Dimensional Crossover in Critical Behavior of Thin XY-films: Equilibrium and Non-equilibrium Properties

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Abstract. In the present work it is studied the dimensional crossover in the critical behavior of the thin XY-films. Increasing the thickness $N$ of XY-film leads to a gradual transition from the Berezinskii-Kosterlitz-Thouless phase transition in the two-dimensional XY-model to the “ferromagnetic-paramagnetic” phase transition in the three-dimensional XY-model. It is investigated how phenomena associated with the topological phase disappears when film thickness $N$ is increased. The main consideration is focused on the dependence of the spin stiffness $\rho_s$ on the thickness $N$. In this work a generalization of Pokrovsky-Uimin equation for spin-wave approximation is introduced. The dynamical dependencies of thermodynamic values in non-equilibrium relaxation from low-temperature and high-temperature initial states are investigated.

1. Introduction
The study of critical behavior causes considerable fundamental and applied scientific interest. In recent years, of particular interest is the study of quasi-two-dimensional systems [1], in particular, the question of the dimensional crossover in the transition from two-dimensional to three-dimensional systems [2]. In this aspect, the XY-model has 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 at temperature $T = T_{BKT}$, and there is a Berezinskii low-temperature phase at $T < T_{BKT}$, 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 $T < T_C$ [7–9]. It is interesting to investigate the crossover in the XY-model when changing 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. 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, in particular [10] 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], including quite specific ones Rb$_2$CrCl$_4$ [13], (C$_6$H$_3$CH$_2$NH$_3$)$_2$CrBr$_4$ [14], (CH$_3$NH$_3$)$_2$MnCl$_4$ [15], (tetrenH$_5$)$_{0.5}$Cu$_4$W(CN)$_8$·7H$_2$O [16], are described using XY-model. Singularities in the critical properties of superconducting thin films [17,18]; arrays of Josephson junctions [3,19,20] and SFS-junctions [21–23]; two-dimensional crystals [5] and smectic liquid crystals [24–28]; some correlation properties of two-dimensional turbulence [29]; singularities in the critical properties of superfluid thin films of liquid helium [30–33]; melting of several layers of sorbed xenon in single-crystal graphite [34]; the process of sorbing hydrogen on tungsten W(011) p(2 × 2) [35]; and some properties of many other physical systems [3,36] are described using XY-model. Also, to the phenomena described by the XY-model, it is possible to relate dynamic properties of such exotic systems as flocks of birds [37] and some other forms of collective behavior of living organisms [38,39].

2. Model and methods

The Hamiltonian of the system in this work was chosen in the form

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

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 $N$; $\varphi_i$ is a phase of spin $S_i$; $\sum_{\langle i,j \rangle}$ is a summation over all pairs of the nearest neighbors. Periodic boundary conditions were set in the film plane and free boundary conditions in the perpendicular direction.

The simulation of critical dynamics and relaxation properties of the system was carried out by Metropolis algorithm.

The dynamics of the relaxation model is characterized by the existence of topological defects. In the two-dimensional case with $N = 1$, they are vortices and antivortices. In quasi-two-dimensional $N > 1$ and three-dimensional $N \to \infty$ cases, they are vortex-loop configurations (see Fig. 1).

Figure 1. Vortex-loop configurations in a thin XY-film with thickness $N = 3$.

Figure 2. The temperature dependences of equilibrium values for thin XY-films with linear size $L = 32$: the magnetization $m$ (a); layered magnetization $m_n$ for the film with thickness $N = 10$ (b); magnetic susceptibility $\chi$ (c); energy $\epsilon$ (d).

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

The temperature dependences of equilibrium values of the total magnetization $m$, layered magnetization $m_n$, magnetic susceptibility $\chi$ and energy $e$ for thin XY-films are shown in Fig. 2.

The main results for equilibrium values for the layered XY-model are obtained using Metropolis algorithm [6]. Therefore, dependence of phase transition temperature $T_BKT(N)$ on thickness $N$ was calculated for testing and verification of the Wolff algorithm developed in this work.

3. Dependence of phase transition temperature $T_BKT(N)$ on thickness

The temperature of BKT phase transition in the two-dimensional XY-model, with $N = 1$, $T_{BKT} = 0.893(4)$ [40, 41]. In the three-dimensional XY-model there is a “ferromagnetic-paramagnetic” phase transition with a critical temperature $T_C = 2.208(5)$ [6–9]. For definiteness we will designate the temperature of phase transition at all thicknesses $N$, except the value $N \to \infty$, as $T_{BKT}(N)$.

The methods of finite-size scaling analysis for magnetic susceptibility $\chi$ and specific heat $C$, method of fourth-order Binder cumulants $U_4$ and spatial correlation function ratio $R$ on two different scales were used to determine the dimensional dependence of phase transition temperature $T_{BKT}(N)$.

The simulations for dimension dependent phase transition temperature $T_{BKT}(N)$ determination were performed for thicknesses of the system $N = 1 \ldots 10$. Linear sizes $L = 12 \ldots 36$ were used for the methods of finite-size scaling analysis. The Wolf algorithm was used to obtain equilibrium values. One MCS/s corresponded to 20 cluster flips. The relaxation time was chosen equal to 1000 MCS/s for the initial temperature step and 100 MCS/s for subsequent temperature steps. The averaging time was chosen equal to 10000 MCS/s. Statistical averaging was performed over 100 initial configurations.

The dependence of the phase transition temperature $T_{BKT}(N)$ on the thickness $N$ is shown in Fig. 3. Also a comparison with the dimensional dependence from the work [6] is given. Approximation of $T_{BKT}(N)$ has the form $T_{BKT}(N) = T_{C}^{-1} + a(1.0 - bN^{-\omega})N^{-1.0}/\nu$, where $T_{C}^{-1} = 0.4541655$, $a = 1.15(2)$ and $b = 0.61(1)$. $\nu = 0.6717(1)$ [7–9] is a critical exponent of the correlation length of the three-dimensional XY-model and $\omega = 0.785(1)$ is an exponent of finite-size scaling corrections. These parameters in [6] are: $a = 1.1545(46)$ and $b = 0.70(2)$. The dependence $T_{BKT}(N)$ obtained in this work agrees well with the results of the work [6].

4. Transverse spin stiffness and Berezinskii-Kosterlitz-Thouless phase transition

The BKT topological phase transition in the XY-model is physically associated with the dissociation of coupled vortex-antivortex pairs at the transition point [3, 5].
A formal condition [4, 42, 43] is representable, as a condition of zeroing the free energy of a vortex, in the form $\rho_b(T_{BKT}(N)) = 2T_{BKT}(N)/\pi$ for the two-dimensional XY-model. However, for the three-dimensional limit there is a condition $\rho_b(T_{BKT}(N \to \infty)) = 0$ which is the case for the “ferromagnetic-paramagnetic” phase transition, and $T_{BKT}(N \to \infty) \equiv T_C$ is a critical temperature for the three-dimensional XY-model.

In a general case of an arbitrary thickness $N$ of a thin XY-film the transverse spin stiffness at the transition temperature $\rho_b(T_{BKT}(N))$ should change from $2T_{BKT}(N)/\pi$ for $N = 1$ to 0 for $N \to \infty$. To study the dimensional crossover in critical behavior of thin XY-films, in this paper we introduced the relation

$$\Im(N) = \frac{\rho_b(T_{BKT}(N))}{T_{BKT}(N)}.$$  

The relation $\Im(N)$ is equal to $2/\pi$ for the two-dimensional case with $N = 1$ and is equal to 0 for the three-dimensional case with $N \to \infty$.

![Figure 4](image)

Figure 4. Fig. (a): The temperature dependence of the transverse spin stiffness $\rho_b$ of the thin XY-film with $L = 128$ for various thicknesses $N$. The arrows indicate the positions of $T_{BKT}(N)$. Fig. (b): The dependence of the ratio $\Im(N)$ on the thickness $N$.

The simulations for the temperature dependence of the transverse spin stiffness $\rho_b$ determination were performed for thicknesses of the system $N = 1 \ldots 10$ and linear size $L = 128$. As before in this work, the Wolf algorithm was used to obtain equilibrium values. The relaxation time was chosen equal to 5000 MCS/s for the initial temperature step and 500 MCS/s for subsequent temperature steps. The averaging time was chosen equal to 50000 MCS/s. Statistical averaging was performed over 1000 initial configurations. The transverse spin stiffness $\rho_b$ was calculated by the method [44].

![Figure 5](image)

Figure 5. The dimensional dependence of the value $\Omega(N)$. In the case of a three-dimensional system with $N \to \infty$.

5. Pokrovsky-Uimin equation and spin-wave approximation

The Pokrovsky-Uimin equation was introduced in works [42, 43] and allows to obtain a spin-wave approximation of the temperature dependence of the transverse spin stiffness $\rho_b(T)$ for the two-dimensional XY-model. This transcendental algebraic equation has a simple form

$$\Omega(N) = \frac{\rho_b(T_{BKT}(N))}{T_{BKT}(N)}.$$  

The dimensional dependence of the value $\Omega(N)$.
\( \rho_s = \exp \left(-T/(4\rho_s)\right) \). To study the dimensional crossover in critical behavior of thin XY-films, in this paper we introduced a generalization of Pokrovsky-Uimin equation in the form \( \rho_s = \exp \left(-T/(\Omega(N)\rho_s)\right) \) with dimensional parameter \( \Omega(N) \). Numerical calculations of this equation’s roots were carried out for different values \( \Omega(N) \) for the purpose of sewing the spin-wave solution with numerical results in Fig. 4 (a), to determine the dimensional dependence of the parameter \( \Omega(N) \) on the thickness \( N \). The dimensional dependence of the parameter \( \Omega(N) \) on \( 1/N \) obtained in this work is shown in Fig. 5. The dependence obtained is well approximated by a linear relation \( \Omega(N) = 5.7 - 1.7/N \). If \( N = 1 \), as in the two-dimensional XY-model, \( \Omega(N = 1) = 4 \), as it was in the original Pokrovsky-Uimin equation. For a three-dimensional system, the value \( \Omega(N \rightarrow \infty) = 5.7 \pm 0.3 \).

6. Relaxation dynamical dependences of thin XY-films

The non-equilibrium critical relaxation depends on the selected initial state of the system. Two different types of initial non-equilibrium states in the XY-model can be distinguished: a low-temperature initial state with \( T_0 = 0 \) and a high-temperature initial state with \( T_0 \gg T_{BKT}(N) \). The initial state is prepared by thermalization with a thermostat with temperature \( T_0 \).

The simulation of the non-equilibrium critical relaxation of the system was performed using the Metropolis algorithm. Systems with thicknesses \( N = 1 \ldots 36 \) were studied. The dynamical dependencies of the magnetization \( m(t) \) and its dispersion \( D_m(t) \), the second and fourth order cumulants \( U_2(t) \) and \( U_4(t) \) of magnetization for non-equilibrium relaxation of the system from the high-temperature and low-temperature initial states were investigated. The dynamical dependences of the magnetization \( m(t) \) of the system with thickness \( N = 36 \) and linear size \( L = 128 \) are presented in Fig. 6. A detailed discussion of the dimensional crossover in the relaxation dynamics of the XY-films is planned in future works.

7. Conclusion

In this paper, we study the dimensional crossover in the critical behavior of the thin XY-films. Increasing the XY-film thickness \( N \) leads to a gradual transition from the Berezinskii-Kosterlitz-Thouless phase transition in the two-dimensional XY-model to the “ferromagnetic-paramagnetic” phase transition in the three-dimensional XY-model. It is shown that this manifests itself in the dependence of the spin stiffness \( \rho_s(T_{BKT}(N)) \) on the thickness \( N \) of the film in the asymptotics \( N \rightarrow \infty \) with the form \( 3(N) \equiv \rho_s(T_{BKT}(N))/T_{BKT}(N) = 2N^{-\sigma} \). The dependence of the temperature \( T_{BKT}(N) \) of the phase transition on the film thickness \( N \) is defined, and it was shown that \( T_{BKT}(N \rightarrow \infty) \equiv T_C \) for the three-dimensional XY-model. In this work a generalization of Pokrovsky-Uimin equation for spin-wave approximation \( \rho_s = \exp \left(-T/(\Omega(N)\rho_s)\right) \) was introduced, with \( \Omega = \Omega(N) \), and it was shown that the case of film thickness \( N \) is well approximated by expression \( \Omega(N) = 5.7 - 1.7/N \). The dynamical dependencies of thermodynamic values in non-equilibrium relaxation from the low-temperature, with \( T_0 = 0 \), and high-temperature, with \( T_0 \gg T_{BKT}(N) \), non-equilibrium initial states were investigated.
Acknowledgments

The reported study was supported by RFBR according to the research projects 17-02-00279, 18-42-550003, 18-32-00814 and grants MD-6868.2018.2, MK-4349.2018.2 of the President of the Russia. The simulations were supported in through computational resources provided by the Shared Facility Center “Data Center of FEB RAS” (Khabarovsk), by the Supercomputing Center of Lomonosov Moscow State University, by Moscow Joint Supercomputer Center and by St. Petersburg Supercomputer Center of the Russian Academy of Sciences.

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