The dimensional crossover in critical behavior of layered XY-model

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Abstract. The study of critical properties and size transition in a diluted layered XY-model was carried out for the first time. The dimensional dependence of the temperature $T_{\text{BKT}}(p; N)$ of the Berezinskii-Kosterlitz-Thouless phase transition on the system thickness $N$ is obtained for a diluted layered XY-model for a wide range of spin concentrations $p$. The temperature $T$, concentration $p$, and dimensional $N$ dependencies of the vortex density $v(p; N; T)$ in a layered XY-model are obtained.

1. Introduction
The investigation of critical behavior of disordered systems is of both fundamental and applied scientific interest. Recently, the study of quasi-two-dimensional systems [1] becomes increasingly interesting, particularly the study of the dimensional crossover in the transition from two-dimensional to three-dimensional systems [2]. An XY-model provides an opportunity to investigate this subjects due to an important and interesting property. In the two-dimensional system the long-range order is destroyed by transverse fluctuations of the spin density at all nonzero temperatures, but there exists a topological Berezinskii-Kosterlitz-Thouless (BKT) phase transition [3–5] at temperature $T = T_{\text{BKT}}$, and there is a Berezinskii low-temperature phase at $T < T_{\text{BKT}}$, where all temperatures $T$ are critical points. There is a continuous set of fixed points of the renormalization-group transformation for the two-dimensional case, and a quasi-long-range order (QLRO) is present in the system. On the other hand, the critical behavior of the three-dimensional XY-model in vicinity of $T = T_C$ is described by a fixed point of the “ferromagnetic-paramagnetic” phase transition and a classical long-range order (LRO) is present at $T < T_C$ [6–8]. It is interesting to investigate the crossover in the XY-model with changing the dimension of the system. The study of the critical behavior of a thin XY-film, or a layered XY-model, is well suited for this [9]. With increasing system thickness, a transition to the behavior of the three-dimensional system should be observed. However, with a small thickness, the system should behave as a two-dimensional or quasi-two-dimensional one.

The 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 [10], in particular 1-2.5 ML (atomic layers) Fe/Au(100) at temperatures $T$ 300-500 K; 2 ML Fe/W(100) at $T$ 180-220 K; Ag/2.2 ML Fe/W(100) at $T$ 270-330 K; 2 ML Co/Cu(100) at $T$ 230-410 K and 3-6.2 ML Ni/Cu(100) at $T$ 210-388 K. Critical properties of an extensive class of “easy plane” planar magnets [11, 12] are described using XY-model. Singularities in the critical properties of superconducting thin films [13, 14]; arrays of Josephson junctions [3, 15, 16] and
SFS-junctions [17–19]; two-dimensional crystals [5] and smectic liquid crystals [20–23]; some correlation properties of two-dimensional turbulence [24]; singularities in the critical properties of superfluid thin films of liquid helium [25–28]; melting of several layers of sorbed xenon in single-crystal graphite [29]; the process of sorbing hydrogen on tungsten W(011) $p(2 \times 2)$ [30]; and some properties of many other physical systems [3, 31] are described using XY-model. 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 [32].

The equilibrium and some non-equilibrium critical properties of the layered XY-model were studied in [9, 33, 34]. However, the influence of structural disorder on the equilibrium and non-equilibrium critical behaviour of the system has not been investigated. As a result of extensive research (in respect of the XY-model, see refs. in [1, 35–44]), it has been found that the critical behavior can undergo significant changes in diluted systems, compared to pure systems. This work is devoted to the study of the influence of structural disorder on the equilibrium critical behavior of a layered XY-model and on a dimensional transition from a two-dimensional XY-model to a three-dimensional XY-model.

The dynamics of the relaxation of XY-model is characterized by the existence of topological defects (see figure 1 and discussion in Section 4). In the two-dimensional case with $N = 1$, they are vortices and antivortices. In quasi-two-dimensional $N > 1$ and three-dimensional $N \rightarrow \infty$ cases, they are vortex-loop configurations. In 1992 Schmidt and Schneider [33] investigated the features of the vortex configurations in a layered XY-model. In the present work, the temperature, concentration, and dimensional dependencies of vorticity are obtained.

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

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

where $S = \{S_i\}$ is a lattice spin field; $S_i = (S_i^{(x)}, S_i^{(y)}) \equiv (\cos \varphi_i, \sin \varphi_i)$ is a classical planar spin which is associated with $i$-node of a cubic lattice with the plane linear size $L$ and the thickness of the film $N$; $p_i$ is an occupation number of $i$-node; if $p_i = 1$ then $i$-node is occupied by spin, else if $p_i = 0$ by impurity (defect node); $\sum_{\langle i,j \rangle}$ is a summation over all pairs of the nearest neighbors. Impurities are distributed uniformly on the lattice, with spin concentration $p$, i.e. $c_{\text{imp}} = 1 - p$. 

Figure 1. Snapshots of the system configuration in the process of non-equilibrium critical relaxation (Metropolis dynamics) from the high-temperature initial state, with a small value of magnetization $m_0 \ll 1$. The color indicates the area of vorticity localization. The system being demonstrated has a thickness $N = 16$ and a linear size $L = 64$; spin concentration $p = 1.0$ (pure system); temperature $T = 0.5 < T_{\text{BKT}}(p,N)$; observation time $0$ (initial state), 100 and 500 MCS/s.
is the concentration of impurity. Periodic boundary conditions were set in the film plane and free boundary conditions in the perpendicular direction.

The study was carried out for the spin concentrations $p = 1.0$ (pure system), 0.95, 0.9, 0.85, 0.8 and 0.75 (diluted systems).

The simulation of the system was carried out by Wolf algorithm [45]. A random unit vector $\mathbf{r}$, determining the direction, was chosen for each cluster. The spin $\mathbf{S}_j$, a neighbour of spin $\mathbf{S}_i$ in the cluster, may join the growing cluster provided both spins lie at the same side of the line perpendicular to the unit vector $\mathbf{r}$, that is, $(\mathbf{S}_i \cdot \mathbf{r})(\mathbf{S}_j \cdot \mathbf{r}) > 0$. The probability of a spin joining a growing cluster was determined by the expression $P(\mathbf{r}; \mathbf{S}_i, \mathbf{S}_j) = 1 - \exp \left(-2(\mathbf{S}_i \cdot \mathbf{r})(\mathbf{S}_j \cdot \mathbf{r})/T\right)$.

The difference between the Wolf algorithm used in this work and the standard implementation is the choice of neighboring spins for surface nodes where free boundary conditions are established. One MCS/s corresponded to 20 cluster flips.

The relaxation time was chosen equal to 5000 MCS/s for the initial temperature step and 1000 MCS/s for subsequent temperature steps. The averaging time was chosen equal to 20000 MCS/s. Statistical averaging was performed over 1000 initial configurations for pure system and 500 impurity configurations and 25 statistical configurations for each impurity configuration for diluted system.

3. The dependence of phase transition temperature $T_{BKT}(p, N)$ on thickness and spin concentration

The concentration dependence of temperature of BKT phase transition in the diluted two-dimensional XY-model was determined in [36]. In the three-dimensional XY-model there is a “ferromagnetic-paramagnetic” phase transition with a critical temperature for pure system $T_C = 2.2018(5)$ [6–9]. In 2011 Santos-Filho, et al. [35] carried out a detailed study of the equilibrium critical behavior of a three-dimensional diluted XY-model and determined the concentration dependence of the critical temperature $T_C(p)$. For definiteness we will designate the temperature of phase transition at all thicknesses $N$, except the value $N \rightarrow \infty$, as $T_{BKT}(N)$. In the limiting case $N \rightarrow \infty$, the system demonstrates the properties of a three-dimensional XY-model [9], and the relative contribution of free boundary decreases. The transverse correlation length $\xi_L$ (limited by system thickness $N$) at the phase transition point increases indefinitely, and the transition temperature represents the classical critical point $T_C$ (see discussion in [9, 33, 46]).

![Figure 2](image_url)

**Figure 2.** The temperature dependence of the fourth order Binder cumulant $U_4(p, N, T)$, for a system with spin concentration $p = 0.8$ and thickness values $N = 8$ (a), 12 (b) and 16 (c), for different values of the linear size $L = 16$, 24, 32, 40, 48 and 64 of the system. In the vicinity of the phase transition temperature $T_{BKT}(p, N)$, there is an intersection of the curves $U_4(p, N, T)$ for different linear sizes $L$, with the formation of a typical triangular region.

We determine the dimensional dependence of phase transition temperature $T_{BKT}(p, N)$ for various spin concentrations $p$ using the methods of finite-size scaling, such as method of fourth-order Binder cumulants $U_4$ (see figure 2); spatial correlation function ratio $R$ and peak analysis
for magnetic susceptibility $\chi$ and specific heat $C$. In figure 3 is shown the dependence of the phase transition temperature $T_{BKT}(p, N)$ on the thickness $N$ for different spin concentrations $p = 1.0$ (pure system), 0.95, 0.9, 0.85, 0.8 and 0.75 of the system. The points $T_{BKT}^{(\text{sim})}(p, N)$ denote the values of phase transition temperature obtained from simulation of the system at various thicknesses $N$. In 2009 Hasenbusch [9] used the approximation dependence of the form

$$T_{BKT}^{-1}(N) = T_C^{-1} + a(1.0 - bN^{-\omega})N^{-1.0/\nu},$$

where $\nu$ and $\omega$ are the critical exponents (correlation length exponent and scaling correction exponent) of the three-dimensional XY-model, $a$ and $b$ are the approximation parameters. The critical exponents of the three-dimensional diluted XY-model [35] are not significantly different from those of the pure system (the exponent $\alpha$ of specific heat is negative, and in accordance with the Harris criterion, point uncorrelated quench impurities do not change the characteristics of the system’s equilibrium critical behavior). The obtained approximation in the case of a three-dimensional ($N \to \infty$) system allows to obtain the value of the critical temperature $T_C(p)$. As a result of the calculations, the values of the approximation parameters $a$ and $b$ were evaluated (Tab. 1). The concentration dependence of the coefficient $a = a(p)$ can be approximated by form $a(p) \approx 1.15 + 0.4(1.0 - p) \equiv 1.15 + 0.4\epsilon_{\text{imp}}$. The concentration dependence of the coefficient $b = b(p)$ shows a more complex form, and its study is complicated due to the significant magnitude of the approximation and statistical errors. Hasenbusch in [9] suggested the values of the coefficients $a = 1.1545(46)$, $b = 0.70(2)$ for a pure system ($p = 1.0$) and obtained more accurate results. Our results coincide with the results [9]. The relatively large deviation of the obtained coefficient $b$ value (0.63(6) vs 0.70(2)) in our work from the work [9] output may be due to the fact that we did not consider thicknesses $N > 16$, while in the [9] thicknesses $N = 32$ was chosen. The obtained dimensional and spin concentration dependencies are shown in figure 3 as $T_{BKT}^{(\text{app})}(p, N)$. In future work, it is proposed to carry out a study of the dimensional and concentration dependencies of the specific value of the spin stiffness $\Theta(p, N)$ for a diluted layered XY-model, similar to the study performed in the work [34] for a pure system.

Figure 3. The dependence of the phase transition temperature $T_{BKT}(p, N)$ on the thickness $N$ for different spin concentrations $p = 1.0$ (pure system), 0.95, 0.9, 0.85, 0.8 and 0.75 of the system. Points $T_{BKT}^{(\text{sim})}(p, N)$ with error bars denote the values of phase transition temperature obtained from simulation of the system at various thicknesses $N$. Points $T_C(p)$ represent the results [35] and indicate the critical temperature of three-dimensional diluted XY-model. Dependence $T_{BKT}^{(\text{app})}(p, N)$ denote the approximation curve.

4. Vortex structures

In the final part of the article we will discuss some aspects of the behavior of the vortex density in the system. The dynamics of the relaxation of XY-model is characterized by the existence of topological defects (see figure 1). In the two-dimensional case they are vortices and antivortices, and in quasi-two-dimensional $N > 1$ and three-dimensional $N \to \infty$ cases, they are vortex-loop configurations. These vortex-loop configurations, or more generally vortex “filaments” (figure 1), are one-dimensional and quasi-one-dimensional structures with vorticity localization. In 1992 Schmidt
Table 1. The concentration dependence of the approximation (2) coefficients $a$ and $b$. Comparison with results from other work.

| $p$  | $a$     | $b$     | $a$     | $b$     | refs. |
|------|---------|---------|---------|---------|-------|
| 1.00 | 1.15(1) | 0.63(6) | 1.1545(46) | 0.70(2) | [9]   |
| 0.95 | 1.17(1) | 0.63(6) | $-$     | $-$     |       |
| 0.90 | 1.19(2) | 0.63(6) | $-$     | $-$     |       |
| 0.85 | 1.21(2) | 0.65(6) | $-$     | $-$     |       |
| 0.80 | 1.23(2) | 0.67(6) | $-$     | $-$     |       |
| 0.75 | 1.25(2) | 0.69(7) | $-$     | $-$     |       |

and Schneider [33] investigated the features of the vortex configurations in a layered XY-model. In the present work, the temperature, concentration, and dimensional dependencies of vorticity are obtained. The vortex structures in the layered XY-model differ from the classical vortices and antivortices in the two-dimensional XY-model. Vortex excitations in a two-dimensional XY-model possess a logarithmically increasing energy with increase of linear size (and entropy), and therefore are the determining subsystem in the thermodynamic limit $L \to \infty$ in a two-dimensional case. With increase of the thickness of the system, in a layered XY-model, the vortex structures take the form of vortex lines and loops. Examples of typical configurations are shown in figure 1. Vortex lines connect the opposite sides of the system. Vortex “filaments” can close, creating vortex loops.

In the XY-model the vorticity $v$ of a plaquette of four spins is defined (in analogy to a contour integral over a continuous field) by [4, 5, 33]

$$\sum_{\text{plaquettes}} f(\varphi_{i+1} - \varphi_i) = 2\pi v_{\text{plaq}}, \quad (3)$$

where $\sum_i$ is the sum by plaquette nodes and $f$ is the shifts of the difference of the phases $\varphi_i$, of spin $S_i = (\cos(\varphi_i), \sin(\varphi_i))$, into the interval $[0, 2\pi)$. The vortex density $v$ is then defined as [33]

$$v = \frac{1}{N_{\text{plaq}}} \sum_{\text{plaq}} |v_{\text{plaq}}|, \quad (4)$$

where the sum $\sum_{\text{plaq}}$ is taken over all possible plaquettes on the lattice, taking into account the periodic boundary conditions in two directions and the free boundary condition in another

Figure 4. The temperature dependence of the vortex density $v$ of the system for different values of the system thickness $N$ and different spin concentrations $p = 1.0$ (a), 0.9 (b) and 0.8 (c). Linear size of system $L = 128$. 

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direction. For the elementary plaquette the vorticity \( v \) can only have the values 0, \( \pm 1 \) (except for a set of measure zero, where it can be \( \pm 2 \)) [33]. Figure 1 shows areas of increased vortex density, where the vortex lines and loops are localized in the system.

The obtained temperature dependencies \( v(p, N, T) \) of the vortex density for various values of the system thickness \( N \) and various spin concentrations \( p \) are shown in figure 4. The results obtained clearly demonstrate an increase in the equilibrium values of the vortex density \( v \) with increasing temperature \( T \). It is seen that at low temperatures \( T \ll T_{\text{BKT}}(p, N) \) the vortex density \( v \) is sufficiently low, whereas with increasing temperature occurs a increase of the vorticity. At low temperatures \( T \ll T_{\text{BKT}}(p, N) \), the temperature dependence can be locally approximated by an exponential function of the inverse temperature \( 1/T \). This is consistent with the results [33]. Deviations from a strict exponential dependence on the inverse temperature \( 1/T \) are associated with the existence in the system of several different elementary types of vorticity [33]: vortex lines connecting two opposite faces of the system; open vortex loops adjacent to both ends of the same face; and closed vortex loops, when the ends of the line are closed in the bulk of the system. With increasing temperature, this approximation disappears, and a point of sharp return of vortex density is observed. The study of this aspect is beyond the scope of this work and will be considered in future articles.

5. Conclusion
In conclusion, we note that in the present work, the study of critical properties and size transition in a diluted layered XY-model was carried out for the first time. The dimensional and concentration dependencies of the temperature of the Berezinskii-Kosterlitz-Tauless phase transition \( T_{\text{BKT}}(p, N) \) in the system are obtained for a wide range of spin concentrations \( p \). In the present work, the temperature \( T \), concentration \( p \), and dimensional \( N \) dependencies of the vortex density \( v(p, N, T) \) in a layered XY-model are obtained. Prospects for further research are indicated.

Acknowledgments
The reported study was supported by RFBR according to the research projects 18-32-00814, 17-02-00279, 18-42-55003 and grants MK-4349.2018.2, MD-6868.2018.2 of the Council of the President of the Russian Federation. The simulations were supported in through computational resources provided by the Shared Facility Center “Data Center of FEB RAS” (Khabarovsk), Supercomputing Center of Lomonosov Moscow State University, Moscow Joint Supercomputer Center of RAS.

We would like to thank Dr. João Batista dos Santos-Filho, for the provided numerical data from the work [35]. This allowed us to focus on other aspects of the study, as well as ensure the correctness of our results.

The visualizations in figure 1 were created using Mayavi version 4.1.0 [49].

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