Non-equilibrium critical vortex dynamics of disordered 2D XY-model

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Abstract. Vortex dynamics and clustering in non-equilibrium critical relaxation of disordered 2D XY-model are investigated for different initial states. Time dependencies of vortex concentration and clusters sizes are studied for different spin concentrations. The anomalous slow down of clustering in disordered system are explained by pinning of vortices on defects. The calculated temperature dependence of transverse stiffness allows to estimate critical temperature $T_{BKT}$ and applicability of spin-wave approximation for disordered system.

1. Introduction
Investigations of low-dimensional systems with continuous symmetry represents a considerable scientific interest. These systems are characterized by specific topological phase transitions with realization of special phases without long-range order [1]. Non-equilibrium behavior of these systems demonstrates slow dynamics with such characteristic effects as an aging [2–4] and the memory about the initial states and about any intermediate state in the course of the relaxation process [5,6]. The critical coarsening is an important non-equilibrium phenomenon in such systems, characterized by the emergence of larger scale structures from smaller ones and accompanied by the decrease of total number of these structures [4,7]. Systems with the coarsening process are called ”coarsening dynamical systems” [8–10]. As opposed to ”coarsening” can be introduced the concept of ”fragmentation” as a process with fragmentation large structures to smaller ones with an overall increase in the number of objects.

The 2D XY-model takes an important position in the set of an low-dimensional systems [1]. This model describes the behavior of a wide class of physical systems, such as the planar magnetics [11,12] and ultrathin magnetic films [13], in particular the films of Co and Ni on Cu-substrate and Fe on Au-substrate [13]. Also, the 2D XY-model is used for description of various properties of the superconducting films [14] and the superfluid helium films [15], Josephson-junction arrays [16], especially tailored nematic liquid crystals [17], toy models for two-dimensional turbulence [18], and many others [1,19].

The 2D XY-model demonstrates the Beresinskii-Kosterlitz-Thouless topological phase transition [20,21] which is associated with the dissociation of coupled vortex-antivortex pairs at the transition point $T_{BKT}$. An important feature of the Beresinskii-Kosterlitz-Thouless phase transition in the 2D XY model is that each temperature in the low-temperature phase becomes critical; i.e., a continuous cascade of second-order phase transitions is observed [20,21]. This allows a certain analogy between non-equilibrium effects in the 2D XY model and the features of spin glass [22].
The equilibrium behavior and statical properties of the 2D XY-model are relatively complete explored scientific area, but investigations of non-equilibrium properties and influence of structural disorder on these properties are of significant interest. According to the Harris criterion [23], the presence of structural defects can be significant if the critical exponent of the heat capacity $\alpha$ is positive. It is predicted that the presence of structural defects does not affect to the 2D XY-model behavior near the critical temperature $T_{BKT}$. However, in low-temperature phase for $T < T_{BKT}$, as shown by analytical and numerical study of the equilibrium and non-equilibrium properties of the model [24–26], the presence of defects leads to changing of the equilibrium characteristics for the correlation functions and their concentration dependence.

2. Description of the model and methods

In this work, we take the Hamiltonian of the disordered system in the form

\[ H = -J \sum_{\langle i,j \rangle} p_i p_j \mathbf{S}_i \mathbf{S}_j, \]  

where $J$ is a exchange integral, $\mathbf{S}_i$ is the classical planar spin fixed in $i$th site of square lattice with linear size $L$, $p_i$ are the occupation numbers: $p_i = 1$ and 0 if the $i$th site is occupied by spin and defect, respectively. Summation occurs on a nearest neighbors of sites $(i, j)$. The distribution of defects are taken as uncorrelated and the concentration of defects $c_{imp}$ is determined by spin concentration $p$: $c_{imp} = 1 - p$.

For simulation of non-equilibrium relaxation it was used the Metropolis algorithm of flipping individual spins which appropriately realizes dynamics of 2D XY-model [27] in low-temperature phase for $T < T_{BKT}$. The dynamics of the Metropolis algorithm corresponds to dissipative processes which described by dynamic model A in Halperin-Hohenberg classification [28].

3. The transverse stiffness

Low-temperature phase $T < T_{BKT}$ is characterized by non zero transverse stiffness $\rho(T, p)$ [20, 27, 29]. For calculation of stiffness it was used numerical method from [30]. The simulation were carried out for linear size of lattice $L = 256$, full random initial conditions, spin concentration $p = 1.0$, 0.9, 0.8. It was used $3 \cdot 10^7$ Monte Carlo steps per spin ($MCS/s$) for equilibration and $5 \cdot 10^7$ $MCS/s$ for statistical averaging. Results of simulation are presented on Fig. 1. These curves have been obtained by averaging over 100 different initial configurations for pure system and by averaging over 50 defects configurations for disordered system with 5 statistical runs for each sample.

The relation [29] $\rho(T_{BKT}) = (2/\pi)T_{BKT}$ allows to calculate the value of $T_{BKT}$. Values $T_{BKT}(p)$ for different spin concentrations are marked by arrows on Fig. 1. Obtained values are in well agreement with the results from [25] which $T_{BKT}(p)$ were determined by method of correlation functions.

In [29] it was introduced relation for pure system $\rho(T) = e^{-T/4\rho(T)}$ in spin-wave approximation (i.e. without vortex component). It let us conclude that $\rho(T = 0) = 1.0$. Spin-wave approximation is works well in low-temperature limit $T \ll T_{BKT}$. If we consider the case $T/4\rho(T) \ll 1$, then $e^{-T/4\rho(T)} \simeq 1 - T/4\rho(T)$ with assuming the relation $\rho_{SW}(T) = 1 + \alpha_{SW}(T)$,
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where $|\alpha_{SW}(T)| \ll 1$ it was obtained the following relation $1 + \alpha_{SW}(T) \simeq 1 - \frac{T}{4[1+\alpha_{SW}(T)]} \simeq 1 - T/4[1 - \alpha_{SW}(T)]$ and the final solution $\alpha_{SW}(T) = -\frac{T}{1-T/4} \simeq -T/4$. Thus, the spin-wave form of $\rho$ is $\rho_{SW}(T) \simeq 1 - T/4$ in low-temperature limit $T \ll T_{BKT}$. The temperature dependence of $\rho_{SW}(T)$ is presented in Fig. 1 by dash line.

The spin-wave form $\rho_{SW}(T) \simeq 1 - T/4$ doesn’t work for disordered system with $p < 1$ by reason of $\rho(T = 0, p < 1.0) \neq 1$.

4. Non-equilibrium vortex dynamics and clustering

In the 2D XY-model where are two different types of critical coarsening: vortex coarsening [7, 31] and quasi-long-range order (quasi-LR order) coarsening [24, 32]. Applied to lattice models it can using concept of “clustering”, where coarsening is the emergence of larger scale structures. The ”fragmentation” is the fragmentation large structures on smaller.

Numerical simulation are performed for 2D XY-model with $L = 256$ and spin concentration $p = 1.0$ (pure system) and 0.9 and 0.8 (disordered system). Values $T_{BKT}(p)$ for this spin concentrations $p$ are used from [25]. Simulation of critical relaxation are performed from two different non-equilibrium initial states: low-temperature initial state ($T_0 = 0$) and high-temperature initial state ($T_0 \gg T_{BKT}(p)$). For relaxation from high-temperature initial state (HT) excessive amount of vortex excitations are present in system originally. As opposed to relaxation from low-temperature initial state (LT) vortex excitation in system are not presented originally and are generated in system in the process of relaxation by energy of temperature fluctuations.

Non-equilibrium relaxation are investigated until the time $10^6 \text{MCS}/s$. For pure system ($p = 1.0$) it was used 20000 different initial configuration, 10000 different defects configuration for $p = 0.9$, and 15000 different defects configuration for $p = 0.8$ and 5 different initial configuration for low-temperature phase $T \leq T_{BKT}(p)$. 

Figure 2. Time dependence of large clusters size $\zeta_m$ in system for different temperature $T < T_{BKT}(p)$, different spin concentration $p$ and different initial state: low-temperature initial state (LT) and high-temperature initial state (HT).
be reduced to two simpler problems: problem of clustering curve and problem of everywhere

\[ T < T_{\text{BKT}}(p) \]

for pure system and takes values \( \varphi \). When defects are introduced to system, the size of clusters is decrease, but this effect can be explained by violation of the translational symmetry in disordered system i.e. areas of quasi-LR order become smaller. The violation of the translational symmetry can not be explained by slow down effects of cluster relaxation.

On Fig. 3 it were presented parametric dependencies average clusters size \( \zeta_m \) in system for different parameters it have been selected large clusters size \( \zeta_m \) – linear size of largest cluster in system, average cluster size \( \zeta \) and quantity of clusters \( \kappa \) in system. Linear size of cluster was selected as square root of square of cluster.

On Fig. 2 it were presented time dependencies of large clusters size \( \zeta_m \) in system for different temperature \( T < T_{\text{BKT}}(p) \), different spin concentration \( p \) and different initial state. As seen from this dependencies the dynamics of relaxation of system is significantly slow because curves of time dependencies for different initial states are intersected and tend to line for large times for pure system \( \sim 10^6 \) MCS/s, but for disordered system and for low-temperature \( T \) these times \( \gg 10^6 \) MCS/s and takes values \( \sim 10^{12} - 10^{18} \) MCS/s. When defects are introduced to system, the size of clusters is decrease, but this effect can be explained by violation of the translational symmetry in disordered system i.e. areas of quasi-LR order become smaller. The violation of the translational symmetry can not be explained by slow down effects of cluster relaxation.

On Fig. 3 it were presented parametric dependencies average clusters size \( \zeta \) on quantity of clusters \( \kappa \) for all studied temperatures \( T < T_{\text{BKT}}(p) \) all spin concentration \( p \) and different initial state. As noted, these dependencies well described dependencies by the relation of the form \( \zeta \sim \kappa^{-1/2} \). It should pay attention that \( \zeta \) is determined as \( \sqrt{S} \), where \( S \) is the square of cluster and only after the averaging of different clusters and not vice versa. If averaging over different clusters designated as \( || \ldots || \) then dependencies on the type \( \zeta \sim \kappa^{-1/2} \) are indicate the relation \( \|\sqrt{S}\| \sim \|S\| \), because \( \sqrt{\|S\|} \sim \kappa^{-1/2} \) obvious from the geometric considerations about clustering of square lattice. Relation \( \|\sqrt{S}\| \sim \sqrt{\|S\|} \) is demonstrated that clustering in lattice of 2D XY-model in non-equilibrium relaxation can be represented as everywhere dense in the lattice of mapping without self-intersections clustered curve. So problem of quasi-LR order clustering in non-equilibrium critical relaxation of 2D XY-model can be reduced to two simpler problems: problem of clustering curve and problem of everywhere

\[ T < T_{\text{BKT}}(p) \]

Figure 4. Time dependence of free vortex concentration \( \Omega_F \) in system for different temperature \( T < T_{\text{BKT}}(p) \), different spin concentration \( p \) and different initial state.

Figure 5. Time dependence of pinning vortex concentration \( \Omega_P \) in system for different parameters of simulation.
and parametric dependence of pinning vortex concentration \( \Omega \) disordered system with multimode regimes \( \Omega \) is not arising possibly because of existence subsystem of vortex excitations originally in system. Temperature dynamics of system with relaxation from high-temperature initial state this effect more complex and can not be reduced to two different independent problems. For low-temperature dynamics of system with relaxation from high-temperature initial state this effect is not arising possibly because of existence subsystem of vortex excitations originally in system.

![Figure 6](image_url)

Figure 6. Parametric dependence of free vortex concentration \( \Omega_F \) on quantity of clusters \( \kappa \) for pure system (left) and parametric dependence of pinning vortex concentration \( \Omega_P \) on large clusters size \( \zeta_m \) for disordered system with \( p = 1.0 \) (right). Relaxation from high-temperature initial state.

For investigation of vortex dynamics it was created special algorithm, when vortex is identified as contour with phase increment \( \Delta \varphi \) which multiple \( 2\pi \). In structure disordered system it were searched all minimal contours around defects clusters and vortex are identified by the phase increment. This algorithm can calculated quantity of free and pinning vortex and antivortex in pure and disordered system. With using this algorithm it were calculated dynamical dependencies of free vortex excitation concentration (quantity of vortex excitations divided on quantity of spins \( N = pL^2 \)) \( \Omega_F \), pinning vortex excitation concentration \( \Omega_P \).

On Fig. 4 and Fig. 5 are presented time dependencies of free vortex in system for different temperature \( T \ll T_{BKT}(p) \), different spin concentration \( p \) and different initial state. Of these dependencies can draw conclusions that concentration of free and pinning vortex have a multimode time dependencies for relaxation from high-temperature initial state. It is connected with complex process of non-equilibrium annihilation vortex and antivortex and non-equilibrium pinning of vortex excitations on defects of structure. In disordered system significantly slowing are observed, i.e. relaxation times in order of magnitude equal to relaxation times of quasi-LR order clustering.

This slowing can well explained by non-equilibrium pinning process. The vortex excitations are "pinned" on defects and their mobility is reduced considerably. It can be explaine the slowing process of quasi-LR order clustering in disordered system. On Fig. 6 it were presented parametric dependence of free vortex concentration \( \Omega_F \) on quantity of clusters \( \kappa \) for pure system and parametric dependence of pinning vortex concentration \( \Omega_P \) on large clusters size \( \zeta_m \) for disordered system with \( p = 1.0 \). From these dependencies it can conclude that vortex excitations constrained growth of quasi-LR order areas – quantity of clusters \( \kappa \) is increase and large clusters size \( \zeta_m \) is decrease with increase vortex concentration \( \Omega_F \). Thus, slowing of vortex dynamics in disordered system by non-equilibrium pinning is slowing quasi-LR order clustering by boundariong effect. As seen on Fig. 6 the power parametric dependencies \( \Omega_F \sim \kappa \) for pure system and multimode regimes \( \Omega_P \sim \zeta_m^{\alpha_1} \) and \( \Omega_P \sim \zeta_m^{\alpha_2} \) on different time intervals for disordered system are appeared.

5. Conclusion

Vortex dynamics and clustering in non-equilibrium critical relaxation of disordered 2D \( XY \)-model are investigated for low-temperature and high-temperature initial states. It was showed
for the first time that quasi-LR order clustering in non-equilibrium critical relaxation of 2D XY-model can be reduced to problem of clustering curve and problem of everywhere dense mapping curve without self-intersections on the plane. The slow down effect of quasi-LR order clustering and slow dynamics of vortex subsystem were demonstrated for disordered system. It was found boundaring effect of vortex for clustering process. The calculated temperature dependence of transverse stiffness allows to estimate values of critical temperature $T_{BKT}(p)$ for disordered system.

Acknowledgments

Work is supported by the Ministry of Education and Science of the Russian Federation, project No. 1627 and grant of Omsk State University for young scientists, project MU-4/2015. Numerical studies were performed with the support by supercomputer center of Moscow State University, Moscow and St.Petersburg Joint Supercomputer Center.

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