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Inhomogeneity of vortices in 2d classical XY-model : a microcanonical Monte Carlo simulation study

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Abstract : The extended 2d classical XY-model has been studied using microcanonical Monte Carlo simulations. Simulations have been carried out on 30 × 30 spin system on a square lattice. We find that the maximum inhomogeneity of vortex distribution occurs at a temperature which coincides with the position of specific heat peak in the Kosterlitz-Thouless (KT) case and in the coexistence region in the first order case. The inhomogeneity is found to be more in the KT case as compared to the first order one.

Keywords : XY-model, vortices, microcanonical

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Study of the two dimensional (2d) classical XY-model has unfolded several interesting physical properties of 2d system [1] and still demands further investigations. The 2d XY-model has been considered in the literature to understand the high temperature superconductors (HTSC), which is however not completely successful [2]. The experimental data can lead to interesting information on HTSC if one knows the right extension of the XY-model that explains them [3]. Thus, there is a need to understand the nature of the vortex-driven transition in 2d XY-model. The lack of long range order, the presence of topological defects called vortices, and the Kosterlitz-Thouless (KT) transition are some of its notable properties known as yet [4–21]. The two types of excitations that dominate at low temperatures are spin waves and vortices. The low-temperature phase has only bound vortex-antivortex pairs and the KT transition is associated with the unbinding of the vortex-antivortex pairs. Investigations have been carried out for the possibility of a first order transition in this model, without disturbing the essential symmetry. Domany, Schick and Swendsen [22] suggested that by sufficiently reducing the width of the nearest neighbour interaction potential in this model a first order transition can be observed. The first order transition is understood to result as due to

/ of vortices. In this paper, we report the .he classical 2d XY-system, which has sofar

2d classical XY-model is given by :

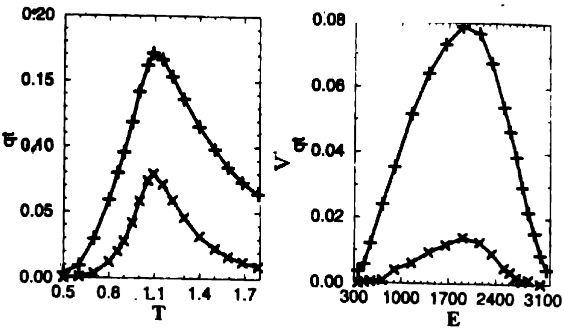
$$^{p^2}\left((\theta_i - \theta_j)/2\right)\Big], \quad (1)$$

al meaning. For $p^2 = 1$; the Hamiltonian reduces to the nich admits the KT transition. By increasing the value of ıde narrower and for $p^2 > 10$ the transition becomes first-

We r canonical MC simulations on a square lattice having 30 × 30 spins [23,24]. We periodic boundary conditions and have calculated system temperature (T), vorticity, magnetization square and their respective standard deviations at each given total energy (E). We used 1×10^5 MCSS for equlibration and 1×10^5 MCSS for averaging. The accuracy of the mean value of the physical quantities was estimated by performing block averages consisting of 5×10^3 MCSS each and then finding the standard deviation of block averages. The KT transition temperature occurs at 0.9 and the maximum of temperature dependence of specific heat occurs at 1.09.

We analysed the Monte Carlo configurations evolved during the simulation to study the inhomogeneity of the vortices across the transition. To this end we estimated the average number ($V_n(r)$) of vortices/antivortices at a distance r from any given vortex. From this we obtained the number of positive (negative) vortices (V_{q+} (V_{q-})) surrounding a positive vortex within a distance of $\sqrt{2a}$ and $2\sqrt{2a}$ (a is the lattice spacing). For $p^2 = 1$, it is seen that V_{q-}, when determined over a distance of $\sqrt{2a}$, decreases with temperature initially upto $T = 1.1$ and then increases with further increase in temperature. The decrease of V_{q-} with temperature is not observed, when determined over a larger distance of $2\sqrt{2a}$. Whereas, V_{q+} shows a steady increase with increase in temperature. On the other hand, for $p^2 = 50$, both V_{q+} and V_{q-} are seen to increase with increase in energy even when determined over a smaller distance of $\sqrt{2a}$ [25].

We next determined the net vortex charge (V_{qt}) within a distance of $\sqrt{2a}$ and $2\sqrt{2a}$ from a vortex as functions of T (or E). Figure 1(a) shows the temperature dependence of V_{qt} for $p^2 = 1$, and comments on some features of this graph are in order. Firstly, V_{qt} goes through a maximum. Secondly, the magnitude of V_{qt} is reduced as the distance increases. Finally, the maximum occurs at $T = 1.1$, which corresponds to the specific heat peak. Similar graph is shown in Figure 1(b), for $p^2 = 50$. The behaviour is qualitatively similar to the case for $p^2 = 1$, except for the following differences. The magnitude of V_{qt} is comparatively smaller. The maximum of V_{qt} occurs in the coexistence region of the first-order transition. The vortices are therefore, not distributed homogeneously in the lattice. Examination of the configurations revealed the presence of vortex clusters in the critical region, which has also been pointed out by Toboknik and Chester [13].



(a) (b)

Figure 1. (a) The temperature dependence of net vortex charge V_{qt} in a radius of $\sqrt{2a}$ (+) and $2\sqrt{2a}$ (×) for $p^2 = 1$. (b) The energy dependence of net vortex charge V_{qt} in a radius of $\sqrt{2a}$ (+) and $2\sqrt{2a}$ (×) for $p^2 = 50$. The data represents averages over 1×10^5 MCSS.

We have not yet come across an explanation of the observed inhomogeneity of vortices. However, certain features can be understood as follows. In the low temperature (energy) insulating phase the vortices are bound tightly which results in a small value of V_{qt}. In the high temperature (energy) Debye-Hückel regime, V_{qt} is also small due to the presence of large number of free charges in the liquid phase. We speculate that clusters of vortices in the critical region are responsible for the peak in V_{qt}. The difference between $p^2 = 50$ and 1 cases can be attributed to the change in interaction from $\ln(r/a)$ to r/a as p^2 changes from 1 to 50 [3].

In conclusion, we have studied the vortices in the classical 2d XY-model undergoing KT and first-order transition. We have reported a subtle aspect of the vortices, that is the inhomogeneity of vortex distribution.

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