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Helicity modulus near a three-state Potts-like transition

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Abstract

By employing Monte Carlo simulations, both the helicity modulus and the heat capacity of a coupled classical XY model in two dimensions have been calculated. The model is based on the Hamiltonian proposed by Bruinsma and Aeppli [Phys. Rev. Lett. 48, 1625 (1982)]. For the first time, the model enables us to study the temperature dependence of the helicity modulus and obtain the associated critical exponent near a three-state Potts transition.

In 1973 Fisher, Barber, and Jasnow [1] introduced an elegant concept, namely the helicity modulus, to characterize the nature of a phase transition. The free energy difference between the antiperiodic (F_a) and the periodic (F_p) boundary conditions is proportional to the helicity modulus,

$$F_a - F_p = 2\pi^2\gamma(\beta)\,. \tag{1}$$

In a two-dimensional $N\times N$ square lattice, while a periodic boundary condition is applied in the y-direction, in calculating F_p (F_a), a periodic (antiperiodic) boundary condition is imposed along the x-direction. The coefficient $\gamma(\beta)$ is the helicity modulus, measuring the rigidity of the system under an applied phase twist as a function of temperature ($\beta = 1/T$). By utilizing thermodynamic relations, the derivative of the helicity modulus can be related to the internal energy difference between the antiperiodic boundary condition ($\langle U_a\rangle$) and the periodic boundary condition ($\langle U_p\rangle$) as follows:

$$d[\beta\gamma(\beta)]/d\beta = 2[\langle U_a\rangle - \langle U_p\rangle]/\pi^2\,. \tag{2}$$

By employing Monte Carlo simulations, it is rather straightforward in most of the cases to calculate the internal energy ($\langle U\rangle$) for a given model system. A clever argument allows one to relate γ to the superfluid density in liquid helium [1]. Thus the calculation

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of γ becomes an important method to characterize the XY model [2,3] and a related model [4] in two dimensions.

It is rather straightforward to impose an antiperiodic boundary condition for some model systems, e.g., the Ising model and calculate the corresponding helicity modulus. To the best of our knowledge, there exists no simple way to impose an antiperiodic boundary condition in the standard three-state Potts model. Thus the corresponding helicity modulus has not yet been calculated. While investigating a coupled classical XY model [5], we have discovered a unique way to calculate the helicity modulus near a three-state Potts transition in two dimensions.

To provide a plausible explanation for the X-ray [6] and calorimetric [7] results near the smecitc-A-hexatic-B transition in bulk liquid-crystal systems [8], Bruinsma and Aeppli [5] proposed a coupled XY Hamiltonian which can be simplified as follows:

$$H = -J_1 \sum_{\langle i,j \rangle} \cos(\psi_i - \psi_j) - J_2 \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j) - J_3 \sum_i \cos(\psi_i - 3\phi_i). \qquad (3)$$

In the light of our remarkable calorimetric and optical-reflectivity measurements from two-layer substrate-free liquid-crystal films (approximately 50Å in thickness) near the smectic-A-hexatic-B transition of 3(10)OBC compound [9], we have recently reconsidered this model and conducted extensive Monte Carlo simulations in two dimensions [10]. Here 3(10)OBC refers to n-propyl-4'-n-decyloxy-biphenyl-4-carboxylate. The simulation studies from this coupled XY model provide reasonable explanations for our experimental results. Here ψ and ϕ represent the phase factors of two proposed molecular orderings, namely, the bond-orientational order ($\Psi = |\Psi| \exp(6i\psi)$) of a system with six-fold symmetry and the herringbone order ($\Phi = |\Phi| \exp(2i\phi)$) [5]. The coefficients J_1 and J_2 account for the nearest-neighbor ($\langle i,j \rangle$) coupling strength for the variables ψ and ϕ, respectively. The coefficient J_3 denotes the coupling strength between these two types of order at the same lattice site. We are interested in situations in which Ψ and Φ are strongly coupled. Therefore, we choose $J_3 = 2.1$ (larger than both J_1 and J_2) for all of the simulations and discussions.

Let us consider the following simple scenario. Take $J_1 > J_2$ (say, $J_1 = 1.0$ and $J_2 = 0.3$). At sufficiently high temperatures ($T > J_3$), the system is in a completely disordered phase. For $J_3 > T > J_1$, the system remains disordered but the phase factors (ψ_i and ϕ_i) of the two order parameters become coupled through the J_3 term. In the temperature range $3J_2/2 < T < J_1$, bond-orientational order is established, and the ordered state corresponds to $\psi_i \approx \psi_j$ for all sites i and j. Without loss of generality, one can choose $\psi_i = 0$. Consequently, in this temperature range, there are three equivalent degenerate minima of the free energy at $\phi_i = 0$, $2\pi/3$, and $4\pi/3$. Further decreasing the temperature below $3J_2/2$ [1] causes the J_2 term to single out one of the three values for ϕ_i to be the lowest energy state leaving the other two degenerate states at a higher value. This is equivalent to the three-state Potts transition [11]. Thus, for $J_3 \gg J_1 > 3J_2/2$,

[1] In the three-state Potts transition, the transition temperature (T_c) is related to the energy difference between two energy states (ΔE), namely, $T_c = \Delta E/1.005$. In our model, $\Delta E = 3J_2/2$, thus $T_c = 3J_2/(2 \times 1.005)$.

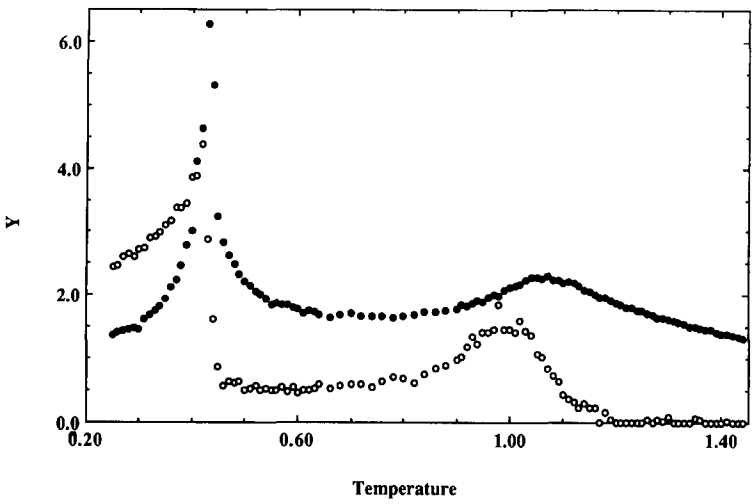

Fig. 1. Temperature dependence of the heat capacity (C_v, solid dots) and the energy difference (ΔU, open circles) for $J_1 = 1.0$, $J_2 = 0.3$, and $J_3 = 2.1$. The size of lattice is 30×30.

the Hamiltonian exhibits an XY transition at $T_{c_1} \approx J_1$ and a three-state Potts transition at $T_{c_2} \approx 3J_2/2$ (see footnote 1). A defect-mediated transition is followed by an order–disorder transition as a function of temperature.

Employing standard Monte Carlo simulations [12], we have carried out detailed calculations of heat capacity and helicity modulus on a 30×30 lattice for the case with $J_1 = 1.0$, $J_2 = 0.3$, and $J_3 = 2.1$. The calculated internal energies from simulations with periodic and antiperiodic boundary conditions enable us to obtain both the heat capacity (C_v) and $\frac{1}{2}d[\beta\gamma(\beta)]/d\beta$. The antiperiodic boundary condition has been imposed on both variables ψ and ϕ along one of the directions in the two-dimensional lattice. We have performed fairly long Monte Carlo calculations (500 000 Monte Carlo steps (MCS) per site). The results are shown in Fig. 1. In order to achieve a reasonable statistics in the values of $\frac{1}{2}d[\beta\gamma(\beta)]/d\beta$, a large number of MCS is necessary. The difference between $\langle U_p \rangle$ and $\langle U_a \rangle$ is generally less than 1%. The heat-capacity data yielded the expected results, a defect-mediated XY transition in the vicinity of $T \approx 1$ (a broad heat-capacity hump) followed by an order–disorder-type three-state Potts transition near $T = 0.43$ (a diverging heat-capacity anomaly) [2]. Finite-size scaling analyses on this heat-capacity anomaly yielded a heat-capacity critical exponent $\alpha = 0.36 \pm 0.05$ [10] which is in good agreement with the theoretical predicted value ($\alpha = 1/3$) for the three-state Potts transition in two dimensions [11].

Similar to the heat-capacity data, the energy difference [$\delta U = (\langle U_a \rangle - \langle U_p \rangle)/\pi^2$] gives us very distinct features associated with these two different types of phase transitions. At sufficiently high temperatures in the disordered state, the imposed antiperiodic boundary condition does not change the internal energy. Thus $\delta U = 0$ for $T > 1.16$. Near the two-dimensional XY transition, both the heat capacity and energy difference (δU) display

[2] We believe that finite values of J_1 and J_3 lead to the fact that $T_{c_2} < 3J_2/2$.

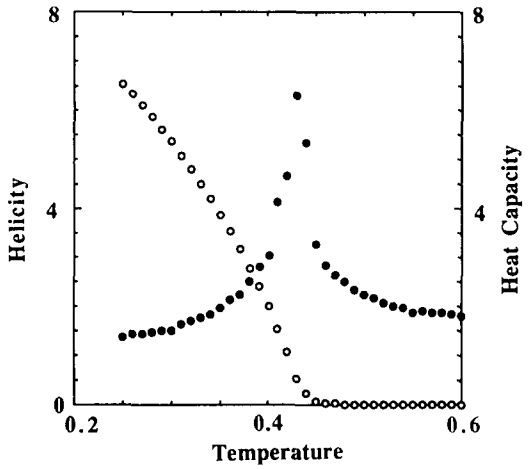

Fig. 2. Temperature variation of the heat capacity (solid dots) and the helicity modulus (open circles) in the vicinity of $T = 0.43$.

broad humps and their maxima are located near $T = 1.07$ and 0.98, respectively with the peak position of the energy difference closer to the reported defect-mediated transition temperature ($T_{KT} = 0.90$) [13]. In the vicinity of $T = 0.43$ (order of Φ), while the heat-capacity data display a symmetric peak, the energy difference shows a precipitous rise followed by a gradual decrease as temperature decreases. The onset of the sharp rise in energy difference coincides with the peak position of the heat capacity at $T = 0.434$. The energy difference remains a constant in the temperature range, $0.46 < T < 0.6$, which is due to the small temperature variation of helicity modulus of the Ψ-order. After subtracting this constant value, the helicity modulus (γ) can be calculated for $T < 0.6$, primarily, due to the order of Φ. Fig. 2 displays the temperature dependence of helicity modulus and heat capacity in the vicinity of $T \approx 0.43$. As predicted theoretically, near the order–disorder transition, $\gamma \to 0$ as $T \to T_c^-$ and $\gamma = 0$ for $T > T_c$. To the best of our knowledge, this is the first calculation of the helicity modulus for a model possessing the three-state Potts symmetry. Due to the unique properties of this two-dimensional coupled XY Hamiltonian, there exists no other known method to impose an antiperiodic boundary condition to the ordinary three-state Potts model. The helicity data can be well described by the following power law:

$$\gamma = \gamma_0 |(T_c - T)/T_c|^{\nu}. \tag{4}$$

The least-square fitting yields $\nu = 0.45 \pm 0.05$ and $T_c = 0.426$. The fitting results are displayed in Fig. 3 as a log–log plot of helicity modulus versus $(T_c - T)$.

In summary, a unique coupled classical XY model enables us, for the first time, to investigate the temperature variation of helicity modulus near a two-dimensional three-state Potts transition. The corresponding critical exponent is found to be 0.45.

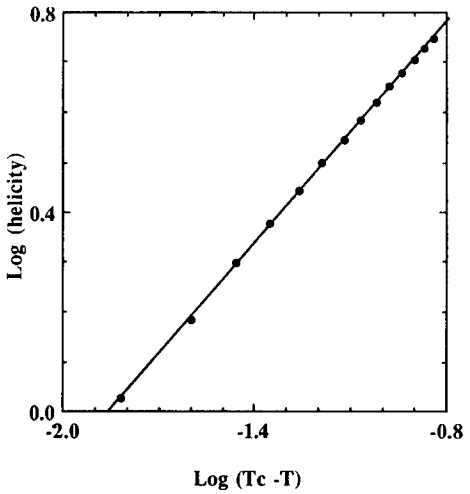

Fig. 3. Log–log plot of helicity modulus versus $(T_c - T)$.

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