Non-universal behavior of helicity modulus in a dense defect system

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Extensive Monte Carlo simulation has been performed on a 2D modified XY model which behaves like a dense defect system. Topological defects are shown to introduce disorders in the system which makes the helicity modulus jump non-universal. The results corroborate the experimental observation of non-universal jump of the superconducting density in high-$T_c$ superconducting films.

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The two-dimensional (2D) XY model of planar spins has been the subject of intense interest since the last four decades. The 2D XY model was believed to be without a phase transition for a long time until Kosterlitz and Thouless (KT) proved that a phase transition indeed occurs and clarified its topological nature [1, 2]. KT transition is a continuous phase transition of infinite order from a high-temperature isotropic phase with exponential decay of spin-spin correlation functions to a low-temperature pseudo-long-range or quasi-long-range order (QLRO) phase with power law decay of spin-spin correlations. KT pictured this transition in terms of vortex unbinding. In the low-temperature phase the charges (vortices) are bound together into dipole-pairs while in the high-temperature phase some dipole-pairs are broken. KT theory [2] leads to the famous universal jump prediction [3] of the helicity modulus [4] or equivalently of the superfluid density [3, 5]. Kosterlitz RG equations for the 2D Coulomb gas (CG) are constructed in the low-temperature phase and are valid in the limit of small particle densities [6]. Later Minnhagen has suggested on the basis of a new set of RG equations for the 2D CG that the conclusions based on Kosterlitz RG equations may break down for larger dipole-pair fugacities [7, 8]. As a result charge unbinding transition with non-universal jumps may, in principle, be possible and it was shown that for higher particle densities, the charge-unbinding transition is first order [9]. Later Zhang et.al [10] on the basis of sine-Gordon (SG) field theory, showed that the nature of the transition in the dense 2D classical CG is of discontinuous first order type. The evidence of a first order phase transition for higher particle densities was supported by Monte Carlo (MC) simulations [11-13]. Such first order phase transitions are related to high-$T_c$ superconductivity [14]. Leemann et.al, in their experimental measurements of the inverse magnetic penetration depth $\Lambda^{-1}$ in thin films of YBa$_2$Cu$_3$O$_7$ [15], observed that the jump of the superconducting density (or equivalently the helicity modulus) did not obey the universal prediction of KT theory. These systems thus cannot be described by conventional XY model. Mila [16] attempted to understand the the non-universal jump of the superconducting density in thin films of high-$T_c$ superconductors in terms of XY model with a modified form of interaction potential. Such kind of model was first introduced by Domany and co-workers [17]. They introduced an extension of the 2D XY model where the classical spins (of unit length), located at the sites of a square lattice and free to rotate in a plane, say the XY plane (having no Z-component) interact with nearest-neighbors through a modified potential

$$V(\theta) = 2J \left[1 - \left(\cos^2\frac{\theta}{2}\right)^{\frac{1}{2}}\right]$$

where $\theta$ is the angle between the nearest neighbor spins, $J$ is the coupling constant and $p^2$ is a parameter used to alter the shape of the potential, or in other words, $p^2$ controls the nonlinearity of the potential well, although variation in $p^2$ does not disturb the essential symmetry of the Hamiltonian. For $p^2 = 1$, the potential reproduces the conventional XY model while for large values of $p^2$ (say $p^2 = 50$), the model behaves like a dense defect system [18] and gives rise to a first order phase transition as all the finite size scaling (FSS) rules for a first order phase transition were seen to be nicely obeyed [19]. The first order phase transition is associated with a sharp jump in the average defect pair density [18, 20]. The change in the nature of the phase transition with the additional parameter $p^2$ is in contradiction with the prediction of RG theory according to which systems in the same universality class (having same symmetry of the order parameter and same lattice dimensionality) should exhibit the same type of phase transition with identical values of critical exponents. In this context, I refer to the work of Curty and Beck [21] who showed that in three dimension (3D), continuous phase transition can be preempted by a first order one.

Enter and Shlosman finally provided a rigorous proof [22, 23] of a first order phase transition in various SO($n$)-invariant $n$-vector models which have a deep and narrow potential well. The model defined by Eqn. [11] is a member of this general class of systems. Moreover, Enter and Shlosman argued that in spite of the order parameter in the 2D systems with continuous energy spectrum being predicted to vanish by Mermin-Wagner theorem [24], the first order transition is manifested by the long range or-

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der in higher-order correlation functions. Recently Sinha and Roy [19] verified this argument by numerical simulations and showed that while the lowest-order correlation function decays to zero, the next higher-order correlation function has a finite plateau. Later they investigated the role of topological defects on the phase transition exhibited by the model described by Eqn. (1) by means of extensive MC simulations and observed that the system appears to remain ordered at all temperatures when configurations containing topological defects are not allowed to occur [18].

However, the connection of spin-stiffness (helicity modulus) with topological defects has not yet been studied for systems exhibiting first order transition. The present Communication aims at studying this aspect of phase transition which allows us to check whether the universal drop in the helicity modulus. I also find that the transition is associated with a non-universal jump predicted in the KT picture is valid in systems defined by the interaction potential given by Eqn. (1)

For the purpose of investigation, I choose the model defined by the interaction potential given by Eqn. (1) too or not. The present paper also explores the fact how disorder influences the properties of phase transition in these 2D systems. The effect of disorder on the KT transition has become relevant since the experimental observation of superconductor-insulator transition in thin disordered films [25, 26].

The variation of average defect pair density \( \rho \) with the dimensionless temperature \( T \) for lattice size \( L = 64 \) is shown in Fig. 1. The coupling constant \( J \) (in Eqn. (1)) has been conventionally set to unity. The method for calculating average defect pair density and the simulation techniques are discussed in Ref. [18]. A sharp variation of \( \rho \) as \( T \) increases through the transition temperature \( T_c(p^2) \) is observed. \( \rho \) is found to show a sharp jump at \( T_c(p^2) \), particularly for large values of \( p^2 \).

Next I plot the average defect pair density \( \rho \) as a function of the parameter \( p^2 \), shown in Fig. 2. The plot is for three different system sizes at a temperature \( T = 1.1200 \), which is above the transition temperature of the model for \( p^2 = 50 \). The data for \( \rho \) versus \( p^2 \) are nicely fitted by the following expression

\[
\rho(T) = \rho_{\text{max}} - \alpha(T) \exp(-\delta \sqrt{p^2})
\]

Eqn. (2) takes into account both vortices and antivortices. \( \rho \) increases monotonically with \( p^2 \) and saturates to a maximum value \( \rho_{\text{max}} \approx 0.28 \), which is independent of the temperature. The values of \( \rho_{\text{max}} \) for the three system sizes are listed in Table I. There is no significant system size dependence of the parameters as is evident from Table I. The maximum defect density \( \rho_{\text{max}} \) is usually achieved in the high-temperature limit \( T \to \infty \) but here it is achieved in the high-\( p^2 \) limit \( \rho^2 \to \infty \). Therefore it seems reasonable to interpret the parameter \( p^2 \) to play the role of disorder. In the high-\( p^2 \) limit, the system contains only vortex excitations. This means that in the high-\( p^2 \) limit, the system must be disordered even at very small temperature and consequently the transition temperature decreases with increase in \( p^2 \) which we observe.

![FIG. 1. (Color online) Average defect pair density \( \rho \) plotted against dimensionless temperature \( T \) for \( L = 64 \) for various values of \( p^2 \).](image1)

![FIG. 2. (Color online) Average defect pair density \( \rho \) plotted as a function of \( p^2 \) at \( T = 1.28 \) for three system sizes. The error bars are smaller than the dimension of the symbols used for plotting.](image2)

**TABLE I. parameters for the fit of \( \rho(T) = \rho_{\text{max}} - \alpha(T) \exp(-\delta \sqrt{p^2}) \) for different \( L \)**

| \( L \) | \( \rho_{\text{max}} \) | \( \alpha(T) \) | \( \delta \) |
|--------|----------------|---------------|--------|
| 32     | 0.2866 ± 0.002 | 0.411 ± 0.005 | 0.301 ± 0.008 |
| 48     | 0.2876 ± 0.002 | 0.406 ± 0.006 | 0.297 ± 0.009 |
| 64     | 0.2878 ± 0.002 | 0.406 ± 0.006 | 0.296 ± 0.009 |
where \( \omega \) is the angle of twist and \( d \) is the spatial dimensional. In the present case, the twisted boundary condition being anti-periodic and \( d \) being 2, the definition of \( \gamma \) simplifies to

\[
\gamma = \lim_{L \to \infty} 2L^{2-d} \frac{F(\omega) - F(0)}{\omega^2}
\]

(3)

Anti-periodic boundary condition is imposed only along one direction, say along X-direction. Our calculation of \( \gamma \) involves a direct simulation of Eqn. (1) using multiple reweighting histogram method, a sophisticated MC technique first proposed by Ferrenberg and Swendsen [29, 30]. In the simulations, \( 10^7 \) MC steps per site were used for computing the raw histograms and \( 10^6 \) MC steps per site were taken for equilibration.

The variation of \( \gamma \) with temperature for various lattice sizes is displayed in Fig. 3. The transition is signaled by an abrupt decrease of the helicity modulus in the vicinity of the transition temperature as the temperature is increased and the drop at the transition gets steeper as the system size \( (L) \) is increased. It is also manifested that instead of the subtle and the smooth KT transition, the transition coincides with a non-universal jump in \( \gamma \). The physical picture can be explained as follows. As \( p^2 \) increases, short-scale fluctuations (rotation of separate spins by large angles) are favored over long-wavelength fluctuations (spin waves and vortices) and when this happens disordering is induced at a lower temperature than the KT transition temperature, but the vortex-vortex interaction still remains stronger at that lower temperature, thus making the helicity modulus jump non-universal. The ratio of \( \gamma/T \) at \( T = T_c \) for different \( L \) is listed in Table II. I point out that Minnhagen [7] also showed the possibility of a KT transition in a 2D CG with a non-universal jump in \( \gamma \).

I have also computed the temperature derivative (\( \tau \)) of the helicity modulus. The internal energy difference under anti-periodic and periodic boundary conditions gives the derivative of helicity modulus in the form

\[
\tau = \frac{1}{2} \frac{d}{d\beta} \left[ \beta \gamma(\beta) \right] = \frac{\langle E \rangle_a - \langle E \rangle_p}{\pi^2}
\]

(5)

The MC data for the right hand size of Eqn. (5) as a function of temperature for different lattice sizes are shown in Fig. 4. The transition is manifested by a huge peak height in \( \tau \) and the data display a divergent behavior with increasing \( L \), indicative of a discontinuous jump in \( \gamma \) in an infinite lattice.

Now I present the FSS of \( \tau \). Since \( \tau \) is a response function like specific heat \( (C_v) \) or susceptibility \( (\chi) \), it is expected to show an identical behavior in scaling as for \( C_v \) or \( \chi \). From Fig. 5 where the maxima of \( \tau \) are plotted

FIG. 3. (Color online) Helicity modulus \( \gamma \) against temperature \( (T) \) for various lattice sizes for \( p^2 = 50 \) with the errorbars shown (for three lattice sizes).

FIG. 4. (Color online) Derivative of \( \frac{1}{2} \beta \gamma(\beta) \) as a function of temperature \( T \) for different lattice sizes for \( p^2 = 50 \) with the errorbars shown (for three lattice sizes).
against $L^2$, it is clear that the peak heights of $\tau$ scale as $L^d$ which confirms the first order nature of the present model for $p^2 = 50$. We recall here that for first order transition standard scaling rule for $C_v$ goes like $C_v \sim L^d$.

In this Communication I have used extensive MC simulation to show that for strong enough nonlinearity (i.e., for large values of $p^2$) in the interaction potential of Eqn. (1), there is a sudden proliferation of topological defects which makes the system disordered. Consequently the transition is associated with a discontinuous non-universal jump in the helicity modulus. Thus our simulation has given some support to the idea that the type of phase transition in thin superconducting films may be changed due to influence of disorder. As high-$T_c$ superconducting films are believed to have a irregular structure, it seems reasonable to relate the non-universal jump to disorder.

However, some studies\cite{16, 32, 33}, mostly based on RG analysis of Migdal-Kadanoff type contested the first order nature of the transition in the model defined by Eqn. (1). Since renormalization arguments hold good only for small disorder, the possibility that disorder may change the nature of phase transition always remains there. Perhaps this is the reason behind the different interpretation of results by the authors of Ref.\cite{16, 32, 33}.

Finally, the present work could shed light on the nature of 2D melting which remains controversial for decades. Experimental works and numerical simulations favor a KT-like transition in some cases and a discontinuous one in others\cite{34}. After all, it is possible that the nature of the melting transition in 2D depends on the specific system and the parameters of the model which in turn translate into different values of the nonlinearity parameter $p^2$.

I end this paper with a comment. It is observed in Fig. 3 that the graphs for helicity modulus ($\gamma$) against temperature for different lattice sizes intersect at a point which is the transition temperature of the model (within an error of 0.03%). I offer no explanation for this interesting result and this issue is left for future research.

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