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Hexatic and Herringbone Orderings in 2D Liquid Crystals

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We investigate the universality class of Bruinsma-Aeppli (BA) model in two dimensions. This model is consisting of two coupled XY order parameters, six-fold and two-fold symmetry, and is proposed to describe the Smc-A to Hex-B transition in some Smectic liquid crystal compounds. Using high resolution Monte Carlo simulation technique based on multi-histogram method and cluster algorithm, and also finite size scaling, we compute the critical exponents of this model with high accuracy. We find that for some ranges of coupling constants this model undergoes transition from disordered phase to a symmetry broken phase with both hexaitc and herringbone orderings.

Keywords 3-state Potts universality class; Critical exponents; histogram method; Monte Carlo simulations; Wolf algorithm

1. Introduction

The explanation of the critical properties of liquid crystal compounds, representingthe phase transition from smectic-A (SmA) phase, with liquid-like in-plane behavior, to Hexatic-B (HexB) phase, with long-range bond-orientational order but short-range in-plane positional order, has remained a challenge for both experimental and theoretical physicists for about 3 decades. The Hexatic-B phase was first observed in x-ray diffraction study of liquid crystal compound 65OBC(n-alkyl-4-m-alkoxybiphenyl-4-carboxylate, $n = 6$, $m = 5$) [1,2], where a hexagonal pattern of diffuse spots was found in intensity of scattered x-rays, indicating the existence of long-range bond-orientational order. In addition to this hexagonal pattern, it was also found that some broader peaks appeared in the diffracted intensity, which indicates the onset of another ordering. These broad peaks are related to herringbone-like packing of molecules, perpendicular to the Smectic layer stacking direction. The accompanying of the hexatic and herringbone orders make it a physically rich phase, which is simply called Hexatic-B (HexB) phase.

The unusual critical behavior at SmA-HexB transition was revealed in heat capacity measurements on bulk samples of 65OBC [1,3] and other calorimetric

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studies on many other components in the nmOBC homologous series [1,4]. These measurements yielded very sharp specific heat anomalies near SmA-HexB transition with no detectable thermal hysteresis and with very large value for the heat capacity critical exponent, $\alpha \approx 0.6$. It is now widely accepted that the reason for αbeing large, is that SmA-HexB transition for the above compounds is weakly first order [5–8]. Interestingly, the heat capacity measurements of two-layer free standing films of different nmOBC compound show a second order SmA-HexB transition, described by the heat capacity exponent $\alpha \approx 0.3$ [1]. This is obviously in contrast with the usual broad and nonsingular specific heat hump of the KT transition in the 2D XY model, suggesting that SmA-HexB transition cannot be described simply by a unique XY order parameter.

A first attempt to describe theoretically this transition was done by Bruinsma and Aeppli (BA) [9], who formulated a Ginzburg-Landau theory with two XY order parameters corresponding to hexatic and herringbone orders. The six-fold symmetry of the hexatic phase suggests that bond-orientational order parameter to be defined by $\Psi = |\Psi|\exp(i6\psi)$, describing the six-fold azimuthal modulation. Because of the broadness of x-ray diffracted peaks associated to herringbone order (which is the reason of being short-range), they considered an XY order parameter with two-fold symmetry for herringbone ordering ($\Phi = |\Phi|\exp(i2\varphi)$). Based on symmetry arguments, they also made a minimal coupling between the hexatic andherringbone order parameters as $V_{hex-her} = h\mathrm{Re}\left(\Psi^{*}\Phi^{3}\right)$.

A discrete version of the BA model has been studied by Monte Carlo simulation method in 2D [10,11] and also in 3D [12]. While the high-resolution Monte Carlo simulation of the BA model in 3D reveals the existence of a tricritical point on the transition line betweenSmA and hexatic (herringbone) phases [12], a 2D simulation shows a continuous phase transition in which two different orderings are simultaneously established [10,11].The specific heat exponent of this transition as obtained from Monte Carlo simulations in 2D is $\alpha \approx 0.3$, in good agreement with experimental values. In this paper we use high performance Monte Carlo and finite size scaling methods to obtain all critical exponents of the continuous transition observed in the two-dimensional BA model and show that this transition is in 3-state Potts universality class.

2. Monte Carlo Simulation

Recalling the six-fold symmetry of hexatic order and two-fold symmetry of the herringbone order, the BA Hamiltonian which describes both orderings can be expressed as follows

$$H = -J_1 \sum_{\langle i,J\rangle} \cos(\psi_i - \psi_J) - J_2 \sum_{\langle i,J\rangle} \cos(\phi_i - \phi_J) - J_3 \sum_{\langle i,J\rangle} \cos(\psi_i - 2\phi_i),$$

where ψ and ϕ denote, respectively, hexatic and herringbone orderings. We are interested in investigating those regions in the coupling constants space for which the two kinds of ordering establish together, so we fix $J_3 = 2.0$ and then start to get data for $J_2 = 0.6$, 0.7, 0.8, 0.9, and 1.0. The basic thermodynamic quantities of interest are the specific heat $c = \frac{(\langle E^2\rangle - \langle E\rangle^2)}{L^2T^2}$, the herringbone order parameter $M = \frac{\left(\sum_i \cos(\Phi_i)\right)^2 + \left(\sum_i \sin(\Phi_i)\right)^2}{L^2}$ and the herringbone susceptibility $\chi = \frac{(\langle M^2\rangle - \langle M\rangle^2)}{L^2T}$.

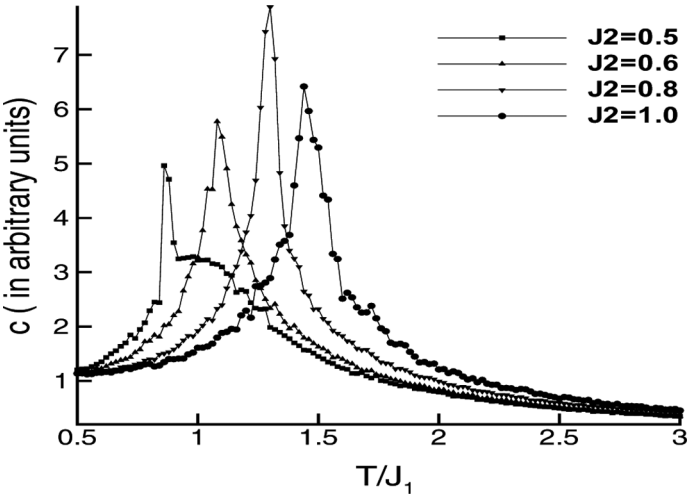

Figure 1. Temperature dependence of specific heat for $J_1 = 1.0$, $J_3 = 2.0$, and $J_2 = 0.5$, 0.6, 0.8, and 1.0.

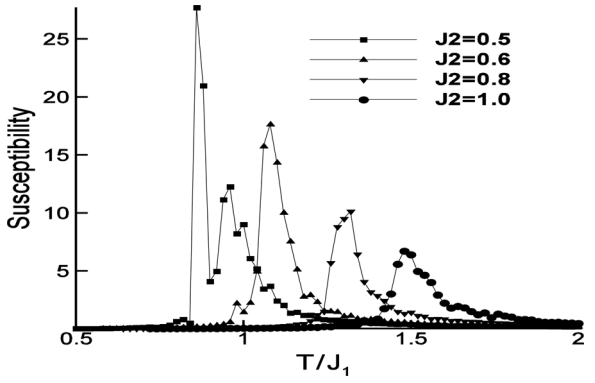

Figure 2. Temperature dependence of susceptibility for $J_1 = 1.0$, $J_3 = 2.0$, and $J_2 = 0.5$, 0.6, 0.8, and 1.0.

We have obtained the specific heat, order parameter and susceptibility as a function of temperature. They are shown in Figures 1 and 2.

3. Order of the Transition

One of the main problems in Monte Carlo data analysis of phase transitions is in determining the order of the transition. Strong first order transitions will show marked discontinuities in thermodynamic quantities such as the internal energy and the order parameters, and present no real problems. Weakly first order transitions are much more difficult to recognize. To determine the order of transition we use the Binder fourth energy cumulant, defined as

$$U_4(L) = 1 - \frac{\langle E^4 \rangle}{3\langle E^2 \rangle}$$

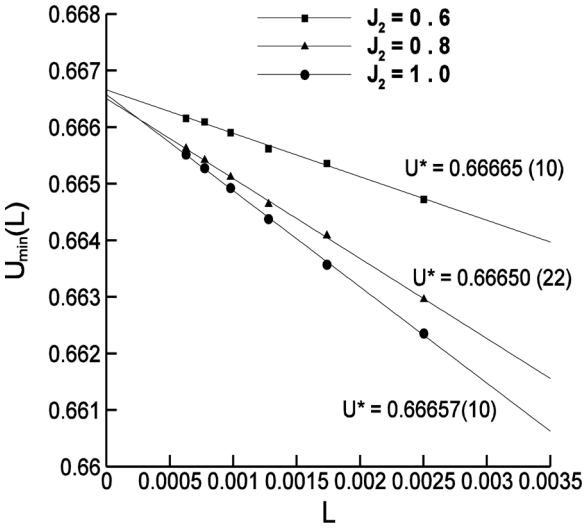

Figure 3. Size dependence of Binder fourth energy cumulate minima, calculated by optimized reweighing for $J_1 = 1.0$, $J_3 = 2.0$, and $J_2 = 0.5$, 0.6, 0.8, and 1.0.

This quantity reaches a minimum near the transition points. It has been shown that the size dependence of this minimum behaves as

$$U_{\min}(L) = 2/3 - \left(\frac{e_1}{e_2} - \frac{e_2}{e_1}\right)^2 /12 + BL^{-d} + O(L^{-2d})$$

whose value approaches $2/3$ in the thermodynamic limit for a continuous transition and approach some nontrivial value less than $2/3$ at a first-order transition. Here e_1 and e_2 are the values of energy per site at the transition point of a first order phase transition. We have plotted the size dependence of $U(L)$ for $J2 = 0.6$, 0.8 and 1 in Figure 3. This indicates that the transitions are continuous for this range of couplings. After determining the order of transitions we proceed to estimate the critical temperatures and the critical exponents, using the finite-size scaling [13–17].

4. Finite Size Scaling

According to the finite-size scaling theory, the scaling form for magnetization density, susceptibility, and specific heat in zero field are as follows:

$$m \approx L^{\beta/\nu} M(tL^{1/\nu}), \quad \text{and } \chi \approx L^{\gamma/\nu} K(tL^{1/\nu}), \quad \text{and } c \approx c_\infty(t) + L^{\alpha/\nu} C(tL^{1/\nu})$$

in which α, β, γ, and ν are the static critical exponents. The logarithmic derivatives of total magnetization (mL^d) are also very useful for high accuracy estimation of the critical temperature Tc and the correlation length critical exponent ν. For example, defining the following quantities:

$$V_1 \equiv 4[M^3] - 3[M^4], V_2 \equiv 2[M^2] - [M^4], V_3 \equiv 3[M^2] - 2[M^3], V_4 \equiv \frac{4[M] - [M^4]}{3},$$
$$V_5 \equiv \frac{3[M] - [M^3]}{2}, \quad \text{and} \quad V_6 \equiv 2[M] - [M^2]$$

Table 1. Universality class of a coupled XY model for the two dimensional BA hamiltonian

J_1/J_2	T_C	ϑ	β	γ	α	δ
0.6	0.79 (9)	0.9645 ± 0.08	0.0711 ± 0.006	1.7761 ± 0.14	0.07078 ± 0.16	25.9673 ± 4.3
0.7	0.91 (8)	0.8810 ± 0.05	0.10867 ± 0.006	1.5421 ± 0.08	0.2379 ± 0.1	15.1900 ± 1.5
0.8	1.02 (3)	0.8303 ± 0.06	0.0923 ± 0.006	1.4754 ± 0.1	0.33933 ± 0.12	16.9752 ± 2.2
0.9	1.11 (3)	0.8503 ± 0.02	0.1171 ± 0.0027	1.5173 ± 0.03	0.2994 ± 0.04	13.9513 ± 0.55
1.0	1.19 (7)	0.8406 ± 0.02	0.1261 ± 0.003	1.4305 ± 0.03	0.3187 ± 0.04	12.3365 ± 0.5
3state-potts model		5/6	1/9	13/9	1/3	14

(where $M = mL^d$ is the total magnetization of the system and $[M^n] \equiv \ln \frac{\partial \langle M^n \rangle}{\partial T}$), it can be shown that the above moments obey the following scaling: $V_j \approx (\frac{1}{\nu}) \ln L + \nu_j (tL^{\frac{1}{\nu}})$ for $j = 1,2,\ldots, 6$.

Therefore, at the critical temperature ($t = 0$) the slope of V_j *vs* ln(L) should be constant, independent of L. We use this method to high-precision evaluation of both the critical temperature and the correlation length exponent ν. The obtained critical exponents are listed in the Table 1, and show to be very close to the values for 3-state Potts model in 2D [18].

5. Conclusion

In summary, using the optimized Monte Carlo simulation based on multi-histogram and Wolf's embedding methods, we investigated the critical properties associated with BA Hamiltonian in 2D. This Hamiltonian contains two coupled XY order parameters, a hexatic field with six-fold symmetry and a two-fold symmetric field corresponding to the herringbone packing and has been proposed for modeling the critical behavior of Smectic-A to Hexatic-B in some liquid crystal compounds. Using fourth Binder cumulates method; we found that the orders of transitions for the couplings range, where both kinds of orderings appear simultaneously, are second order. All the static critical exponents were derived by finite-sizes caling analysis for this range of couplings. The static critical exponents are in excellent agreement with the two dimensional three-state Potts model, indicating that the two dimensional BA Hamiltonian is in the universality class of the 3-state Potts model in 2D.

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