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

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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

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

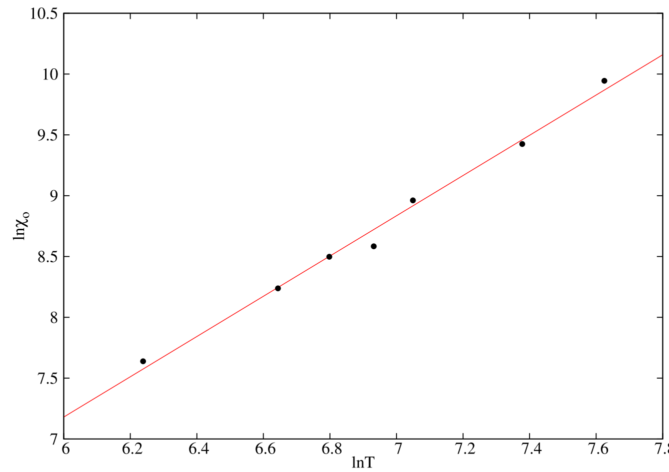

Fig. 1. Linear fit showing variation of susceptibility with system size. The line has a slope $\frac{\gamma}{\nu} = 1.655$.

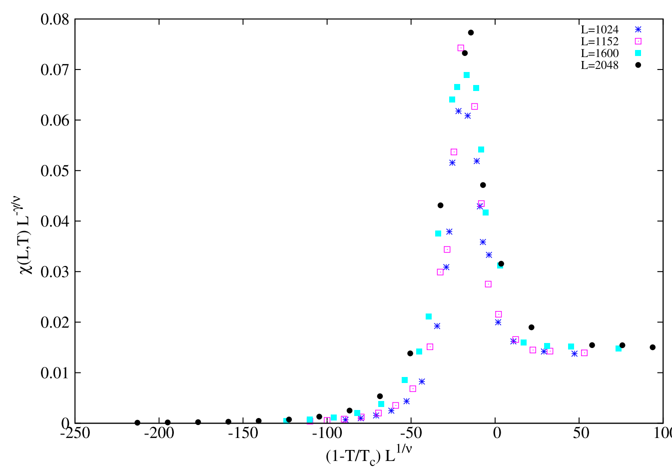

Fig. 2. Data collapse curves of susceptibility. Four system sizes have been used and the collapse has been designed to be best near $T = T_C$. The fit shown gives $T_C = 0.526$, $\nu = 1.01$ and $\gamma = 1.656$.

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

$$T_C = 0.526$$

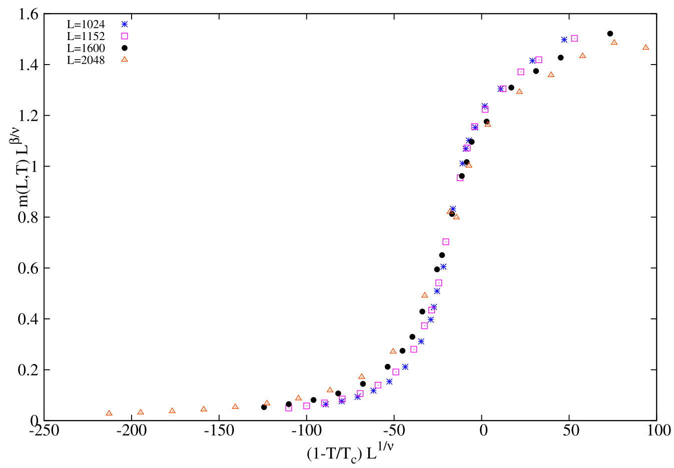

Fig. 3. Data collapse curves of order parameter. Four lattice sizes have been used and maximum overlap has been designed to be near $T = T_C$. The fit gives $T_C = 0.526$, $\nu = 1.01$ and $\beta = 0.202$.

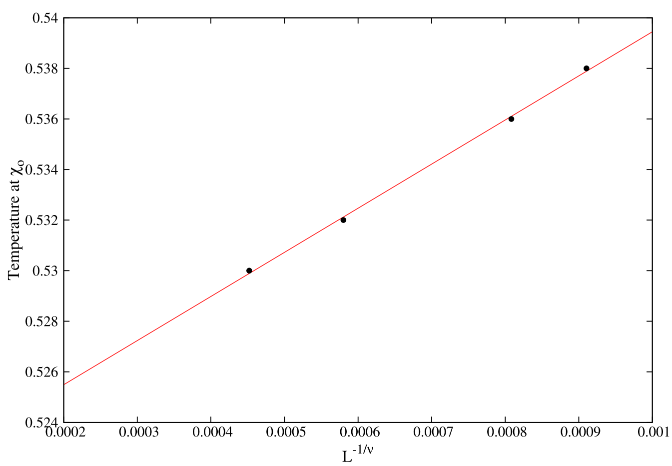

Fig. 4. Value of T_C obtained from the linear fit of temperatures at which susceptibility has a maximum value (χ_0) for different lattice sizes.

$\nu = 1.01$

$\beta = 0.202$

The value of T_C obtained by us may appear to be different from previously quoted results in the literature (e.g. [10]). This is due to the fact, as already mentioned above, that we have used a Hamiltonian which differs by a factor of 1.5 from the Hamiltonian used by Kunz and Zumbach in their work.

For the data collapse analysis of order parameter and susceptibility we have used the higher lattice sizes.

A common method for circumventing the question of size of the critical region is to perform data collapse of the susceptibility curves at a single point, the point x_0 at which the scaling function (in this case susceptibility) is a maximum. T_0 is given by

$$T_0 = T_C(1 + x_0 L^{-\frac{1}{\nu}}) \tag{4}$$

By plotting T_0 vs. $L^{-\frac{1}{\nu}}$ as shown in Fig. 4 and obtaining the value of the intercept we get an estimate of $T_c = 0.522$. This value of T_C nearly matches the value of $T_c = 0.526$ obtained from data collapse analysis of order parameter and susceptibility curves. The value of $\frac{1}{\nu}$ is taken to be 0.99 which was obtained from data collapse analysis of order parameter and susceptibility.

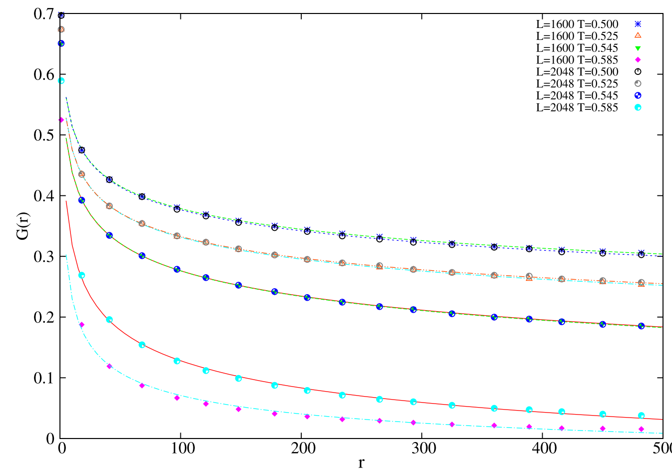

Fig. 5. Variation of correlation function with distance showing power law fits for $T < T_c$ and exponential decay for $T > T_C$. Two system sizes $L = 1600, 2048$ have been plotted here.

3.3. Variation of correlation function

In Fig. 5 we have shown the pair correlation function for two lattice sizes 1600×1600 and 2048×2048. The pair correlation function is defined by

$$G(r) = < P_2(\cos \gamma_{ij}(r)) > \tag{5}$$

where γ_{ij} is the angle between two particles which are at a distance r apart. In systems exhibiting quasi-long range order (QLRO) the correlation function decays according to a power law whereas in a disordered system it dies off exponentially. As can be seen from Fig. 5 it is evident that for the temperatures below $T_C = 0.526$ (as predicted from the data collapse results) the decay exhibits a power law behavior whereas for higher temperatures the decay of the correlation function becomes sharper and is closer to an exponential one.

3.4. Verification of hyperscaling relations

Using finite size scaling for the system susceptibility χ it is possible to estimate the value of correlation function exponent η within the temperature range $T \leq T_{BKT}$. On a line of critical points χ should scale with the exponent ratio $\frac{\gamma}{\nu}$ which is related to η through the hyperscaling relation

$$\frac{\gamma}{\nu} = 2 - \eta \tag{6}$$

Using Eq. (6) and the value of the $\frac{\gamma}{\nu}$ ratio obtained from data collapse of susceptibility curves we estimate the value of η at $T_C = 0.526$ to be 0.36.

Similarly from the hyperscaling relation

$$\beta = \frac{1}{2}(d - 2 + \eta)\,\nu \tag{7}$$

and the value of the ratio $\frac{\beta}{\nu}$ obtained from data collapse of order parameter curves we have estimated η at $T_C = 0.526$ to be 0.40. Here d stands for the dimensionality of the system which in our case is 2.

The scaling relation

$$\gamma + 2\beta = d\nu \tag{8}$$

is also satisfied. By replacing the ratios $\frac{\gamma}{\nu}$ and $\frac{\beta}{\nu}$ with those obtained from data collapse of susceptibility and order parameter we get $d = 2.056$.

Table 1
The $\frac{\gamma}{\nu}$ at different temperatures were obtained by plotting $\ln\chi$ vs. $\ln L$ (as in Fig. 1 but using χ at the respective temperatures, instead of the peak values χ_0). The exponent η has been obtained from the power law fits of $G(r)$ vs r for $L = 2048$ and using the relation $G(r) \sim r^{-\eta(T)}$. For these systems η varies little with temperature and the constant value has been taken. The last column is for testing to what extent the scaling law $\frac{\gamma}{\nu} + \eta = 2$ is satisfied.

Temperature	$\frac{\gamma}{\nu}$	η	$\frac{\gamma}{\nu}+\eta$
0.5	1.79 ± 0.03	0.120 ± 0.001	1.91
0.505	1.80 ± 0.14		1.92
0.51	1.77 ± 0.03		1.89
0.515	1.89 ± 0.14		2.01
0.52	1.75 ± 0.09		1.87
0.525	2.17 ± 0.07		2.29
0.53	2.64 ± 0.07		2.76

The Josephson's identity

$$\alpha = 2 - d\nu \tag{9}$$

yields $\alpha = -0.02$ and the Rushbrooke relation

$$\gamma + 2\beta + \alpha = 2 \tag{10}$$

gives $\alpha = -0.056$. The negative value of α obtained from both the relations is consistent with the cusp we observed in the specific heat curves (not presented in this paper).

3.4.1. Possibility of a line of critical points

Correlation function critical exponent η may depend on T on a line of critical points. An interesting result that we have come across here which has been highlighted in Table 1 is that the hyperscaling relation $\frac{\gamma}{\nu} + \eta = 2$ is approximately satisfied on a possible line of critical points when we evaluate $\frac{\gamma}{\nu}$ by doing a linear fit of $\ln\chi$ vs. $\ln L$ curve. This has been done for each temperature as shown in Table 1 so that we obtain the temperature variation of $\frac{\gamma}{\nu}$. η has been calculated from a power law fit of correlation function $G(r)$ at the same set of temperatures.

From the above data we can see that the hyperscaling relation holds till $T = 0.525$. This points towards the existence of a line of critical points. The power law decay of correlation function as has been discussed earlier also strongly points towards an existence of a line of critical points below a particular temperature.

3.5. Variation of correlation length with T

In Fig. 6 we have plotted the correlation lengths of system sizes $L = 256, 512, 768, 896, 1024, 1152, 1600$ and 2048 with temperature. Here the correlation length has been obtained by using dependence of correlation function $G(r)$ with r till half of the lattice size ($\frac{L}{2}$) and Eq. (11)

$$\xi^2 = \frac{\sum r^2 G(r)}{\sum G(r)} \tag{11}$$

At low temperatures the corresponding correlation lengths appear to saturate thus confirming that for all these lattice sizes $L >> \xi$. For the maximum lattice size 2048×2048 the saturation temperature seems to be around 0.53. The low temperature region lying below 0.53 can be conjectured to lie on a line of critical points.

3.6. Binder's Cumulant check

For continuous phase transition the Binder's Cumulant

$$U_4 = 1 - \frac{<m^4>}{3<m^2>^2} \tag{12}$$

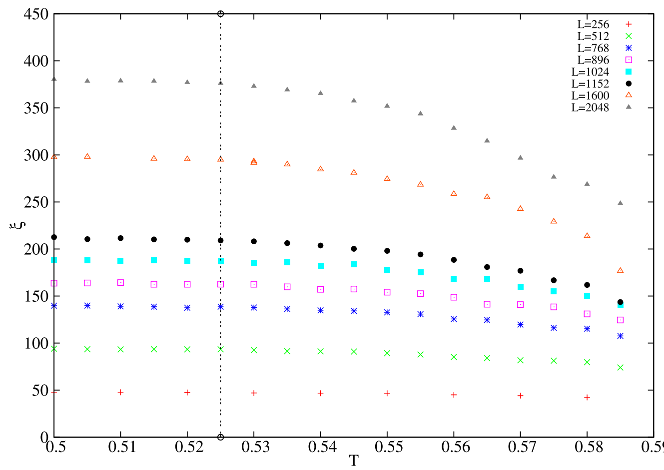

Fig. 6. Variation of correlation length with temperature for different lattice sizes (the vertical line denotes $T = 0.525$).

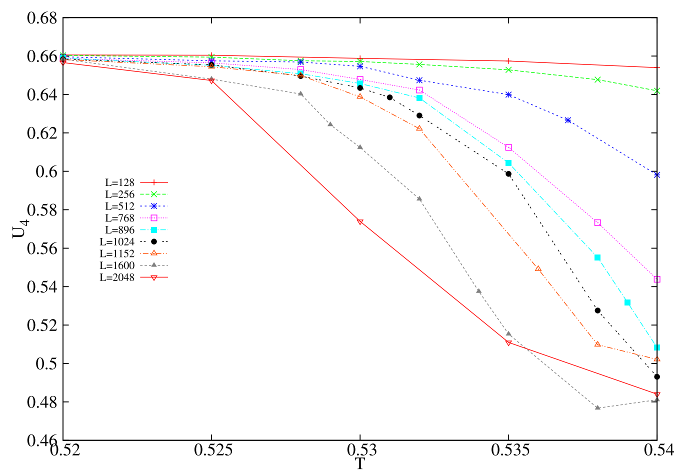

Fig. 7. Variation of Binder Cumulant with temperature for different lattice sizes.

is known to be a universal quantity independent of L at the critical point [24] (see Fig. 7). For the XY model it was seen by Farinas-Sanchez et al. [23] that the Binder Cumulants for different lattice sizes cross over at a single point which is close to the reported BKT temperature. The behavior of U_4 obtained by us for the different lattice sizes is however completely different. The Binder Cumulants decrease with L but does not cross over at any single point close to our predicted BKT temperature.

4. Conclusions

From the results obtained by us though we have not been able to reach definitive conclusions we are certainly in a position to highlight some interesting features. The Binder Cumulants calculated for different lattice sizes do not show any cross over thus indicating the absence of a phase transition. However, from data collapse of susceptibility and order parameter we could predict a transition at a temperature, $T_C = 0.526$ and the value of critical exponents γ, β, ν obtained agrees well with the different hyperscaling relations. The correlation function changes from a power law behavior below $T = 0.525$ to an exponential decay for temperatures above $T = 0.53$ thus confirming the presence of QLRO at around T_C which has been predicted by us from data collapse studies.

Values of η obtained from a power law fit of correlation function and the ratio $\frac{\gamma}{\nu}$ values obtained from susceptibility data satisfy the hyperscaling relation $\frac{\gamma}{\nu} = 2 - \eta$ for a small temperature range between $T = 0.50$ and $T = 0.525$. This region corresponding to $T < 0.525$ can be considered to lie on a probable line of critical points. The evidence of this comes from the nature of the correlation function $G(r)$ as well as from the hyperscaling relations. Paredes et al. in their work in 2008 [13] had concluded against the existence of QLRO in 2D systems but our work within errors and with large system sizes used points closer to the existence of a BKT transition at $T = 0.525$.

The values of η obtained using the hyperscaling relations and the results obtained from the data collapse curves of susceptibility and order parameter do not agree well with those obtained from the power law fit of $G(r)$. With our present resources we have not been able to generate quantitatively more accurate results as the computation presented in this communication has consumed enormous CPU time. We believe that the quantitative predictions of our work could perhaps be improved by reducing the statistical errors present in the work. By taking MC averages over more configurations ($\sim 10^7$ sweeps) or by doing multiple histogram reweighting the errors could be significantly reduced. The merit of the model certainly deserves such work to be performed before a final conclusion may be thought to have been reached. It also needs to be seen if the Binder Cumulants in a better MC work points towards a BKT transition. As discussed by Tomita [15] the fixed scale factor finite size scaling (FSF-FSS) analysis is quite useful in distinguishing the genuine critical behavior present in the 2D XY model from the pseudocritical behavior exhibited by the 2D Heisenberg model. In the case of the RP^2 model the FSF-FSS analysis seems to show that the model is pseudocritical while some studies [10,11] mention that this model possesses a genuine critical region. This discrepancy arises from a subtle and persistent crossover in the model. In case of a LL model the existence of a line of critical points can be further corroborated using this FSF-FSS analysis.

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