Non-equilibrium vortex annealing of structural disorder in the critical relaxation of diluted two-dimensional XY-model

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Abstract. The study of the effects of aging in the non-equilibrium critical relaxation of a two-dimensional XY-model with a non-equilibrium vortex annealing of structural disorder has been carried out. Two-time dynamic dependencies of the spin-spin and defect-defect autocorrelation functions \(C_{SS}(t; t_w)\) and \(C_{DD}(t; t_w)\) are obtained for the entire Berezinskii low-temperature phase \(T < T_{BKT}(p)\), for a wide range of waiting times \(t_w\) and spin concentrations \(p\). Near the BKT phase transition point \(T_{BKT}(p)\), the dynamic dependencies \(C_{DD}(t; t_w)\) become uniform with time. However, with a decrease in temperature in the low-temperature phase \(T < T_{BKT}(p)\), this relaxation uniformity breaks down, and \(C_{DD}(t; t_w)\) does not exhibit canonical aging properties. The formation of a declining family of dynamical scaling curves is clearly observed at large observation times \(t > t_w\) which may indicate the presence of an asymptotic scaling dependence of \(C_{DD}(t; t_w)\).

1. Introduction
The study of non-equilibrium critical behavior and non-equilibrium relaxation processes is of considerable fundamental and applied scientific interest [1]. Systems at the critical point are characterized by intense fluctuation behavior. Reducing the dimension of the system leads to a significant increase in fluctuation effects [2]. Of particular interest is the study of the influence of structural disorder on the behavior of systems at a critical point [3]. Introducing even a weak structural disorder into the system can significantly change critical behavior [2–7]. Systems with a continuous symmetry of the ground state are characterized by an increase in fluctuations compared with discrete systems [8]. In two-dimensional systems with continuous degeneration of the ground state, the long-range order is destroyed by the strong fluctuations. The two-dimensional XY-model occupies a special place among low-dimensional spin systems with non-continuous symmetry [9]. The long-range order in the two-dimensional XY-model is absent at all non-zero temperatures. However, the features of topological structures arising in the system lead to the emergence of a Berezinskii-Kosterlitz-Thouless (BKT) topological phase transition [10–13] at a temperature \(T_{BKT}\) and a low-temperature Berezinskii phase \(T < T_{BKT}\) [10, 11].

The XY-model is used to describe the critical properties of a wide range of real physical systems [9], such as critical properties of ultra-thin magnetic films, extensive class of “easy plane” planar magnets and critical properties of some other physical systems. Some physical systems exhibit two-dimensional XY-like behavior under certain conditions, such as the frustrated Heisenberg antiferromagnets on a triangular lattice in non-equilibrium relaxation [14].
The equilibrium critical behavior of the two-dimensional XY-model has now been studied [9], at least the basic processes and phenomena that accompany the equilibrium critical behavior of a pure system are well known. However, the study of the non-equilibrium critical relaxation of the system from the initial non-equilibrium state and the influence of structural disorder on the critical properties of the system is a modern scientific problem [3, 4, 6, 7, 14–24].

Figure 1. Typical snapshot configurations of large clusters of defects growths by interaction of structural disorder with vortex in the system with the linear size $L = 64$ and the spin concentration $p = 0.9$. Arrows demonstrate spins, red squares – defects.

The inclusion of structural disorder in a two-dimensional XY-model leads to the emergence of pinning of vortices on defects associated with the appearance of an attractive potential [25] between the vortex and the impurity site. The study of the influence of vortex pinning on defects in a two-dimensional XY-model was carried out in [3, 4, 6, 7, 17–23], however, the quench structure disorder was mainly considered in them. The study of the non-equilibrium critical relaxation of a two-dimensional XY-model with thermalization and vortex annealing of structural disorder were carried out in [24, 28]. It was shown that non-equilibrium pinning of vortices on defects leads to a non-equilibrium process of the coarsening of defects into clusters (see figure 1 and figure 2). This leads to the formation of non-equilibrium coherent structures, such as stripes and clumps, which were previously observed in the equilibrium critical behavior of the model when the additional long-range potential is included in the system with annealed disorder [26, 27]. In the state of equilibrium in the low-temperature phase, the vortices formed vortex pairs, as a result of which the non-equilibrium effects disappeared and the non-equilibrium structures of the defects were destroyed. Thus, a non-equilibrium vortex annealing of structural disorder in a two-dimensional XY-model has properties and processes that have a substantially non-equilibrium nature and are not manifested in the state of thermodynamic equilibrium, unless explicitly including additional long-range potentials.

Figure 2. Snapshot configuration of the defects in system with the linear size $L = 256$ and the spin concentration $p = 0.9$ by time $0$ (initial state), $500$, $10000$ and $50000$ MCs/s.
This paper is devoted to the study of one of the important manifestations of non-equilibrium critical relaxation, especially in disordered systems – non-equilibrium aging effects. The aging have been studied in sufficient detail for a pure and quench diluted two-dimensional XY-model [15, 16, 18–22]. However, in certain situations, the two-dimensional diluted model demonstrates a rather complex behavior, which leads to the emergence of super-aging and sub-aging effects [19]. Therefore, the question of aging in a two-dimensional quench diluted XY-model cannot be considered closed. In this paper, an attempt has been made to consider the effect of thermalization and vortex annealing of structural disorder on aging in a two-dimensional model.

2. Model and methods
The Hamiltonian of the two-dimensional diluted XY-model in this work was chosen in the form

\[ H = -\frac{1}{2} \sum_{i,j} p_i p_j S_i S_j, \]  

where \( S_i \) is a classical planar spin which is associated with \( i \)-node of square lattice with the linear size \( L \), \( p_i \) is occupation number of \( i \)-node. Defects on the lattice are distributed uniformly at time \( t = 0 \) with probability \( P(p_i) = (1 - p)\delta(p_i) + p\delta(1 - p_i) \), where \( p \) is a spin concentration, i.e. \( c = 1 - p \) is a concentration of defects.

Simulation of non-equilibrium critical relaxation was performed in the low-temperature Berezinskii phase at quenched temperatures \( T < T_{\text{BKT}}(p) \) [24] with the Metropolis algorithm. It was shown [17] that the Metropolis algorithm correctly describes a non-equilibrium critical properties of the two-dimensional XY-model. To include the mobility of defects, the elementary step of the Metropolis algorithm was modified. As a time unit, we used the Monte Carlo step per spin (MCs/s) corresponding to \( L^2 \) spin flips or defects moves per unit time. The study was carried out for the spin concentrations \( p = 0.9, 0.8, 0.7 \) and 0.6.

The system started from the non-equilibrium high-temperature initial state with the initial magnetization \( m_0 \ll 1 \), which was prepared at the temperature \( T_0 \gg T_{\text{BKT}}(p) \). The non-equilibrium critical relaxation of the system from such an initial state is accompanied by non-equilibrium vortex dynamics and an intense interaction of the vortices with each other and with defects. To study the non-equilibrium characteristics of the system, we considered a lattice with the linear size \( L = 256 \).

3. Spin-spin autocorrelation function and aging
Aging is a nontrivial dynamic effect in the slow dynamics of relaxation of the system, from the initial non-equilibrium state. Physically, aging is manifested in slowing relaxation processes with increasing age, waiting time \( t_w \), of the system. Mathematically, aging is manifested primarily in the dynamic dependencies of the two-time dynamic characteristics of the system, such as autocorrelation functions \( C(t, t_w) \) and response functions \( R(t, t_w) \). On the dynamic scales of the aging system, these functions depend not only on the difference \( t - t_w \) of their arguments, but also on each argument \( t \) and \( t_w \) separately. In the two-dimensional XY-model, the aging effects are manifested not only near the phase BKT transition temperature \( T_{\text{BKT}}(p) \), but also throughout the low-temperature Berezinskii phase \( T < T_{\text{BKT}}(p) \). The study of the effects of aging, in particular in the two-dimensional XY-model, is devoted to an extensive set of works. Some aspects of aging in a two-dimensional model are not sufficiently explained. In the non-equilibrium critical relaxation of the diluted two-dimensional XY-model, the effects of super-aging and sub-aging are detected [19]. In this work, we carried out a basic study of the manifestation of aging in a two-dimensional XY-model with thermalization of structural disorder.
Two-time dynamic dependence of the spin-spin autocorrelation function $C_{SS}(t, t_w)$ of the vortex non-equilibrium critical relaxation of system for a wide range of observation times $t_w$, for spin concentrations $p = 0.9$ (a, b, c) and 0.6 (d, e, f), and for frizzing temperatures $T$ in BKT transition point $T_{BKT}(p)$ (a, d), and in low-temperature Berezinskii phase $T < T_{BKT}(p)$: $T_{BKT}(p)/2$ (b, e) and $T_{BKT}(p)/8$ (c, f).

Two-time dynamic dependence of the defect-defect autocorrelation function $C_{DD}(t, t_w)$ of the vortex non-equilibrium critical relaxation of system for a wide range of observation times $t_w$, for spin concentration $p = 0.9$, and for quenched temperatures $T$ in BKT transition point $T_{BKT}(p)$, and in low-temperature Berezinskii phase $T < T_{BKT}(p)$: $T_{BKT}(p)/2$ and $T_{BKT}(p)/32$.

The investigation of aging in this work was studied on the two-time dynamic dependencies of the spin-spin autocorrelation function $C_{SS}(t, t_w)$:

$$C_{SS}(t, t_w) = \frac{1}{pL^2} \left[ \sum_i p_i(t)p_i(t_w)S_i(t)S_i(t_w) \right], \quad (2)$$

where the brackets $[\ldots]$ and $\langle \ldots \rangle$ denote statistical averaging and averaging over the initial realisations of structural disorder in the system respectively. The results of the simulation results are presented in figure 3. Two typical aging regimes are observed in the presented two-time dynamic dependencies of the spin-spin autocorrelation function $C_{SS}(t, t_w)$. The short-time regime is observed at small observation times $t - t_w \ll t_w$, the long-time regime is observed at large times $t - t_w \gg t_w$. Modes are characterized by a power-law decay of the dynamic
dependence of the autocorrelation function $C_{SS}(t, t_w)$ with increasing observation time $t - t_w$. Between these two dynamic regimes, there is a dynamic crossover $t - t_w \sim t_w \gg 1$ corresponding to the transition from the short-time regime to the long-time regime. At large observation times $t - t_w \gg t_w$ there is a power-law dynamic dependence of the form $C_{SS}(t, t_w) \sim (t/t_w)^{-\Delta C}$. With a decrease in the quenched temperature $T$ of the system, there is a decrease in the value of the exponent $\Delta C$, while enhancing the aging of the system. In contrast to the system with quench disorder, in the process of non-equilibrium annealing of structure defects, there is no significant increase in aging with a decrease in the spin concentration $p$. From this we can conclude that the thermalization of the disorder does not lead to an additional slowing down of dynamic processes in the system in a non-equilibrium vortex critical relaxation, compared with the quench disorder. The study of dynamic scaling in the two-time dependencies of the spin-spin autocorrelation function is of considerable interest in the study of non-equilibrium aging, but this is supposed to be done in future works.

![Graphs](image)

**Figure 5.** Two-time dynamic dependence of the defect-defect autocorrelation function $C_{DD}(t, t_w)$ of the vortex non-equilibrium critical relaxation of system for a wide range of observation times $t_w$, for quenched temperature $T$ in low-temperature Berezinskii phase $T_{BKT}(p)/16$, and for spin concentrations $p = 0.8$ (a), 0.7 (b) and 0.6 (e). Similar graphs for concentration $p = 0.9$, see figure 4 (e).

### 4. Defect-defect autocorrelation function and aging

In the process of thermalization and annealing by vortices, defects move on the lattice. In this case, the occupation numbers $p_i$ obviously depend on time $t$, which allows one to introduce an autocorrelation function $C_{DD}(t, t_w)$ for defects. The investigation of aging in this work was studied on the two-time dynamic dependencies of the defect-defect autocorrelation function $C_{DD}(t, t_w)$:

$$C_{DD}(t, t_w) = \frac{1}{(1-p)L^2} \left[ \sum_i (1-p_i(t)) (1-p_i(t_w)) \right].$$

(3)

Similarly, it was possible to introduce a node-node autocorrelation function $C_{NN}(t, t_w)$:

$$C_{NN}(t, t_w) = \frac{1}{pL^2} \left[ \sum_i p_i(t)p_i(t_w) \right].$$

(4)

However, it is connected by a one-to-one ratio with the defect-defect autocorrelation function $C_{DD}(t, t_w)$ by relation (similarly for $C_{DN}(t, t_w)$ and $C_{ND}(t, t_w)$):

$$C_{DD}(t, t_w) = \frac{1 - 2p}{1 - p} + \frac{p}{1 - p}C_{NN}(t, t_w).$$

(5)
The results of the simulation are presented in figure 4 and figure 5. At the phase transition temperature $T_{\text{BKT}}(p)$, the dependence of the dynamic behavior of the autocorrelation function $C_{\text{DD}}(t, t_w)$ on the waiting time $t_w$ is practically absent, and relaxation is uniform over time ($C_{\text{DD}}(t, t_w) \sim f(t - t_w)$). With a decrease in temperature $T < T_{\text{BKT}}(p)$, dependence on the waiting time $t_w$ arises, and becomes especially significant in the region of very low temperatures $T \ll T_{\text{BKT}}(p)$. It can be seen that the two-time dependencies have a rather complex structure, which is not inherent to ordinary aging. With decrease in the spin concentration $p$, there is a decrease (see figure 5) in the differences between dynamic dependencies with different waiting times $t_w$. In the critical dynamics of the autocorrelation function $C_{\text{DD}}(t, t_w)$, the phenomenon of dynamic scaling is characteristic, when the two-time dependence of the autocorrelation function is expressed as

$$C_{\text{DD}}(t, t_w) \sim \Phi\left(\frac{\xi(t - t_w)}{\xi(t_w)}\right),$$

where $\xi(t)$ is the dynamic dependence for the correlation length of the system. The results of the scaling dependence of the defect-defect autocorrelation function $C_{\text{DD}}(t, t_w)$ are presented in figure 4 and figure 5. It is important to note that this dependence is not a “canonical” scaling dependence, as in [15, 16, 18–22], because there are no multipliers of the form $t_w^{-\eta/2}$ or $(t - t_w)^{-\eta/2}$. It is important to note that dynamic dependencies do not collapse for a selected set of waiting time $t_w$. However, at large observation times $t - t_w$, the formation of a declining family of curves is clearly observed. This may indicate the presence of an asymptotic scaling dependence on large times $t - t_w$.

![Figure 6](image.png)

**Figure 6.** Scaling dependence of the defect-defect autocorrelation function $C_{\text{DD}}(t, t_w)$ vs $\xi(t - t_w)/\xi(t_w)$ of the vortex non-equilibrium critical relaxation of system for a wide range of observation times $t_w$, for spin concentration $p = 0.9$, and for quenched temperatures $T$ in BKT transition point $T_{\text{BKT}}(p)$, and in low-temperature Berezinskii phase $T < T_{\text{BKT}}(p)$: $T_{\text{BKT}}(p)/4$ and $T_{\text{BKT}}(p)/32$. The envelope of a family of curves occurs at long observation times $t - t_w$.

5. Conclusion

In conclusion, we note that in the present work, the study of aging was first carried out in a two-dimensional XY-model with thermalization of defects. Two-time dynamic dependencies of the spin-spin autocorrelation function $C_{\text{SS}}(t, t_w)$ are obtained for the entire Berezinskii low-temperature phase $T < T_{\text{BKT}}(p)$, for a wide range of waiting times $t_w$ and spin concentrations $p$. It is revealed that the influence of structural defects annealed by vortices on aging in the dynamic dependencies of the spin-spin autocorrelation function $C_{\text{SS}}(t, t_w)$ is weaker than the influence of quench disorder. Two-time dynamic dependencies of the defect-defect autocorrelation function $C_{\text{DD}}(t, t_w)$ of the annealed disorder are obtained for the entire low-temperature phase $T < T_{\text{BKT}}(p)$ and for a wide range of spin concentrations $p$ and a range of waiting times $t_w$. Dynamic dependencies $C_{\text{DD}}(t, t_w)$ are of a fundamentally different nature than the two-time
dependencies for the spin-spin autocorrelation function $C_{SS}(t, t_w)$ and do not exhibit canonical aging properties. It is shown that near the BKT phase transition point $T_{BKT}(p)$, the dynamic dependencies $C_{DD}(t, t_w)$ become uniform with time, however, with a decrease in temperature in the low-temperature phase $T < T_{BKT}(p)$, this relaxation uniformity breaks down. In the region of extremely low temperatures $T < T_{BKT}(p)$, the dynamic dependencies $C_{DD}(t, t_w)$ become quite complex, and their structure requires further study. Dynamic dependencies $C_{DD}(t, t_w)$ do not collapse as $(t - t_w) = (t_w)^p$ for a selected set of waiting times $t_w$. However, at large observation times $t_w$, the formation of a declining family of curves is clearly observed and this may indicate the presence of an asymptotic scaling dependence.

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