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Existence of a line of critical points in a two-dimensional Lebwohl Lasher model

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ABSTRACT

Controversy regarding transitions in systems with global symmetry group O(3) has attracted the attention of researchers and the detailed nature of this transition is still not well understood. As an example of such a system in this paper we have studied a two-dimensional Lebwohl Lasher model, using the Wolff cluster algorithm. Though we have not been able to reach any definitive conclusions regarding the order present in the system, from finite size scaling analysis, hyperscaling relations and the behavior of the correlation function we have obtained strong indications regarding the presence of quasi-long range order and the existence of a line of critical points in our system.

1. Introduction

The symmetry of a disordered phase is broken by the order present in the phase below a phase transition. In many cases the symmetry which is being broken is continuous. The simplest continuous symmetry is that of rotations in a two-dimensional plane – the XY model. Thermal fluctuations depress order parameter present in a phase from its zero temperature maximum value. Mermin and Wagner established that long range order can [1–4] not appear for systems with continuous symmetry at finite temperature in space dimension $d \leq 2$. This is the phenomenon of fluctuation destruction of long range order. The importance of such fluctuations is reduced in higher dimensions. A large number of vortices can destroy long range order and systems with continuous symmetry might have another type of transition governed by vortex binding–unbinding topological defects at definite positive temperature. This kind of topological phase transition is called Berezinskii, Kosterlitz and Thouless (BKT) transition. The two-dimensional XY model with global symmetry group O(2) exhibits such topological transitions [5–7]. In this system quasi-long range order (QLRO) appears at low temperatures and the order parameter vanishes as a power law at the thermodynamic limit. The system has a line of critical points as is evident from the divergence of the susceptibility of the system at all temperatures below T_{BKT} (the Berezinskii–Kosterlitz–Thouless transition temperature). Another characteristic behavior of this transition is that at temperatures just above the BKT transition the correlation length ξ diverges as the essential singularity $\xi \sim \exp(bt^{-\frac{1}{2}})$ that is much stronger divergent than the second order transition power law $\xi \sim t^{-\nu}$. However there is a controversy regarding phase transition in a system with global symmetry group O(3).

Various experiments on three-dimensional liquid crystals exhibit a weak first order transition [8]. The Lebwohl Lasher (LL) model was designed for the 3D system, however the corresponding two-dimensional problem also has attracted the attention of researchers and is still not well understood. The LL model is a model for a regular 2D liquid crystal [16]. It is based on a lattice version of the mean field model of Maier et al. [17] where the molecule experiences an attractive anisotropic interaction. This model is also referred to as a nematic n-vector model, the RP^{n-1} model, in which to each lattice site is attached a direction in n-dimensional space. There is an interaction between nearest neighbors, which tends to make the corresponding directions parallel. In our system the uniaxial particles are placed at the sites of a square lattice and they interact through a nearest neighbor pair potential of the form

$$H = -\sum_{<i,j>} P_2(\vec{S_i}.\vec{S_j}) \tag{1}$$

where the coupling constant has been absorbed in H and $P_2(x) = (3x^2 - 1)/2$ is the second order Legendre polynomial. The first significant Monte Carlo study of such system was done by Chiccoli et al. [9]. From the behavior of the specific heat their conclusion was for the absence of a true phase transition. However they were not

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very conclusive about the nature of the phase transition. Kunz and Zumbach in 1992 [10] concluded in support of a BKT like topological phase transition. They did a numerical study of a nematic n-vector model which is called the RP^{n-1} model and reported the transition temperature $T_c = 0.356$ for the RP^2 case.

Mondal and Roy in 2003 [11] studied the planar LL model and concluded that the model should present a continuous transition at $T_C = 0.547$. Another work by Dutta and Roy [12] shows results in favor of a topological transition. Contrary to all these and many more numerical studies Paredes et al. in 2008 [13] reported a lack of QLRO phase in a LL liquid crystal and conjectured that the LL liquid crystal in two dimensions cannot experience a transition of the BKT type. The maximum system size on which they carried out their studies was 768×768. Almaraz et al. in 2010 [14] studied the phase transitions of the LL model when confined between planar slits of different widths. Recently in 2014 Tomita [15] did a low temperature study on two-dimensional continuous spin systems. Here a finite size scaling analysis suitable for distinguishing the critical behavior has been applied to the 2D XY, Heisenberg and RP^2 models and a fixed-scale-factor finite size scaling has been done which gives a criterion for judging a system as to whether it is in the critical region or in the pseudocritical region. The Hamiltonian of the RP^2 model differs from that of the LL model by a factor of 1.5 ($P_2(\cos\vartheta)$ as opposed to $\cos^2\vartheta$).

In the present communication we have revisited the problem of the appearance of the QLRO in the 2D LL model using extensive Monte Carlo simulations. For this purpose we have gone upto a lattice size as large as 2048×2048 which is much bigger than that used by Paredes et al. in their work [13]. To analyze our result we have used the technique of finite size scaling.

2. Method

Our work is based on the Monte Carlo simulation technique where we have used the Wolff cluster algorithm [20,21]. We have done simulations on lattices $L \times L$ for $L = 128$, 256, 512, 768, 896, 1024, 1152, 1600 and 2048. All data for lattice size smaller than and equal to 1600×1600 were obtained after 10^6 Monte Carlo (MC) steps for equilibration of the system followed by another 10^6 MC sweeps for production. For the lattice size 2048×2048 larger runs were required and we have performed 3×10^6 MC sweeps for equilibration and another 10^6 MC sweeps for production. The total number of simulations performed are approximately 180 i.e. around 20 temperatures for each lattice size. The simulations were carried out on HP servers DL 360P with 8 core Intel Xeon processors. We have obtained temperature dependence of different thermodynamic quantities like energy, specific heat, order parameter, susceptibility, Binder Cumulant and correlation function. The temperature range has been chosen to be sufficiently wide to cover the region of important thermodynamic changes.

3. Results and discussions

3.1. Data collapse of susceptibility

Standard finite size scaling theory for second order phase transition predicts [18,19] that the peak height (χ_0) of the susceptibility curve scales as $L^{\frac{\gamma}{\nu}}$ where L is the lattice size and γ and ν are the susceptibility and correlation length exponents. Fig. 1 shows the plot of $\ln \chi_0$ against $\ln L$ and we have obtained a linear fit. The slope of the line obtained gives us the ratio $\frac{\gamma}{\nu} = 1.655$.

In the neighborhood of T_c and $L \gg \xi$ where ξ is the correlation length the susceptibility behaves as

$$\chi(T,L) = L^{\frac{\gamma}{\nu}} \widetilde{\chi}\left[\left(\frac{T}{T_C} - 1\right) L^{\frac{1}{\nu}}\right] \tag{2}$$

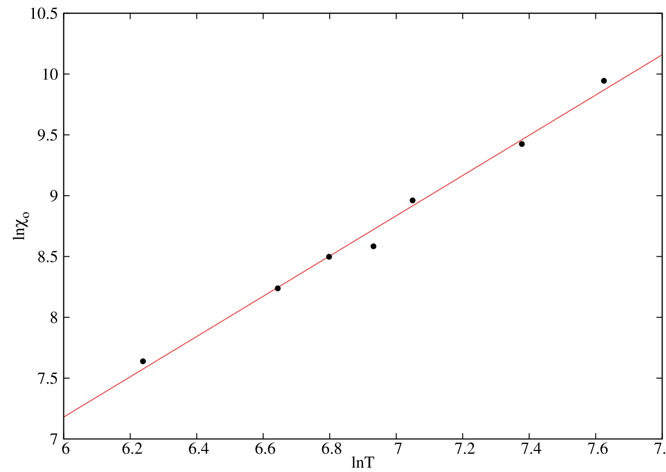

Fig. 1. Linear fit showing variation of susceptibility with system size. The line has a slope $\frac{\gamma}{\nu} = 1.655$.

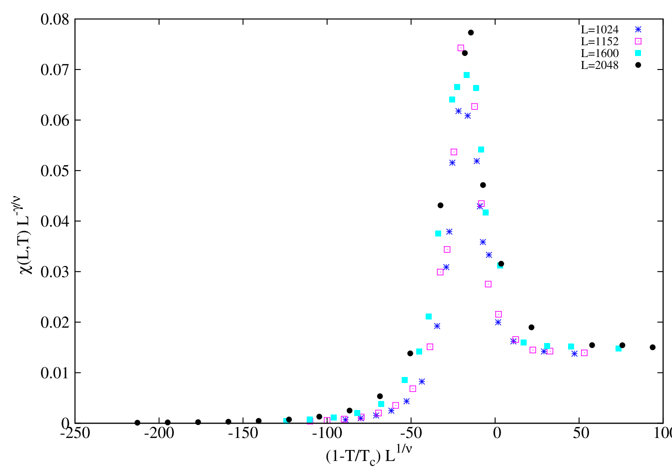

Fig. 2. Data collapse curves of susceptibility. Four system sizes have been used and the collapse has been designed to be best near $T = T_C$. The fit shown gives $T_C = 0.526$, $\nu = 1.01$ and $\gamma = 1.656$.

where $\widetilde{\chi}$ is the scaled susceptibility [22]. By plotting $\chi(T,L)L^{-\frac{\gamma}{\nu}}$ along Y axis and $(1 - \frac{T}{T_C})L^{\frac{1}{\nu}}$ along X axis and by adjusting T_C, the ratio of exponents $\frac{\gamma}{\nu}$ and $\frac{1}{\nu}$ simultaneously the family of curves $\chi(T,L)$ can be collapsed on a single curve as shown in Fig. 2.

The value of critical exponents thus obtained is

$T_C = 0.526$

$\nu = 1.01$

$\gamma = 1.656$

3.2. Data collapse of order parameter

Similarly data collapse analysis of order parameter $\langle P_2 \rangle$ as shown in Fig. 3 is obtained by plotting $m(T,L)L^{\frac{\beta}{\nu}}$ along Y axis (here $\langle P_2 \rangle$ has been written as m) and $(1 - \frac{T}{T_C})L^{\frac{1}{\nu}}$ along X axis. The corresponding scaling relation is given by

$$m(T,L) = L^{-\frac{\beta}{\nu}} \widetilde{m}\left[\left(\frac{T}{T_C} - 1\right) L^{\frac{1}{\nu}}\right] \tag{3}$$

where $\widetilde{m}$ is the scaling function and β is the order parameter exponent. The critical exponents obtained thus are

$T_C = 0.526$