PHYSICAL REVIEW E **84**, 010102(R) (2011)

Nonuniversal behavior of the helicity modulus in a dense defect system

Suman Sinha*

Theoretical Condensed Matter Physics Division, Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700 064, India

(Received 18 April 2011; published 25 July 2011)

An extensive Monte Carlo simulation has been performed on a two-dimensional modified XY model that behaves like a dense defect system. Topological defects are shown to introduce disorder in the system, which makes the helicity modulus jump nonuniversal. The results corroborate the experimental observation of a nonuniversal jump of the superconducting density in high-T_c superconducting films.

DOI: 10.1103/PhysRevE.84.010102 PACS number(s): 05.70.Fh, 64.60.an, 75.40.Mg, 05.10.Ln

The two-dimensional (2D) XY model of planar spins has been the subject of great interest for the past four decades. It had long been thought that the 2D XY model was without a phase transition until Kosterlitz and Thouless proved that a phase transition indeed occurs and clarified its topological nature [1,2]. The Kosterlitz-Thouless (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-order or quasi-long-range-order (QLRO) phase with power-law decay of spin-spin correlations. Kosterlitz and Thouless 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 well-known 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]. On the basis of a different set of RG equations for the 2D CG, Minnhagen suggested that the conclusions based on the Kosterlitz RG equations may break down for larger dipole-pair fugacities [7,8]. As a result, a charge-unbinding transition with nonuniversal jumps may, in principle, be possible and it was shown that for higher particle densities, the charge-unbinding transition is first order [9]. On the basis of sine-Gordon field theory, Zhang *et al.* [10] 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 Λ^{-1} in thin films of $YBa_2Cu_3O_7$ [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 the conventional XY model. Mila [16] attempted to understand the nonuniversal jump of the superconducting density in thin films of high-T_c superconductors in terms of the XY model with a modified form of interaction potential. Such kind of model was introduced by Domany *et al.* [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

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

where θ 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 rules for a first-order phase transition were seen to be 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 universal class (having the same symmetry of the order parameter and the same lattice dimensionality) should exhibit the same type of phase transition with identical values of the 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.

Finally, van Enter and Shlosman provided a rigorous proof [22,23] of a first-order phase transition in various SO(n)-invariant n-vector models that have a deep and narrow potential well. The model defined by Eq. (1) is a member of this general class of systems. Moreover, van 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 order 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. The role of topological defects on the phase transition exhibited by the model described by Eq. (1) was then investigated by means of extensive MC simulations and it was observed that the system appears to remain ordered at all temperatures when

*suman.sinha@saha.ac.in

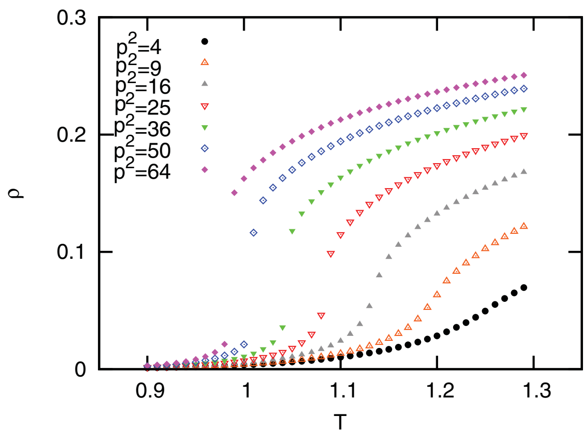

FIG. 1. (Color online) Average defect pair density ρ plotted against dimensionless temperature T for $L = 64$ for various values of p^2.

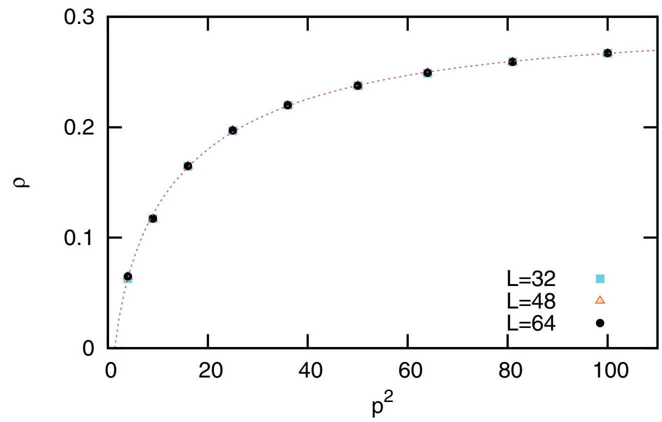

FIG. 2. (Color online) Average defect pair density ρ plotted as a function of p^2 at $T = 1.1200$ for three system sizes. The best fit corresponds to $L = 64$. The error bars are smaller than the dimension of the symbols used for plotting.

configurations containing topological defects are not allowed to occur [18].

However, the connection of spin stiffness (the helicity modulus) to topological defects has not yet been studied for systems exhibiting a first-order transition. The present Rapid Communication aims at studying this aspect of phase transition, which allows one to check whether the universal jump predicted in the KT picture is also valid in systems defined by Eq. (1). The present work also explores how disorder influences the properties of the phase transition in these 2D systems. The effect of disorder on the KT transition has become relevant since the experimental observation of the superconductor-insulator transition in thin disordered films [25,26].

The model defined by the interaction potential given by Eq. (1) is chosen for the present investigation. It is found that the transition is associated with a nonuniversal drop in the helicity modulus. It is also found that when the number density of topological defects increases rapidly, disorder is introduced into the system. The additional parameter p^2 plays the role of disorder here.

The variation of the average defect pair density ρ with the dimensionless temperature T for lattice size $L = 64$ is shown in Fig. 1. The coupling constant J [in Eq. (1)] has been conventionally set to unity. The method for calculating the average defect pair density and the simulation techniques are discussed in Ref. [18]. A sharp variation of ρ as T increases through the transition temperature $T_c(p^2)$ is observed. ρ is found to show a sharp jump at $T_c(p^2)$, particularly for large values of p^2. So, for strong enough nonlinearity, there is a sudden proliferation in the average defect pair density and the system under investigation behaves like a dense defect system for large values of p^2.

Next the average defect pair density ρ is plotted as a function of the parameter p^2 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 ρ versus p^2 are nicely fitted by the expression

$$\rho(T) = \rho_{\max} - \alpha(T)\exp(-\delta\sqrt{p^2}). \tag{2}$$

Equation (2) takes into account both vortices and antivortices. ρ increases monotonically with p^2 and saturates to a maximum value $\rho_{\max} \approx 0.28$, which is independent of the temperature. The values of $\rho_{\max}$ 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 $\rho_{\max}$ is usually achieved in the high-temperature limit $T \to \infty$, but here it is achieved in the high-p^2 limit $p^2 \to \infty$. Therefore, it seems reasonable to interpret the parameter p^2 as playing 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 low temperature; consequently, the transition temperature decreases with increasing p^2, which we observe in Fig. 1. In other words, as we increase the nonlinearity p^2, the influence of disorder becomes stronger and a tendency of a first order transition with a sudden proliferation of topological defects develops.

The concentration is now focused on the behavior of spin stiffness (the helicity modulus). The helicity modulus, introduced by Fisher *et al.* [27], is a thermodynamic function that measures the rigidity of an isotropic system under an imposed phase twist. The free-energy difference between the twisted and the periodic boundary conditions is proportional to the helicity modulus γ. Thus the general definition of the helicity modulus may be regarded as [28]

$$\gamma = \lim_{L\to\infty} 2L^{2-d}\frac{F(\omega) - F(0)}{\omega^2}, \tag{3}$$

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

L	$\rho_{\max}$	$\alpha(T)$	δ
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

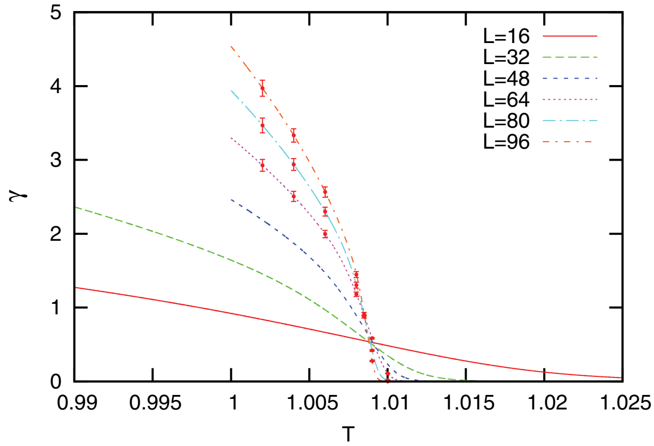

FIG. 3. (Color online) Helicity modulus γ plotted against temperature T for various lattice sizes for $p^2 = 50$; error bars are shown for three lattice sizes.

where ω is the angle of twist and d is the spatial dimension. In the present case, in which the twisted boundary condition is antiperiodic and $d = 2$, the definition of γ simplifies to

$$\gamma = 2\frac{F(\pi) - F(0)}{\pi^2}. \tag{4}$$

Antiperiodic boundary condition is imposed only along one direction, say, along the X direction. Our calculation of γ involves a direct simulation of Eq. (4) using the multiple reweighting histogram method, a sophisticated MC technique proposed by Ferrenberg and Swendsen [29,30]. In the simulations, 10^7 MC steps per site were used to compute the raw histograms and 10^6 MC steps per site were taken for equilibration.

The variation of γ 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 increases and the drop at the transition becomes steeper as the system size L increases. It is also manifested that instead of the subtle and smooth KT transition, the transition coincides

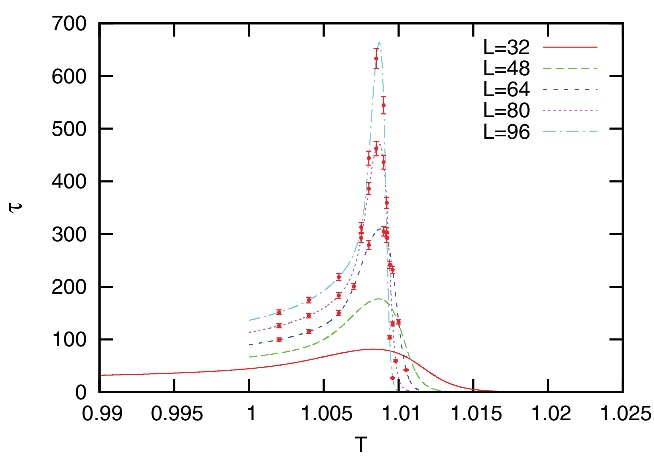

FIG. 4. (Color online) Derivative of $\frac{1}{2}\beta\gamma(\beta)$ as a function of temperature T for different lattice sizes for $p^2 = 50$; error bars are shown for three lattice sizes.

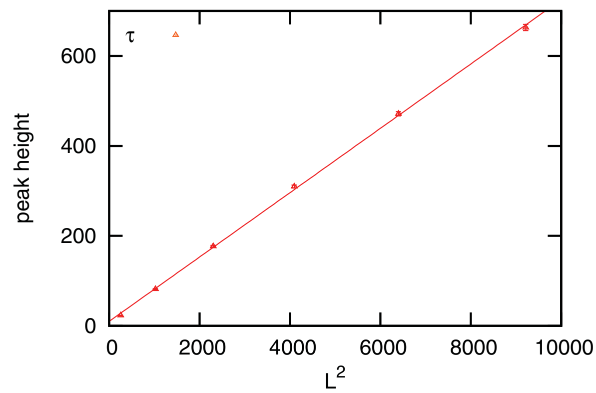

FIG. 5. (Color online) Peak heights of τ plotted against L^2 with the linear fit represented by the straight line. The error bars for most points are smaller than the dimension of the symbols used for plotting.

with a nonuniversal jump in γ. The physical picture can be explained as follows. As p^2 increases, short-scale fluctuations (the rotation of separate spins by large angles) are favored over long-wavelength fluctuations (spin waves and vortices), which induces disordering 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 nonuniversal. The ratio of γ/T at $T = T_c$ for different values of L is listed in Table II. It should be noted that Minnhagen [7] also showed the possibility of a KT transition in a 2D CG with a nonuniversal jump in γ.

The temperature derivative τ of the helicity modulus has also been computed. The internal energy difference under antiperiodic and periodic boundary conditions gives the derivative of the helicity modulus in the form

$$\tau = \frac{1}{2}\frac{d}{d\beta}[\beta\gamma(\beta)] = \frac{\langle E\rangle_a - \langle E\rangle_p}{\pi^2}. \tag{5}$$

The MC data for the right-hand size of Eq. (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 τ and the data display a divergent behavior with increasing L, which is indicative of a discontinuous jump in γ in an infinite lattice.

The finite-size scaling of τ is now presented. Since τ is a response function like specific heat C_v or susceptibility χ, it is expected to show scaling behavior that is identical to that for C_v or χ. From Fig. 5, where the maxima of τ are plotted against L^2, it is clear that the peak heights of τ scale as L^d, which confirms the first-order nature of the present model for $p^2 = 50$. We recall here that for the first-order transition the standard scaling rule for C_v goes like $C_v \sim L^d$ [31].

In this Rapid Communication an extensive MC simulation has been used to show that for strong enough nonlinearity (i.e., for large values of p^2) in the interaction potential of Eq. (1), there is a sudden proliferation of topological defects that makes the system disordered. Consequently, the transition is associated with a discontinuous nonuniversal jump in the helicity modulus. Thus the present simulation has given some support to the idea that the type of phase transition in thin superconducting films may be changed due to the influence

TABLE II. γ/T at $T = T_c$ for different values of L.

L	γ/T
16	0.5742
32	0.6049
48	0.6569
64	0.7192
80	0.6971
96	0.6454

of disorder. As high-T_c superconducting films are believed to have an irregular structure, it seems reasonable to relate the nonuniversal jump to disorder.

Some studies [16,32,33], however, mostly based on RG analysis of the Migdal-Kadanoff type, contested the first-order nature of the transition in the model defined by Eq. (1). Since renormalization arguments hold only for small disorder, the possibility that disorder may change the nature of the phase transition always remains. Perhaps this is the reason behind the different interpretation of results by the authors of Refs. [16,32,33].

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

This Rapid Communication concludes with a comment. It is observed in Fig. 3 that the graphs for the helicity modulus γ against temperature for different lattice sizes intersect at a point that is the transition temperature of the model (within an error of 0.03%). No explanation is offered here for this interesting result; this issue is left for future research.

The author is grateful to S. K. Roy for many fruitful discussions and a number of suggestions after critically reading this manuscript.

[1] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[2] J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).
[3] D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. **39**, 1201 (1977).
[4] T. Ohta and D. Jasnow, Phys. Rev. B **20**, 139 (1979).
[5] P. Minnhagen, Phys. Rev. B **24**, 6758 (1981).
[6] P. Minnhagen, Rev. Mod. Phys. **59**, 1001 (1987).
[7] P. Minnhagen, Phys. Rev. Lett. **54**, 2351 (1985).
[8] P. Minnhagen, Phys. Rev. B **32**, 3088 (1985).
[9] P. Minnhagen and M. Wallin, Phys. Rev. B **36**, 5620 (1987).
[10] G. M. Zhang, H. Chen, and X. Wu, Phys. Rev. B **48**, 12304 (1993).
[11] J. M. Caillol and D. Levesque, Phys. Rev. B **33**, 499 (1986).
[12] J. R. Lee and S. Teitel, Phys. Rev. Lett. **64**, 1483 (1990).
[13] J. R. Lee and S. Teitel, Phys. Rev. Lett. **66**, 2100 (1991).
[14] S. E. Korshunov, Phys. Rev. B **46**, 6615 (1992).
[15] Ch. Leemann *et al.*, Phys. Rev. Lett. **64**, 3082 (1990).
[16] F. Mila, Phys. Rev. B **47**, 442 (1993).
[17] E. Domany, M. Schick, and R. H. Swendsen, Phys. Rev. Lett. **52**, 1535 (1984).
[18] S. Sinha and S. K. Roy, Phys. Rev. E **81**, 041120 (2010).
[19] S. Sinha and S. K. Roy, Phys. Rev. E **81**, 022102 (2010).
[20] J. E. Van Himbergen, Phys. Rev. Lett. **53**, 5 (1984).
[21] P. Curty and H. Beck, Phys. Rev. Lett. **85**, 796 (2000).
[22] A. C. D. van Enter and S. B. Shlosman, Phys. Rev. Lett. **89**, 285702 (2002).
[23] A. C. D. van Enter and S. B. Shlosman, Commun. Math. Phys. **255**, 21 (2005).
[24] N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).
[25] D. B. Haviland, Y. Liu, and A. M. Goldman, Phys. Rev. Lett. **62**, 2180 (1989).
[26] A. F. Hebard and M. A. Paalanen, Phys. Rev. Lett. **65**, 927 (1990).
[27] M. E. Fisher, M. N. Barber, and D. Jasnow, Phys. Rev. A **8**, 1111 (1973).
[28] P. M. Chaikin and T. C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge University Press, Cambridge, England, 2009).
[29] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988); **63**, 1195 (1989).
[30] *Monte Carlo Methods in Statistical Physics*, edited by M. E. J. Newman and G. T. Barkema (Clarendon, Oxford, 1999).
[31] *Monte Carlo Simulation in Statistical Physics*, edited by K. Binder and D. W. Heermann (Springer-Verlag, New York, 1986).
[32] H. J. F. Knops, Phys. Rev. B **30**, 470 (1984).
[33] J. E. Van Himbergen, Solid State Commun. **55**, 289 (1985).
[34] K. J. Strandburg, Rev. Mod. Phys. **60**, 161 (1988).