Disorder Aggregation by Vortices in Non-Equilibrium Critical Annealing of Two-Dimensional XY-model

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Abstract. It is shown that the non-equilibrium vortex annealing of structural disorder in a two-dimensional XY-model leads to a non-equilibrium critical coarsening. Large clusters are separated into an individual subsystem, the relaxation dynamics of which is much slower than the relaxation dynamics of the cluster subsystem as a whole. Despite the fact that the main equilibrium critical properties, even the Berezinskii-Kosterlitz-Thouless phase transition temperature $T_{BKT}(p)$, of the two-dimensional XY-model with disorder thermalization do not change as compared with the system with quench disorder, the non-equilibrium critical relaxation shows significant differences.

The study of critical behavior of disordered systems causes considerable fundamental and applied scientific interest [1, 2]. The critical phenomena are characterized by a strong fluctuation behavior. In the system at the critical state there are anomalously large and long-lived fluctuations of the main thermodynamic quantities, characterized by strong interaction. Lowering the dimension of the system leads to increased fluctuation effects. The systems with continuous symmetry of the ground state are usually characterized by much stronger fluctuation effects than systems with discrete symmetry. Therefore, low-dimensional systems with continuous symmetry are characterized by a significant contribution of fluctuations to critical properties [3]. In two-dimensional systems with continuous symmetry, the long-range order (LRO) is destroyed by anomalously strong transverse fluctuations of the spin density at all non-zero temperatures $T \neq 0$. However, in such systems there are more exotic forms of ordering. The main features of such systems are associated with the existence of topological excitations in them, such as vortices and other topological defects [4–6].

A special place among two-dimensional systems with continuous symmetry is occupied by a two-dimensional XY-model [3–5]. Despite the absence of a long-range order at all non-zero temperatures $T \neq 0$, there exists a Berezinskii-Kosterlitz-Thouless (BKT) topological phase transition at temperature $T = T_{BKT}$ in it. In this system there is a low-temperature Berezinskii phase $T < T_{BKT}$, where each temperature $T$ is a critical point, i.e. there is a continuous set of fixed points of the renormalization group transformation. This makes it possible to study the critical behavior of the system not only in one isolated point $T_C$ (as, for example, in the Ising model), but in the whole temperature range $T \leq T_{BKT}$. The low-temperature phase has a quasi-long-range order (QLRO). In this case, the spatial correlation function decreases by power-law to zero with increasing distance. The critical exponents of the two-dimensional XY-model depend on temperature, for example $\nu = \nu(T)$. The phase transition is physically related to dissociation of the coupled vortex pairs at the transition point. In the two-dimensional XY-model in the...
state of thermodynamic equilibrium in the low-temperature Berezinskii phase $T < T_{BKT}$, all the vortices are connected in coupled pairs, and in the high-temperature phase $T \geq T_{BKT}$ the vortices are uncoupled.

The two-dimensional XY-model is used to describe the critical properties of a wide range of real physical systems [3], such as critical properties of ultra-thin magnetic films [7] and extensive class of easy plane planar magnets [8,9], including quite specific ones $\text{Rb}_2\text{CrCl}_4$ [10], $(\text{C}_6\text{H}_5\text{CH}_2\text{NH}_3)_2\text{CrBr}_4$ [11], $(\text{CH}_3\text{NH}_3)_2\text{MnCl}_4$ [12], $(\text{tetrenH}_5)_0.8\text{Cu}_4\text{[W(CN)]}_8\cdot 7\text{H}_2\text{O}$ [13]; singularities in the critical properties of superconducting thin films [14,15] and superfluid thin films of liquid helium [16–19]; arrays of Josephson junctions [3,20,21] and SFS-junctions [22–24]; two-dimensional crystals [5] and smectic liquid crystals [25–29]; some correlation properties of two-dimensional turbulence [30]; melting of several layers of sorbed xenon in single-crystal graphite [31]; the process of sorbing hydrogen on tungsten $W(011) \ p(2 \times 2)$ [32]; and some properties of many other physical systems [3,33]. Also, to the phenomena described by the XY-model, it is possible to relate dynamic properties of such exotic systems as flocks of birds [34] and some other forms of collective behavior of living organisms [35,36].

**Figure 1.** Snapshot configurations of the system with linear size $L = 64$ and spin concentration $p = 0.9$ at times 0, 500, 2000 and 10000 MCS/s. Arrows indicate the spins, red squares indicate the defects.

**Figure 2.** Snapshot configurations of the defects in the system with linear size $L = 512$ and spin concentration $p = 0.9$ at times 0, 5000, 20000 and 100000 MCS/s.

The non-equilibrium critical relaxation of a two-dimensional XY-model can have vortex and spin-wave characters [37–41]. It depends on the initial non-equilibrium state. If the initial state is the low-temperature one, prepared in contact with a thermostat at zero temperature $T_0 = 0$, then the relaxation dynamics will be spin-wave [37,38,40]. In the case of the initial high-temperature state the system is prepared at a high temperature $T \gg T_{BKT}$ thermostat, and the relaxation is accompanied by vortex dynamics [37–39]. Inclusion the structural disorder in the model leads to a significant qualitative change in critical behavior [39–41]. The effect of structure
defects on spin-wave relaxation is not considered in this work, details are given in another work [40]. The effect of structure defects on the non-equilibrium critical vortex dynamics is accompanied by the appearance of non-equilibrium pinning of vortices on defects [39, 41].

Existing research (see [2, 39–42] and refs. in them) focuses on the study of the quenched disorder influence on the vortex dynamics of a two-dimensional XY-model. The quenched disorder model assumes that the relaxation time of the defect subsystem is significantly longer than the relaxation time of the spin subsystem. In the papers [43, 44] it was shown that the vortex relaxation of the diluted model occurs extremely slowly. This particularly applies to the vortex concentration and geometric characteristics of QLRO-areas. Therefore, there is an interest in the study of the structural disorder thermalization in the diluted two-dimensional XY-model.

In a diluted XY-model with a quenched structural disorder in the process of non-equilibrium pinning, vortices are attracted by defects. If defects are defrosted, a reverse process will occur, when the defects are attracted by vortices. Defects will be collected in vortex cores, thereby creating non-equilibrium defect aggregations. The first produced simple Monte-Carlo simulation shows that this effect does take place (see Fig. 1 and Fig. 2). When the system goes into the thermodynamic equilibrium state, the vortices will gather into the vortex pairs. In this case defects can not be pinned with the vortices, and the defect clusters will be destroyed. Thus, the non-equilibrium annealing of defects by vortices in the diluted two-dimensional XY-model will be accompanied by a substantially non-equilibrium effect associated with non-equilibrium aggregation. This paper is devoted to research of this disorder aggregation by vortices in non-equilibrium critical annealing of diluted two-dimensional XY-model.

The Hamiltonian of the two-dimensional XY-model in this work was chosen as

$$H[p, S] = -\frac{1}{2} \sum_{\langle i,j \rangle} p_i p_j S_i S_j - \frac{1}{2} \sum_{\langle i,j \rangle} p_i p_j \cos(\varphi_i - \varphi_j),$$  \hspace{1cm} (1)

where $S = \{S_i(t)\}$ and $p = \{p_i(t)\}$ – spin and defect lattice fields; $S_i = (S_{i,x}, S_{i,y}) \equiv (\cos \varphi_i, \sin \varphi_i)$ is a classical planar spin which is associated with $i$-node of a square lattice with the linear size $L$; $\varphi_i$ is a phase of spin $S_i$; $p_i$ is an occupation number of $i$-node: if $p_i = 1$ then $i$-node is occupied by a spin, else, if $p_i = 0$, by a defect; $\sum_{\langle i,j \rangle}$ is a summation over all pairs of the nearest neighbors. Defects on the lattice are distributed uniformly at time $t = 0$ with probability $P(p_i) = (1 - p)\delta(p_i) + p\delta(1 - p)$, where $p$ – spin concentration, i.e. $c_{imp} = 1 - p$ is the concentration of impurity. Simulation of critical dynamics of the system was carried out by Metropolis algorithm, as it adequately sets the dynamic properties of this system [45]. To include the mobility of defects, the elementary step of the Metropolis algorithm was modified. If a randomly selected node is occupied by a spin, then the classical elementary step is produced. But if a node is occupied by a defect, then an attempt is made to swap this defect with a random neighboring spin. Similarly, the calculation of $\Delta E$ is carried out and the elementary step of Metropolis algorithm is used. For analysis of defect cluster structure the Hoshen-Kopelman algorithm [46–48] is used. The study was carried out for spin concentrations $p = 0.9, 0.8, 0.7$ and 0.6. Spin concentration $p = 0.6$ is close to the spin percolation threshold $p_c \approx 0.592745(2)$ [49] by the nearest neighbors on the two-dimensional square lattice.

Initially in this work the temperatures of Berezinskii-Kosterlitz-Thouless phase transition $T_{\text{BKT}}(p)$ were determined for considered spin concentrations $p$. To do this, we used Binder cumulants $U_4 = \frac{1}{2} \langle 3 - |M^4|/|M^2|^2 \rangle$ and spatial correlation function $C(r)$ ratio at two different scales $R = \{C(L/2)|/|C(L/4)|\}$. The temperature dependences of these quantities for three different values of $L$ have triangles in the region $T_{\text{BKT}}(p)$. As a result of simulation, $T_{\text{BKT}}(p = 0.9) = 0.679(6)$, $T_{\text{BKT}}(p = 0.8) = 0.487(9)$, $T_{\text{BKT}}(p = 0.7) = 0.339(9)$ and $T_{\text{BKT}}(p = 0.6) = 0.161(5)$. Also it is important to note that the temperatures $T_{\text{BKT}}(p)$ for spin concentrations $p = 0.9, 0.8, 0.7$ and 0.6 are equal within the statistical error to the corresponding
values for the two-dimensional XY-model with quenched disorder [50]. However, this result is not unexpected. It is well known that annealed structural disorder does not significantly affect the equilibrium critical behavior [51]. In this case, the influence of annealed structural disorder did not even lead to a change in the temperature of the Berezinskii-Kosterlitz-Thouless phase transition $T = T_{BKT}(p)$.

![Figure 3](image1)

**Figure 3.** The dynamic dependences of the size of the largest cluster of defects $S_m(t)$ (a, b) and of the average size of clusters of defects $S(t)$ (c, d) for the system with spin concentrations $p = 0.9$ and linear sizes $L = 32$ (a, c) and $L = 256$ (b, d).

![Figure 4](image2)

**Figure 4.** The dynamic dependences of the size of the largest cluster of defects $S_m(t)$ (a, b) and of the average size of clusters of defects $S(t)$ (c, d) for the system with spin concentrations $p = 0.6$ and linear sizes $L = 32$ (a, c) and $L = 256$ (b, d).

Subsequent research in this work was focused on the study of the non-equilibrium critical annealing of defects by vortices. The expected behavior of the subsystem of defects showed that there is a non-equilibrium aggregation of defects in vortex cores (see Fig. 1 and Fig. 2). In the vortex cores, defects are collected in clusters. Therefore, the geometric characteristics of defect clusters were chosen to characterize the non-equilibrium vortex annealing of defects. In works [44,52–54] it was shown that non-equilibrium vortex dynamics in a two-dimensional model is accompanied by coarsening of the vortex subsystem. During coarsening, the concentration of the vortices decreases with time, and the effective “size” of the vortices increases. For a detailed description of the clustering of defects in a non-equilibrium vortex annealing, we calculated the average values of the sizes $S(t)$ of defect clusters and the sizes $S_m(t)$ of the largest defect clusters. Fig. 3 and Fig. 4 show the results for $p = 0.8$ and 0.6. Immediately, attention should be paid to an important feature of the defect clustering dynamics in the system: dynamic dependences for the average cluster sizes do not depend on the linear size $L$ of the system. This is manifested in the absence of changes for systems with linear sizes $L = 32$ and $L = 256$. Dynamic dependences of the sizes of defect clusters clearly demonstrate the process of coarsening of the subsystem of defects. One can immediately notice the inertial feature of cluster growth. At first, the sizes of defect clusters reach the maximum value, the peak, and then decrease to their equilibrium values. The initial value ($t = 0$) of cluster size can be considered equal to the size of similar defect clusters in the simulation of quenched structural disorder, since the preparation of the defect distribution in both cases is identical. The equilibrium values ($t \rightarrow \infty$) of cluster sizes do not equal the initial values. This suggests that in the equilibrium state, the defects are distributed uniformly over the lattice, despite the absence of uncoupled vortices in the system. However, since in this work the dynamic dependences of the vortex concentration are...
not investigated, one can say that few unpaired vortices remain and exist in the system longer than was simulated in this work. With increasing system temperature $T$, the peak amplitude decreases, and at the phase transition point $T = T_{BKT}(p)$ the peak disappears from the dependences. Dynamic dependences of the average values of the sizes $S(t)$ of defect clusters and the sizes $S_m(t)$ of the largest defect clusters in Fig. 3 for system with linear size $L = 32$ show a clear time retard in the dynamics of cluster growth on average $S(t)$ and large clusters $S_m(t)$. In the low-temperature region, for example at a temperature $T = T_{BKT}(p)/16 \ll T_{BKT}(p)$, the dynamic dependence for the average cluster size peaks at times of 200-300 MCS/s, while for large clusters the peak occurs at time 1000 MCS/s. For large linear sizes $L$, this effect is enhanced. In particular, for the linear size of $L = 256$ the time to reach the peak of the dynamic dependence for the average cluster size $S(t)$ is also 200-300 MCS/s, while for the sizes of large clusters $S_m(t)$ the peak occurs at times of 10000 MCS/s. With increasing system temperature $T$, the scale of subsystem of large clusters retard, as compared with the cluster subsystem as a whole, gradually decreases and disappears at the phase transition point $T = T_{BKT}(p)$. With an increase in the defects concentration $c_{imp}$ (i.e. decrease in the spin concentration $p$), the process of relaxation of the subsystem of structural defects slows down. At the same time the sizes of clusters $S(t)$ and $S_m(t)$ become larger. Thus, the non-equilibrium vortex annealing demonstrates many interesting features, in particular, requiring further study.

Conclusion

In conclusion, in this work a study of the non-equilibrium vortex annealing of defects in a two-dimensional model was carried out. It is shown that the “defrosting” of defects does not change the values of the Berezinskii-Kosterlitz-Thouless phase transition temperature $T_{BKT}(p)$. The study revealed that the non-equilibrium vortex annealing of structural disorder in a two-dimensional XY-model leads to a non-equilibrium critical coarsening. In this case, large clusters are separated into an individual subsystem, the relaxation dynamics of which is much slower than the relaxation dynamics of the cluster subsystem as a whole.

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