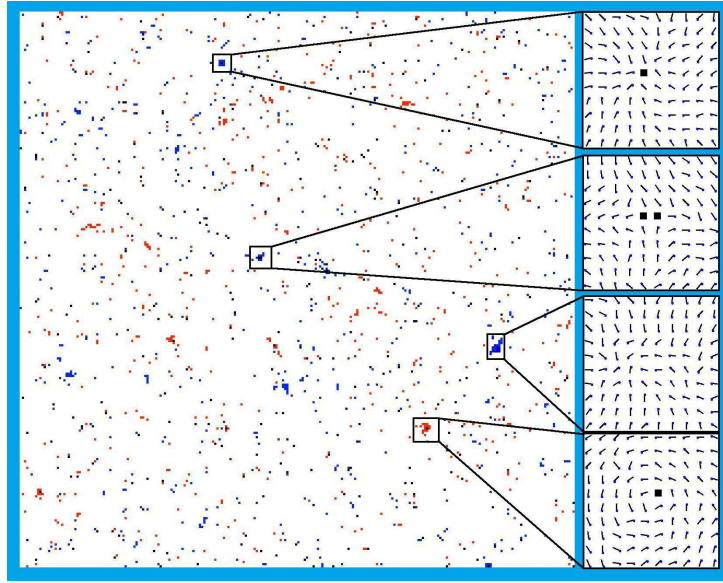


Figure 1. Spin system configuration for $p = 0.995$, $L = 256$, $T = 0.3$ at moment of time $t = 10000$ MCS/s after starting from the initial high-temperature state with $m_0 \ll 1$. Vortex excitations are designated by red points, antivortex excitations – blue points, structural defects – black points

To characterize these time intervals it have been introduced exponent time dependence of the autocorrelation function:

$$A(t, t_w) = (t - t_w)^{-\Delta_A}. \quad (5)$$

The obtained values of exponents Δ_A are presented for system with low-temperature and high-temperature initial state in Table. 1. It was shown that critical slow down and ageing effects becomes stronger with increasing t_w for $T < T_{\text{BKT}}$.

The scaling behaviour of autocorrelation function can be defined by form [22]

$$A(t, t_w) = \frac{1}{(t - t_w)^{\eta(T)/2}} \Phi \left(\frac{\xi(t)}{\xi(t_w)} \right). \quad (6)$$

where $\xi \sim t/\ln(t)$ is the correlation length, η – spatial exponent insuring the best collapse of data, Φ is the scaling function which behaviour is presented in the insets of Fig. 2. $\Phi(x) = 1$ for small values of x . Long-time decay of $\Phi(x)$ is well described by a power law, i.e. $\Phi(x) \sim x^{-\lambda}$ for large x . The calculated values of the exponents λ are presented in Table. 2. The value $\lambda = 0.5384(9)$ for $T = 0.3$ is in good agreement with value $\lambda = 0.54$ obtained in [22].

Presented in Fig. 2 the behaviour of $A(t, t_w)$ demonstrate that for time regime $t - t_w \sim t_w$ the influence of vortex excitations is irrelevant and the main contribution to the relaxation dynamics has only the spin-wave nature. In the time regime $t - t_w \gg t_w$ the role of vortex interaction have been increased and become significant.

It has revealed significant differences in the non-equilibrium evolution from the different initial states. These differences can be explained by role of vortex interaction. In system which started from high-temperature state the initial value of vortex-antivortex excitations is significant and vortex-antivortex interaction produce drastically effect on non-equilibrium dynamics. When system started from low-temperature state it needs energy for formation of vortex and antivortex excitations and the role of vortex interaction is not so significant.

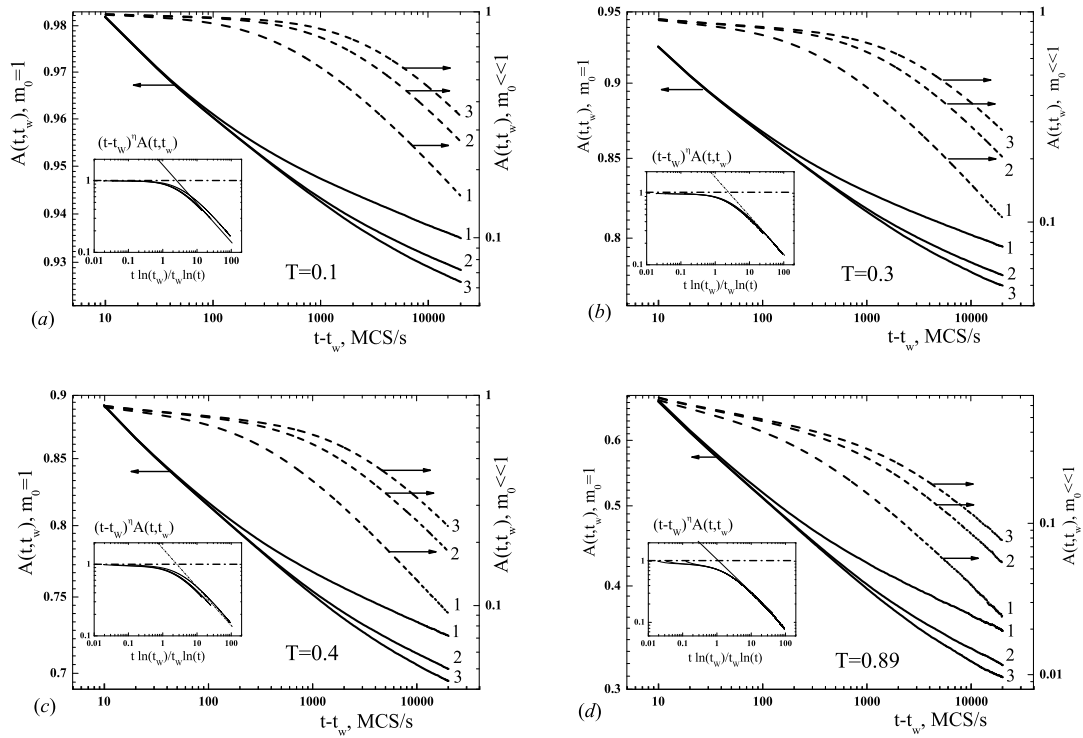


Figure 2. Time dependencies of the autocorrelation function $A(t, t_w)$ as a function $t - t_w$ for different non-equilibrium initial states and values of t_w : 1 – $t_w = 100$, 2 – $t_w = 500$, 3 – $t_w = 1000$ MCS/s. The relaxation curves were presented for low-temperature phase $T < T_{\text{BKT}}$ states for $T = 0.1$ (a), $T = 0.3$ (b), $T = 0.4$ (c), $T = 0.89$ (d). The solid lines correspond to low-temperature initial state, the dashed lines and scaling (insets) – high-temperature initial state

4. The influence of structural disorder on the non-equilibrium critical behaviour

The presence of structural disorder and non-magnetic impurities breaks the interaction of vortices and antivortices. The vortices are pinned 1 at the defects [25].

To estimate the $T_{\text{BKT}}(p)$ dependence on spin concentration p for disordered systems was calculated temperature dependence of the ratio R

$$R = \frac{[\langle C(L/2) \rangle]}{[\langle C(L/4) \rangle]}, \quad (7)$$

where $C(L)$ is the correlation function

$$C(r) = \left\langle p_i p_{i+r} \vec{S}_i \vec{S}_{i+r} \right\rangle, \quad (8)$$

the angle brackets stand for an statistical average over MC realizations and the square brackets stand for additional average over disorder configurations.

Temperature dependencies of $R(L)$ were investigated for spin concentrations $p = 1.0$ (Fig. 3a), $p = 0.9$, $p = 0.8$ and $p = 0.7$ (Fig. 3b) for systems with linear sizes $L = 16, 32, 48$. The averaging was carried out on over 10000 MCS/s and 50 samples with different disorder configurations with 10 MC runs for each sample. The error bars for spin concentration $p = 1.0$ (Fig. 3a), 0.9 and 0.8 are smaller than the size of the symbols. The significant value of error bars for $p = 0.7$ (Fig. 3b) can be explained by the breakdown of the phase transition.

Table 1. The values of exponent Δ_A for different initial states

T/J	$t_w = 100$		$t_w = 500$		$t_w = 1000$	
low-temperature initial state with $m_0 = 1$						
	[0;60]	[1000;10000]	[0;60]	[1000;10000]	[0;100]	[10000;20000]
0.2	0.0185(4)	0.0091(1)	0.0197(3)	0.0093(1)	0.0190(3)	0.0093(1)
0.4	0.0379(8)	0.0193(1)	0.0400(6)	0.0203(1)	0.0389(5)	0.0206(1)
0.6	0.0603(10)	0.0313(1)	0.0635(9)	0.0322(1)	0.0620(6)	0.0356(1)
0.8	0.0903(12)	0.0477(8)	0.0948(12)	0.0483(1)	0.0931(8)	0.0534(1)
0.89	0.1112(15)	0.0623(9)	0.1176(40)	0.0649(2)	0.1164(9)	0.0597(2)
high-temperature initial state with $m_0 \ll 1$						
	[0;60]	[1000;20000]	[0;60]	[5000;20000]	[0;60]	[1000;20000]
0.2	0.041(2)	0.461(3)	0.026(5)	0.457(8)	0.024(6)	0.41(5)
0.4	0.064(1)	0.484(1)	0.050(9)	0.461(8)	0.046(4)	0.42(7)
0.6	0.096(1)	0.499(3)	0.078(1)	0.479(7)	0.071(6)	0.44(3)
0.8	0.148(1)	0.514(9)	0.117(3)	0.489(8)	0.106(5)	0.44(4)
0.89	0.184(1)	0.612(3)	0.146(9)	0.614(7)	0.135(7)	0.56(4)

Table 2. The values of exponents λ

T/J	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.89
λ	0.5216(3)	0.5428(5)	0.5384(9)	0.5267(4)	0.5188(9)	0.5200(8)	0.4983(8)	0.4812(9)	0.6151(3)

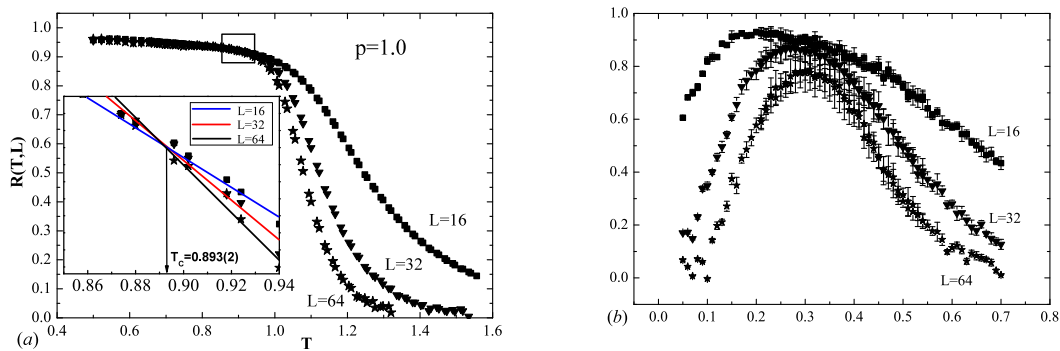


Figure 3. Temperature dependencies of ratio $R(L)$ for the spin concentration $p = 1.0$ (a) and $p = 0.7$ (b) for different L

The MC obtained values of critical temperature are $T_{\text{BKT}}(p = 1.0) = 0.893(2)$, $T_{\text{BKT}}(p = 0.9) = 0.679(7)$, $T_{\text{BKT}}(p = 0.8) = 0.485(4)$. It can be seen that the presence of disorder considerably reduces the temperature of the phase transition. The value of $T_{\text{BKT}}(p = 1.0) = 0.893(2)$ for pure system is in a good agreement with value $T_{\text{BKT}} = 0.894(5)$ [26]. For $p = 0.7$

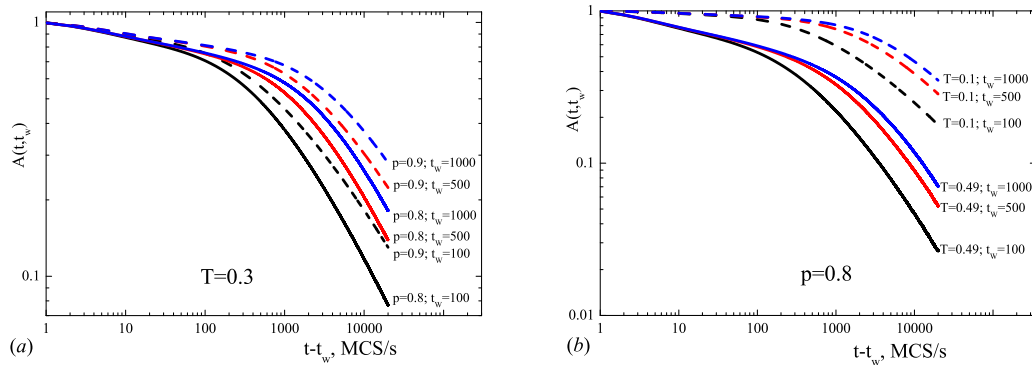


Figure 4. Time dependence of autocorrelation function $A(t, t_w)$ from $t - t_w$ for different p

the intersection wasn't find and this behaviour can be associated with the breakdown of the *Berezinskii-Kosterlitz-Thouless* phase transition.

Feature of non-equilibrium behaviour of systems with slow dynamics is a violation of the translational invariance of time due to the long-term effect of non-equilibrium initial states of such systems. This is manifested primarily in two-time characteristics of the system, such as the correlation function and the response function. When these functions are non-equilibrium processes depend on two variables, the temporary nature of t and t_w (when $t > t_w$), and not only on the difference but also on each separately. Moreover, this dependence is maintained for sufficiently long times observation t .

The ageing effects were investigated for disordered systems with $p = 0.8$ and $p = 0.9$ started from high-temperature initial state. The two-time autocorrelation function is defined for disordered systems by the following expression:

$$A(t, t_w) = \left[\left\langle \frac{1}{pN} \sum_i p_i \vec{S}_i(t) \vec{S}_i(t_w) \right\rangle \right] - \left[\left\langle \frac{1}{pN} \sum_i p_i \vec{S}_i(t) \right\rangle \right] \left[\left\langle \frac{1}{pN} \sum_i p_i \vec{S}_i(t_w) \right\rangle \right]. \quad (9)$$

The two-time dependencies of the autocorrelation function for different p are presented in Fig. 4. The data is clearly shows that the presence of disorder lead to increasing of the system relaxation from initial non-equilibrium high-temperature state.

5. Violation of the fluctuation-dissipation theorem

Another slow dynamics effect at out-of-equilibrium stage is the violation of the fluctuation-dissipation theorem (FDT) [27]. FDT suggests relation between autocorrelation function $A(t, t_w)$ and response function $R(t, t_w)$ on some external field

$$R(t, t_w) = \frac{X(t, t_w)}{T} \frac{\partial A(t, t_w)}{\partial t_w}, \quad (10)$$

where $X(t, t_w)$ is so called fluctuation-dissipation ratio (FDR), and one assumes $t > t_w$. According to FDT $X(t, t_w) = 1$ in equilibrium. The asymptotic value of the FDR

$$X^\infty = \lim_{t_w \rightarrow \infty} \lim_{t \rightarrow \infty} X(t, t_w) \quad (11)$$

can be used as a new universal critical characteristic of a systems with slow dynamics.

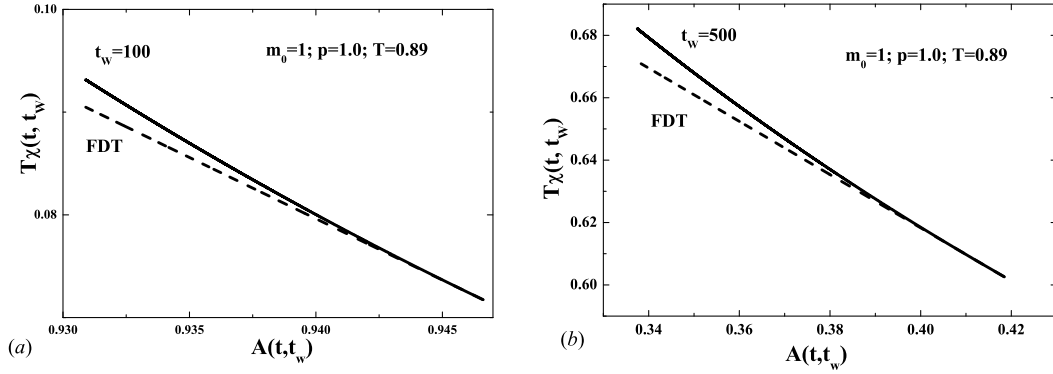


Figure 5. FDR plot for $T = 0.89$: $t_w = 100$ MCS/s (a) and $t_w = 500$ MCS/s (b). The dashed line corresponds to the $X(t, t_w) = 1$

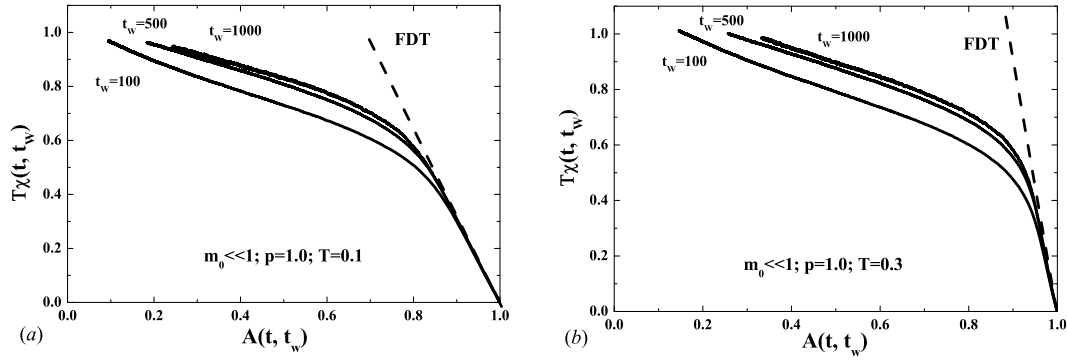


Figure 6. FDR plot for $T = 0.1$ (a) and $T = 0.3$ (b). The dashed line corresponds to the $X(t, t_w) = 1$

FDR can be estimated with application of small magnetic field after waiting time t_w . In this case the response function $R(t, t_w)$ can not be calculated directly and more useful quantity is the integrated response function [28].

$$\chi(t, t_w) = T \int_{t_w}^t dt' R(t, t'). \quad (12)$$

In the large time limit $\chi(A) = \int_A^1 X(q) dq$ and the FDR can be defined as

$$X(t, t_w) = - \lim_{A \rightarrow 0} \frac{\partial T\chi(t, t_w)}{\partial A(t, t_w)}. \quad (13)$$

$\chi(t, t_w)$ for the two-dimensional XY-model can be calculated based on the following relationship:

$$\chi(t, t_w) = \frac{1}{L^2 h^2} \sum_i \overline{< \vec{h}_i(t_w) \vec{S}(t) >}, \quad (14)$$

where the random magnetic field h is characterized by two components which are independently drawn from a bimodal distribution $\pm h$. The overline means an average over the realizations

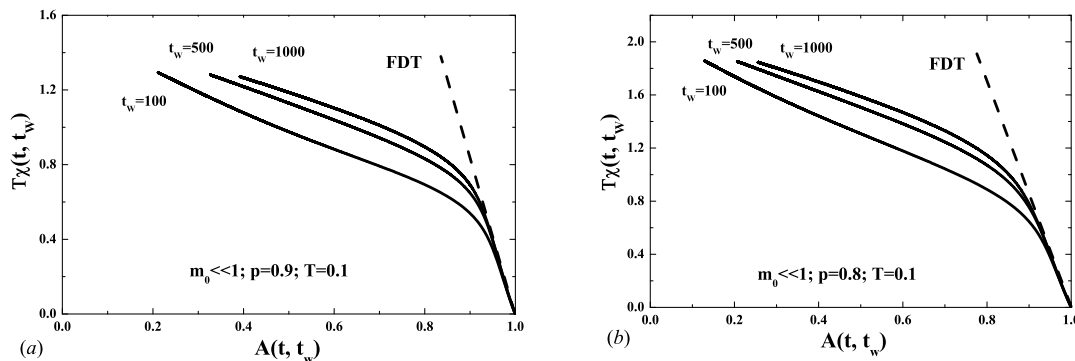


Figure 7. FDR plot for disordered system: $T = 0.1$; $p = 0.9$ (a) and $p = 0.8$ (b). The dashed line corresponds to the $X(t, t_w) = 1$

of the random magnetic field. We checked that the value $h = 0.04$ was small enough for the response to be linear.

In Fig. 5 we present for initial state with $m_0 = 1$ the obtained parametric $T\chi(t, t_w)$ versus $A(t, t_w)$ plot for $T_{BKT} = 0.89$ and for different waiting times t_w . The dashed line represents $X(t, t_w) = 1$, while the solid line represents $X(t, t_w) > 1$, which means that the susceptibility is larger than its equilibrium value and it takes place the violation of FDT. To obtain the FDR on the base of relation (13), we analysed the dependencies $T\chi(t, t_w)$ from $A(t, t_w)$, found the slopes of curves for different t_w , and then made extrapolation $t_w \rightarrow \infty$. The asymptotic value of FDR for system started from low-temperature initial state with $m_0 = 1$ is $X_\infty = 2.49(13)$.

The same procedure was used for describing FDT violation in non-equilibrium behaviour of the system started from high-temperature initial state. The MC obtained data is presented in Fig. 6. The asymptotic value of FDR for system started from initial state with $m_0 \ll 1$ $X_\infty = 0.47(3)$.

The violation of FDT in disordered 2D XY-model were discovered. We present in Fig. 7 the FDR plot for disordered system with different p . It clear demonstrates that the presence of disorder lead to increasing of FDT violation.

6. Conclusion

In this paper we have investigated the non-equilibrium effects in critical behaviour of pure and structural disordered 2D XY-model. It has revealed significant differences in the non-equilibrium evolution from the different initial states. These differences can be explained by role of vortex interaction. In system which started from high-temperature state the initial value of vortex-antivortex excitations is significant and vortex-antivortex interaction produce drastically effect on non-equilibrium dynamics. When system started from low-temperature state it needs energy for formation of vortex and antivortex excitations and the role of vortex interaction is not so significant.

The violation of FDT for different initial non-equilibrium states have been discovered. The final values of the asymptotical fluctuation-dissipation ratio are $X_\infty(m_0 \ll 1) = 0.47(3)$, $X_\infty(m_0 = 1) = 2.49(13)$.

The presence of structural disorder lead to increasing of the system relaxation and violation of FDT. It have been explained by vortex pinning on defects.

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