Vortex annealing of structural disorder in non-equilibrium critical relaxation of the two-dimensional site-diluted XY-model with generalized model of disorder

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Abstract. The work is devoted to investigation of non-equilibrium vortex annealing of structural disorder in the two-dimensional site-diluted XY-model. The system incorporates mobile and fixed structure defects, with concentrations $c(a)$ and $c(q)$ correspondingly. Limiting cases $c(a) \approx c(q)$ and $c(a) \ll c(q)$ were considered. Dynamic clusterization of mobile defects was investigated by analysis of time dependences of size of the largest clusters and of averaged size of clusters. A comparison of the results with behavior of the XY-model with mobile defects only, revealed a qualitative change in non-equilibrium critical relaxation in case of $c(a) \ll c(q)$. That may be related to considerable slowing down of non-equilibrium vortex dynamics due to vortex pinning on fixed defects and attraction of percolation fixed point.

1. Introduction

Classical spin systems with continuous symmetry have been under investigation for long time [1, 2]. The two-dimensional XY-model is of particular interest among such systems. Although the long-range order is broken at any finite temperature in two-dimensional systems with continuous symmetry, the two-dimensional XY-model is characterized by existence of the topological Berezinskii-Kosterlitz-Thouless (BKT) phase transition at temperature $T_{\text{BKT}}$ [3–7]. This transition is related to a vortex-antivortex dissociation at the transition point. There is the low-temperature Berezinskii phase below the transition point, where each temperature can be considered as a critical one.

The two-dimensional XY-model is used to describe the critical properties of a wide range of real physical systems [1], such as critical properties of ultra-thin magnetic films [8] and a class of easy plane planar magnets [9, 10]; and many other systems. The spin mobility and impurity annealing are taken into account for description of granular superconductors [11, 12], high-temperature bulk superconductors [13], two-dimensional superfluids [14] and the superfluid transition of helium in porous media [15] by the two-dimensional XY-model.

The investigation of influence of structural disorder on non-equilibrium critical behavior of the system is also of special interest [2, 16]. Most of such studies are performed with the quenched disorder model (see refs. in [2,17–21]). Investigation of influence of structural disorder thermalization on equilibrium and non-equilibrium critical properties of the two-dimensional XY-model, by the model with annealed disorder, was performed in [21–24]. Introducing of mobile
defects into the two-dimensional XY-model results in formation of essentially non-equilibrium coherent stripe-like structures of defects [25, 26]. Such structures appears also in lattice models with additional special long-range interactions [27–31].

In view of the obtained results concerning the influence of the quenched disorder and of the structural disorder thermalization on equilibrium and non-equilibrium critical properties of the system, an interest is emerging to investigate general features of structural disorder influence on non-equilibrium critical relaxation properties of the two-dimensional XY-model, particularly on non-equilibrium vortex dynamics.

2. Model and methods
The Hamiltonian of the system was chosen in the following form

\[ H = -\frac{1}{2} \sum_{\langle i,j \rangle} p_ip_j S_i S_j, \]

where \( S_i \) is a classical planar spin placed at \( i \)-node of a square lattice with the linear size \( L \), \( p_i \) is an occupation number of \( i \)-node (if \( p_i = 1 \) then \( i \)-node is occupied by spin, else if \( p_i = 0 \) it is occupied by defect), \( \sum_{\langle i,j \rangle} \) denotes a summation over all pairs of the nearest neighbors.

The system contains two types of defects: mobile and fixed ones, with concentrations \( c^{(a)} \) and \( c^{(q)} \) correspondingly. They are uniformly distributed on the lattice 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. \( c = c^{(q)} + c^{(a)} = 1 - p \) is a concentration of defects. If \( c^{(a)} = 0 \) and \( c^{(q)} \neq 0 \) then the system represents that with the quenched disorder. On the contrary, if \( c^{(q)} = 0 \) and \( c^{(a)} \neq 0 \), all defects can move and such a system was previously [22–24] used for investigation of annealing of disorder. The present work is focused on study of a generalized model of disorder with \( c^{(a)} \neq 0 \) and \( c^{(q)} \neq 0 \).

The simulation of non-equilibrium critical relaxation of the model was conducted by the Metropolis algorithm. The dynamics implemented by the Metropolis algorithm corresponds to the dynamical model A according to dynamical and non-equilibrium critical behavior classification by Halperin and Hohenberg [32, 33]. The Metropolis algorithm was demonstrated to correctly describe non-equilibrium critical properties of the two-dimensional XY-model in the whole low-temperature phase \( T < T_{BKT}(p) \), up to the BKT phase transition point [34].

Taking into account the mobility of defects was accomplished by a modification of the Metropolis algorithm elementary step. If a randomly selected node is occupied by a mobile defect, then an attempt is made to swap this defect with random neighboring spin, calculating \( \Delta E_{nm} \) and producing a classical elementary step of Metropolis algorithm. The Monte Carlo step per spin (MCS/s) was used as a time unit, corresponding to \( L^2 \) spin flips or defects moves per unit time.

The annealing of structural disorder was investigated by analysis of disorder clustering, or the formation of clusters of defects. Identification of clusters was performed by the Hoshen-Kopelman algorithm [35–37]. Only mobile defects were included into clusters, as they are directly subjected to annealing. So the lattice was searched through for all clusters, and the sizes of each \( k \)-th cluster \( S_k \) were calculated at each time step \( t \). The size of the cluster was determined as the number of mobile defects in it. Then the size of the largest cluster \( S_{\text{m}}(p, T; t) \) and the average size of cluster \( S_{\text{av}}(p, T; t) \) were determined as follows

\[ S_{\text{m}}(p, T; t) = \left\lceil \max_{k=1 \ldots K} S_k(p, T; t) \right\rceil, \quad S_{\text{av}}(p, T; t) = \left\lceil \frac{1}{K} \sum_{k=1}^{K} S_k(p, T; t) \right\rceil, \]

where \( K = K(p, T; t) \) is the total amount of clusters on the lattice, the brackets (\( \ldots \)) and [\( \ldots \)] correspond to the statistical averaging over spin and impurity configurations respectively.
The investigation was carried out for system with linear sizes \( L = 32, 64, 128 \) and 256 and observation time \( 2 \times 10^4 \) MCS/s. The statistical averaging was performed over 500 impurity configurations and 15 spin configurations for each impurity configuration.

3. Analysis of simulation results

The initial Monte-Carlo simulation of the two-dimensional XY-model with generalized model of disorder demonstrated formation of non-equilibrium coherent structures such as stripes and clumps. They are formed due to vortex annealing of structural disorder. Typical configurations with such structures are demonstrated in figure 1.

![Figure 1.](image1.png)

Figure 1. Configuration fragment \((32 \times 32)\) of the system with the linear size \( L = 256 \) during non-equilibrium critical relaxation. The spin concentration \( p = 0.95 \), the mobile defect concentration \( c^{(a)} = 0.10 \) and the fixed defect concentration \( c^{(q)} = 0.05 \). Observation times from left to right: 0 (initial state), \( 10^2, 10^3, 10^4 \) and \( 10^5 \) MCS/s. Arrows denote classical planar spins; red squares — mobile defects; blue squares — fixed defects.

![Figure 2.](image2.png)

Figure 2. Dynamic dependences of sizes of the largest clusters \( S_n(t) \) (top) and averaged sizes of clusters \( S_n(t) \) (bottom) in non-equilibrium critical relaxation of the two-dimensional site-diluted XY-model with initial high-temperature non-equilibrium state, with spin concentration \( p = 0.9 \), fixed defect concentration \( c^{(q)} = 0.05 \) and mobile defect concentration \( c^{(a)} = 0.05 \).

Dynamic dependences of sizes of the largest clusters \( S_n(t) \) and averaged sizes of clusters \( S_n(t) \) in non-equilibrium critical relaxation of the two-dimensional site-diluted XY-model with initial high-temperature non-equilibrium state, with spin concentration \( p = 0.9 \), fixed defect concentration \( c^{(q)} = 0.05 \) and mobile defect concentration \( c^{(a)} = 0.05 \) are presented in figure 2. These results correspond to the case of small concentrations \( c^{(a)} \ll 1 \) and \( c^{(q)} \ll 1 \) of mobile and fixed defects respectively, with \( c^{(a)} \simeq c^{(q)} \). In this case the behavior is expected to be
qualitatively similar to that of the two-dimensional site-diluted XY-model with mobile defects only and with the same value of spin concentration $p = 0.9$ [22].

The dynamic dependences of $S_m(t)$ and $S_{av}(t)$ clearly demonstrate an “inertial” property of the growth. At first, sizes of clusters are increasing, reaching values greater than equilibrium ones. Then at larger times the growth is replaced by decrease of sizes.

The described dynamics may be characterized as a non-equilibrium critical coarsening, with the largest clusters determining the clusterization process. This can be clearly seen in figure 2 in dependences of dynamic relaxation scales on linear size $L$. In the process of non-equilibrium critical relaxation the correlation length $\xi(t) \ll L$, when finite-size effects are negligible. At times $t$, when $\xi(t) \approx L$, non-equilibrium critical relaxation is replaced by quasi-equilibrium and equilibrium critical behavior. Therefore the major contributions to non-equilibrium behavior are those with characteristic dynamic scales infinitely increasing with $L \to \infty$. Dynamic dependences of $S_m(t)$ in figure 2 demonstrate an increase of characteristic time scales with increase of linear size $L$. Also values of $S_m(t)$ in vicinity of maximum are increased with $L$ — the effect of inertial growth is enhanced and shifted to larger observation times $t$. Dynamic dependences for averaged sizes of clusters $S_{av}(t)$ demonstrate behavior almost independent of linear size of the system $L$. Comparison of dynamic dependences for $S_m(t)$ and $S_{av}(t)$ reveals an important feature: for all linear sizes $L$ under consideration, time region with decrease of $S_{av}(t)$ is partially overlapped with time region with increase of $S_m(t)$. This means that there exist dynamic scales when the growth of the largest clusters is produced by absorption of smaller clusters. At the same time the number of clusters formed by mobile defects is decreased.

The revealed peculiarities have essentially vortical nature, related to non-equilibrium interaction of vortices among themselves and with defects by means of non-equilibrium pinning.

The intensity of non-equilibrium coarsening of structural disorder is increased with decrease of “freezing” temperature $T$. And sizes $S_m(t)$ and $S_{av}(t)$ increase with decrease of temperature. The rate of non-equilibrium clusterization of mobile defects is decreased with increase of temperature $T$, that is clearly observed in the lowering of inertial growth peak value. At the BKT phase transition point $T_{BKT}(p)$ the inertial growth effect disappears: in the equilibrium state vortex pairs are destroyed, that affects the rate of non-equilibrium vortex annihilation.

Thus, dynamic dependences of sizes $S_m(t)$ and $S_{av}(t)$, as well as general characteristics of non-equilibrium critical coarsening, in the case of spin concentration $p = 0.9$, fixed defect concentration $c^{(q)} = 0.05$ and mobile defect concentration $c^{(a)} = 0.05$, qualitatively agree with non-equilibrium vortex annealing of structural disorder in the two-dimensional XY-model with mobile defects only and the same spin concentration $p = 0.9$ [22]. Quantitative differences consist in slight slowing down of relaxation processes and in increase of characteristic time scales. That is accounted for by decrease in mobility of vortices due to pinning on fixed defects [38].

Analogous behavior was observed in simulation with spin concentration $p = 0.8$, fixed defect $c^{(q)} = 0.1$ and mobile defect concentrations $c^{(a)} = 0.1$. However, slowing down of relaxation and increasing of characteristic time scales were observed in comparison with the case of $p = 0.9$.

Dynamic dependences of sizes of the largest clusters $S_m(t)$ and averaged sizes of clusters $S_{av}(t)$ in non-equilibrium critical relaxation of the two-dimensional site-diluted XY-model with initial high-temperature non-equilibrium state, with spin concentration $p = 0.65$, fixed defect concentration $c^{(q)} = 0.30$ and mobile defect concentration $c^{(a)} = 0.05$ are presented in figure 3. This corresponds to the case of small mobile defect concentration $c^{(a)} \ll 1$ and rather large fixed defect concentration $c^{(q)}$, with $c^{(a)} \ll c^{(q)}$. Here a qualitative change in behavior of the system during non-equilibrium critical relaxation is expected in comparison with a general behavior of non-equilibrium vortex annealing of structural disorder in the two-dimensional site-diluted XY-model with $p = 0.6 - 0.7$ [22]. This is connected with significant slowing down of non-equilibrium vortex dynamics due to pinning of vortices on fixed defects and attraction of percolation fixed point [39].
generalized model of disorder. The dynamic dependences for the size of the largest cluster of disorder in non-equilibrium critical relaxation of the two-dimensional site-diluted XY-model with spin concentration $p = 0.65$, fixed defect concentration $c^{(q)} = 0.30$ and mobile defect concentration $c^{(a)} = 0.05$.

An important feature appears in case of $c^{(a)} \ll c^{(q)}$ with a rather large fixed defect concentration: with increase of temperature $T$ the rate of mobile defect clusterization is decreased; however, the inertial effect does not disappear at the BKT phase transition point. That is due to attraction of percolation fixed point in non-equilibrium interaction of vortices and structure defects.

At the vicinity of the temperature $T_{BKT}(p)$ a qualitative change occurs in the cluster growth process (for both $S_m(t)$ and $S_{av}(t)$): there appears a time region with a growth of clusters after decreasing of their sizes.

Analogous behavior is observed for the case of simulation with spin concentration $p = 0.6$, fixed defect concentration $c^{(q)} = 0.3$ and mobile defect concentration $c^{(a)} = 0.1$. However, slowing down of relaxation and increasing of characteristic time scales were observed in comparison with the case $p = 0.65$.

4. Conclusion

The present work was devoted to investigation of non-equilibrium vortex annealing of structural disorder in non-equilibrium critical relaxation of the two-dimensional site-diluted XY-model with generalized model of disorder. The dynamic dependences for the size of the largest cluster $S_m(t)$ and the averaged sizes of clusters $S_{av}(t)$ were obtained in non-equilibrium critical relaxation with initial high-temperature non-equilibrium state, for temperatures $T$ in the entire low-temperature Berezinskii phase, up to the BKT phase transition point $T_{BKT}$, for a wide range of values of spin concentration $p$, fixed defect concentration $c^{(q)}$ and mobile defect concentration $c^{(a)}$.

Limiting cases $c^{(a)} \approx c^{(q)}$ and $c^{(a)} \ll c^{(q)}$ were considered. In case of $c^{(a)} \approx c^{(q)}$, dynamics of sizes of the largest clusters $S_m(t)$ and averaged clusters $S_{av}(t)$, as well as general behavior of critical coarsening, agree qualitatively with those obtained in the two-dimensional site-diluted XY-model with mobile defects only and the same spin concentration $p$ value.

In case of $c^{(a)} \ll c^{(q)}$ a qualitative change in non-equilibrium critical relaxation has been revealed in comparison with a general non-equilibrium vortex annealing of structural disorder in two-dimensional site-diluted XY-model. That may be related to considerable slowing down of non-equilibrium vortex dynamics due to vortex pinning on fixed defects and attraction of

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![Figure 3](image_url)
percolation fixed point.

The change of fixed defect concentration $c^{(q)}$, within limiting cases under consideration, was revealed to result only in quantitative changes of dynamic characteristics, connected with slowing down of relaxation and increasing of characteristic time scales.

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References

[1] Korshunov S E 2006 *Phys. Usp.* 49 225
[2] Prudnikov V V, Prudnikov P V and Mamonova M V 2017 *Phys. Usp.* 60 762
[3] Berezinskii V L 1973 *Sov. Phys. JETP* 32 498
[4] Berezinskii V L 1972 *Sov. Phys. JETP* 34 610
[5] Berezinskii V L 2007 *Low-Temperature Properties of Two-Dimensional Systems* (Moscow: Fizmatlit) p 232 [in Russian]
[6] Kosterlitz J M and Thouless D J 1973 *J. Phys. C* 6 1181
[7] Kosterlitz J M 1974 *J. Phys. C* 7 1046
[8] Vaz C A F, Bland J A C and Lauhoff G 2008 *Rep. Progr. Phys.* 71 056501
[9] Kawabat C and Bishop A R 1986 *Solid State Commun.* 60 167
[10] Elmers H-J, Hauschild J, Liu G H and Gradmann U 1996 *J. Appl. Phys.* 79 4984
[11] Zeng X C, Stroud D and Chung J S 1991 *Phys. Rev. B* 43 3042
[12] Zeng X C, Stroud D and Chung J S 1984 *Phys. Rev. B* 30 134
[13] Carlson E W, Kivelson S A, Emery V J and Manousakis E 1999 *Phys. Rev. Lett.* 83 612
[14] Schultka N and Manousakis E 1994 *Phys. Rev. B* 49 12071
[15] Moon K and Girvin S M 1995 *Phys. Rev. Lett.* 75 1328
[16] Odor G 2004 *Rev. Mod. Phys.* 76 663
[17] Berche B, et al 2003 *Eur. Phys. J. B* 36 91
[18] Kapikranian O, Berche B and Holovatch Yu 2007 *Eur. Phys. J. B* 56 93
[19] Prudnikov V V, Prudnikov P V and Popov I S 2018 *JETP* 126 369
[20] Prudnikov V V, Prudnikov P V and Popov I S 2015 *JETP Letters* 101 539
[21] Popov I S, Popova A P, Prudnikov P V and Popov V V 2019 *J. Phys.: Conf. Series* 1163 012042
[22] Popov I S, Popova A P and Prudnikov P V 2019 *EPL* 128 26002
[23] Popov I S, Popova A P and Prudnikov P V 2019 *J. Phys.: Conf. Series* 1389 012024
[24] Popov I S, Popova A P and Prudnikov P V 2019 *J. Phys.: Conf. Series* 1163 012039
[25] Sandvik A W, Daul S, Singh R R P and Scalapino D J 2002 *Phys. Rev. Lett.* 89 247201
[26] Valdez-Balderas D and Stroud D 2005 *Phys. Rev. B* 72 214501
[27] Valdez-Balderas D and Stroud D 2006 *Phys. Rev. B* 74 147506
[28] Valdez-Balderas D and Stroud D 2008 *Phys. Rev. B* 77 045151
[29] Reichhardt C J O, Reichhardt C and Bishop A R 2010 *Phys. Rev. E* 82 041502
[30] Reichhardt C J O, Reichhardt C and Bishop A R 2011 *Phys. Rev. E* 83 041501
[31] Derzhko V, Jedrzejewski J and Krokhmalski T 2009 *Eur. Phys. J. B* 68 501
[32] Hohenberg P C and Halperin B I 1977 *Rev. Mod. Phys.* 49 435
[33] Folk R and Moser G 2006 *J. Phys. A: Math. Gen.* 39 207
[34] Prudnikov V V, Prudnikov P V, Alekseev S V and Popov I S 2014 *Phys. Metal. Metallogr.* 115 1186
[35] Hoshen J and Kopelman R 1976 *Phys. Rev. B* 14 3438
[36] Hoshen J and Kopelman R 1978 *J. Stat. Phys.* 19 219
[37] Hoshen J and Kopelman R 1979 *J. Stat. Phys.* 21 583
[38] Pereira A R, Mól L A S, Leomel S A, Coura P Z and Costa B V 2003 *Phys. Rev. B* 68 132409
[39] Prudnikov V V, Prudnikov P V and Popov I S 2020 *JETP* 131 [to be translated]