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THE THREE-STATE CHIRAL CLOCK MODEL*

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We give a brief summary of our recent works on the three-state chiral clock model. In these works, we use improved effective field theories with clusters being strips, infinite in the chiral direction and finite in the non-chiral direction. Hence, effective-field transfer matrix methods can be employed in these studies. The effective fields are determined by the Gibbs-Bogoliubov free energy variational principle, leading to Weiss or Bethe approximations in different studies respectively. By systematic improvement of these approximations, i.e. widening the strips, these studies point to the conclusion that there is no Lifshitz point existing at finite non-zero chirality.

1. Introduction

The three-state chiral clock model was introduced independently by Ostlund[1] and Huse.[2] It is the simplest model with only nearest-neighbor interactions which exhibits spatially modulated phases. These spatially modulated phases occur diversely in physical systems.[3] The reduced Hamiltonian for this model on the two-dimensional square lattice is

$$-\beta H(\{n_{i,j}\},\Delta)=\sum_{i,j}\left[K_n\cos\frac{2\pi}{3}(n_{i,j}-n_{i,j+1}+\Delta)+K_t\cos\frac{2\pi}{3}(n_{i,j}-n_{i+1,j})\right], \tag{1}$$

where $\beta=1/k_{\mathrm{B}}T$. From the symmetry within this model, we can restrict ourselves to $0\le\Delta\le 1/2$ without losing generality. Ostlund used free-fermion analysis, which is valid for low temperature and Δ close to $1/2$, to show that there are incommensurate phases in this model. This fact makes the model interesting for the study of commensurate-incommensurate phase transitions and hence it has been the focus of considerable theoretical efforts.

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The model (1) has been studied by finite-size scaling methods,[4–8] Monte-Carlo simulation,[9] hierarchical lattice approximation,[10] Monte-Carlo renormalization group[11] and series expansion methods.[12–14] Important analytical predictions using domain-wall arguments and general topological ideas also have been presented.[15–17] In spite of all these efforts, several features remain controversial, for example, the existence of a Lifshitz point at $\Delta \neq 0$ in the phase diagram of this model. Haldane et al.,[15] Schulz,[16] and Von Gehlen and Rittenberg[7] argue against the idea of a Lifshitz point at $\Delta \neq 0$, while Howes,[12] Huse and Fisher,[17] Selke and Yeomans,[9] Duxbury et al.,[4] and Martins and Tsallis[10] are presenting arguments for it. Apart from this controversy over a qualitative feature, there are also uncertainties concerning the nature of various phase transitions in this model.

In order to shed more light on these problems, we used improved effective field theories with clusters to be taken as strips which are infinite in the chiral direction and finite in the non-chiral direction. This treatment is equivalent to separating the original two-dimensional square lattice into many identical decoupled strips with effective fields on their boundaries and treating interactions within them exactly. Effective-field transfer matrix methods[18] can be successfully used in such strip-related calculations.

Obviously, within an improved effective field theory, we have to pay serious attention to

i) how to put the effective fields on the boundary (so as to partially include the effects of the out-of-cluster part of original system) and

ii) how to relate the typical order parameters of the finite-strip system to ones of the original system.

These two aspects determine whether the approximate critical points obtained will be converging to the true ones and how fast the convergence will be. Currently, the most-commonly used effective field theories employ the Gibbs-Bogoliubov free energy variational principle, resulting in the Weiss and Bethe approximations. It has been found that even an infinite chain with effective fields (which are determined from free energy considerations) on the boundaries can qualitatively improve the simple effective field results.[19]

More interestingly, as advocated by Suzuki, it is possible to apply the coherent anomaly method (CAM)[18] to well-chosen sequences of effective field theories. By systematically treating wider and wider strips—i.e. more and more interactions are treated exactly—one obtains better and better approximations to the exact phase diagram of the original physical system and an excellent extrapolation to the exact results can be expected from these successive approximations, if the strips become wide enough.

This paper is organized as follows. In Section 2, we present our analysis of effective field theories based on the Gibbs-Bogoliubov free energy variational principle.[20] In Section 3, we first show how the approximate wavevector-dependent susceptibility is obtained in two series of effective field theories with either Weiss or

Bethe approximations, resulting in two series of Lifshitz point approximants. From these a new series is constructed showing that possibly no Lifshitz point exists at finite (non-zero) chirality.[21] A brief summary is given in Section 4.

2. Effective Field Theory from Free Energy Considerations

The approximate free energy F_{MF} is obtained by the use of the Gibbs-Bogoliubov inequality

$$F \leq F_{\text{MF}} = \min(F_0 + \langle H - H_0 \rangle), \tag{2}$$

where F is the exact free energy of the original system with H being the original Hamiltonian. H_0 is a trial Hamiltonian and F_0 is the exact free energy of the system defined by H_0. The average $\langle \cdots \rangle$ is carried out in the ensemble defined by H_0 and this convention will be used throughout this paper. For boundary spins, it is more convenient to introduce the vector notation

$$\mathbf{S}_{i,j} = \left(\cos \frac{2\pi}{3} n_{i,j}, \ \sin \frac{2\pi}{3} n_{i,j} \right). \tag{3}$$

H is given in Eq. (1) and H_0 is defined as follows:

$$\begin{aligned} -\beta H_0 = & \sum_{i,j} K_n \cos \frac{2\pi}{3}(n_{i,j} - n_{i,j+1} + \Delta) \\ & + \sum_{p=0}^{N_s-1} \sum_{k=pN}^{(p+1)N-2} \sum_{j} K_t \cos \frac{2\pi}{3}(n_{k,j} - n_{k+1,j}) \\ & + \sum_{p,p'=0}^{N_s-1} \sum_{k=0}^{L-1} K_t \boldsymbol{\eta}_k \cdot (\mathbf{S}_{pN-1,p'L+k} + \mathbf{S}_{pN,p'L+k}), \end{aligned} \tag{4}$$

where $0 \leq i \leq N_s N - 1$, $0 \leq j \leq N_s L - 1$, periodic boundary conditions are imposed on both directions, and $\beta = 1/k_{\text{B}}T$. The trial Hamiltonian H_0 consists of N_s independent strips of width N and length $N_s L$ with effective boundary fields $\{\boldsymbol{\eta}_j = (\eta_{j1}, \eta_{j2})\}$ having period L to replace the exact interactions between strips. To find a good approximation for the free energy, we use Eq. (2) to find the minimum conditions which $\{\boldsymbol{\eta}_j\}$ should satisfy. The necessary minimum conditions can be simplified as

$$\boldsymbol{\eta}_j = \langle \mathbf{S}_{0,j} \rangle \equiv \mathbf{m}_j. \tag{5}$$

The corresponding approximate free energy per site f_{MF} can be given as

$$f_{\text{MF}} = f_0 + \frac{K_t}{NL\beta} \sum_{j=0}^{L-1} (2\boldsymbol{\eta}_j \cdot \mathbf{m}_j - \mathbf{m}_j \cdot \mathbf{m}_j), \tag{6}$$

where f_0 is the free energy per site of the system defined by H_0 and can be calculated by the effective transfer matrix method.[18,20]

It is easy to see that the effective fields in our trial Hamiltonian are essentially the thermal averages of the strip boundary spins whose configuration can be used to characterize the related phase. Eqs. (5) can be solved by iteration methods and interested readers can consult our full paper[20] for technical details. From physical considerations, we may expect three types of solutions to Eqs. (5), i.e.

i) the disordered solution with ($\boldsymbol{\eta} = \mathbf{0}$),
ii) the ordered solution with ($\boldsymbol{\eta} \neq \mathbf{0}$) which can be obtained by setting $L = 1$ in Eqs. (5), and
iii) modulated solutions with unequal effective fields, i.e. $L > 1$.

The thermodynamically stable phase is the one that gives the absolute minimum free energy for all different solutions with all possible L. Hence, for $0 \leq \Delta \leq 1/2$, we can expect that the disordered solution gives the lowest approximate free energy for the disordered phase and the ordered solution for commensurate phase. In the modulated phase, one of the modulated solutions should give the lowest approximate free energy and the choice of solution may vary from point to point.

The numerical results are summarized as follows. We obtain $\Delta_L(1) \approx 0.3143$, $\Delta_L(2) \approx 0.2883$, $\Delta_L(3) \approx 0.2770$, $\Delta_L(4) \approx 0.2709$ for $K_n = K_t$ and $\Delta_L(1) \approx 0.2258$, $\Delta_L(2) \leq 0.2156$ for $K_n = 10K_t$, where the notation $\Delta_L(N)$ is used to denote the approximate Lifshitz point from the effective field theory for a strip of width N. Hence, we can safely claim that the Lifshitz point $\Delta_L(N)$ located by this approximation is systematically decreased when the width N becomes larger. The result for different ratios of K_n/K_t also coincides with our intuition that the larger K_n/K_t leads to faster convergence. Its possible explanation is discussed in our papers 20 and 21.

As reviewed by Wu,[22] simple mean-field theory predicts a first-order phase transition in the three-state Potts model, which is equivalent to the $\Delta = 0$ three-state chiral clock model. Our effective field theory with finite-width strip also predicts a first-order phase transition for $0 \leq \Delta < \frac{1}{2}$ which is characterized by a sudden change of spin profiles (described by the thermal average of the central-row spins in our effective field theory) due to the discontinuity of the effective fields when the system crosses the critical point. However, this artificial feature of the effective field theory can be overcome by systematically improving the effective field approximation.[20] When $N \to \infty$, these effective fields $\{\boldsymbol{\eta}_j\}$ (which are non-vanishing but have no direct physical meanings in the original problem) should give an infinitesimally small effect on the spin profiles (which should approach zero) and on the specific heat. Hence, the extrapolation of these effective field approximations would be able to give the correct nature of the phase transition, i.e. a continuous phase transition.

3. Effective Field Theory from Susceptibility Considerations

When the system changes from the disordered phase into the incommensurate phase as the temperature is lowered, the peak of the wavevector-dependent susceptibility also changes into a divergence. Hence, we only have to approximate the wavevector-dependent susceptibility in the disordered phase. We take the trial Hamiltonian of one strip in the disordered regime as follows:

$$-\beta H' = -\beta H + K_t h \sum_j \sum_{i=1}^{N} \cos\left(\frac{2\pi}{3} n_{i,j} - jq\right) + K_t \eta \sum_j \left[\cos\left(\frac{2\pi}{3} n_{1,j} - jq\right) + \cos\left(\frac{2\pi}{3} n_{N,j} - jq\right)\right] \qquad (7)$$

where H is a restriction of the exact Hamiltonian taking precisely all its terms within the strip, and where η denotes the amplitude of the modulated effective boundary fields, h the amplitude of the auxiliary external bulk fields, and q the wavevector of the external field and modulated effective boundary fields along the chiral direction. (In the disordered phase and with a weak field condition, we can expect the response of the spin average to be characterized by the same wavevector q because of the symmetry of H and $H'|_{\eta=0,h=0}$ under translation. When we introduce our Weiss and Bethe effective-field approximations, the effective fields should be characterized by this wavevector q as well.) Meanwhile, because most of the previous understanding has come from the study of the Hamiltonian limit, which corresponds to either $K_n/K_t \to 0$ or $K_n/K_t \to \infty$,[6–8,12,14] it is kind of natural for us to keep K_n/K_t general.

Since in all calculations below we take ensemble averages based on H' and often with both η and h being zero, we use $\langle \cdots \rangle$ to denote the statistical average with ensemble based on H' and $\langle \cdots \rangle_0$ to denote $\langle \cdots \rangle|_{\eta=0,h=0}$. For convenience, we also define quantities Q_c and $Q_{\partial,j}$ as follows:

$$Q_\mathrm{c} = \begin{cases} \exp\left(\mathrm{i}\frac{2\pi}{3} n_{m+1,0}\right), & \text{if } N = 2m+1, \\ \frac{1}{2}\left[\exp\left(\mathrm{i}\frac{2\pi}{3} n_{m,0}\right) + \exp\left(\mathrm{i}\frac{2\pi}{3} n_{m+1,0}\right)\right], & \text{if } N = 2m, \end{cases} \qquad (8)$$

$$Q_{\partial,j} = \frac{1}{2}\left[\exp\left(\mathrm{i}\frac{2\pi}{3} n_{1,j}\right) + \exp\left(\mathrm{i}\frac{2\pi}{3} n_{N,j}\right)\right]. \qquad (9)$$

These quantities have a direct interpretation: Q_c is the spin in the middle row of the 0-th column, if the number of rows N is odd. If the number of rows N is even, we take the average over the two middle rows. $Q_{\partial,j}$ is the average of the two spins in the boundary rows $i = 1$ and $i = N$ of the j-th column ($j = -\infty, \cdots, \infty$).

We put the self-consistency conditions

$$\langle Q_\mathrm{c} \rangle = \eta \qquad \text{for Weiss approximation,} \qquad (10)$$

$$\langle Q_\mathrm{c} \rangle = \langle Q_{\partial,0} \rangle \qquad \text{for Bethe approximation.} \qquad (11)$$

The wavevector-dependent susceptibility has a peak located at q_m which gives an approximation to the characteristic wavevector of the corresponding correlation function. By some tedious calculation, the critical point that demarcates the paramagnetic-incommensurate phase transition can be located from

$$\min_q \Big(1 - K_{\rm c} \sum_j \langle Q_{\rm c} Q^*_{\partial,j}\rangle_0 \exp({\rm i}jq)\Big) = 0 \quad \text{for Weiss approximation,} \tag{12}$$

$$\min_q \sum_j \Big(\langle Q_{\partial,0} Q^*_{\partial,j}\rangle_0 - \langle Q_{\rm c} Q^*_{\partial,j}\rangle_0\Big) \exp({\rm i}jq) = 0 \quad \text{for Bethe approximation,} \tag{13}$$

where the minimum condition is over all q. The corresponding $q_{\rm m}$ will give an approximation to the wavevector $q_{\rm c}$, characteristic of the correlation function at the phase transition point. Here and in the following we write $K \equiv K_t$ and $K_{\rm c} \equiv K_{t{\rm c}}$, its value at the critical point separating the disordered and modulated phases. K_n and K_t vary proportionally.

In both approximations, the susceptibility near $K_{\rm c}$ ($K < K_{\rm c}$) can be presented in the form

$$\chi = \overline{\chi}/(\frac{K_{\rm c}}{K} - 1). \tag{14}$$

where $\overline{\chi}$ is the coherent anomaly coefficient and has been worked out for both cases.[21]

From the above, we can obtain two series of approximations. However, both series are short and hence difficult to extrapolate. To circumvent this problem, we construct a new extrapolation method as follows.

If there exist two sequences $\{a(n)\}$ and $\{b(n)\}$, which satisfy

i) $\lim_{n\to\infty} a(n) = c$, $\lim_{n\to\infty} b(n) = c$ and $a(n)$, $b(n) \neq c$ for any n,
ii) $\lim_{n\to\infty} \big(a(n+\delta n) - a(n)\big)/\big(b(n+\delta n) - b(n)\big)$ exists and is not 1,

it is possible to construct a third sequence $\{c(n)\}$ with $\lim_{n\to\infty} c(n) = c$ by

$$c(n) = \frac{a(n+\delta n)b(n) - a(n)b(n+\delta n)}{a(n+\delta n) - a(n) - b(n+\delta n) + b(n)}. \tag{15}$$

Under certain conditions, we can expect that the sequence $\{c(n)\}$ will converge faster than either $\{a(n)\}$ or $\{b(n)\}$.

We find that this new construction works very well for the square lattice Ising model and Potts cases with various ratios of K_n/K_t.[21] Here we only present the Potts model results, i.e. the case with $\Delta = 0$ and $K_n = K_t$, in Table 1, where

Table 1. Table of $T_{\rm b}$, $T_{\rm w}$ and $T_{\rm n}$.

N	3	4	5	6	7
$T_{\rm b}$	1.56208	1.55004	1.54073	1.53471	1.52965
$T_{\rm w}$	1.65702	1.62624	1.60251	1.58794	1.57563
$T_{\rm n}$	1.5010	1.4992	1.4974		

critical temperature $T_{\rm b}(N)$ is obtained by Bethe approximation, $T_{\rm w}(N)$ by Weiss approximation, N being the width of the finite strip, and $T_{\rm n}(N)$ is obtained by Eq. (15) with $\delta N = 2$. The exact value for $N = \infty$ is $T^*_{\rm c} = 1.4925$. We clearly see good convergence of series $\{T_{\rm n}(N)\}$. We have also used this construction to find the range of critical temperatures for $\Delta \neq 0$.[21] More interestingly, we use this construction to find the characterizing wavevector along the critical line.

As is well-known,[4] we should be able to get phase transition information through the analysis of the wavevector at the phase transition point. If a Lifshitz point Δ_L exists at finite chirality, the characterizing wavevector along the critical line should vanish for $\Delta \leq \Delta_L$. Although we are not sure how this Lifshitz point Δ_L will depend on K_n/K_t, old works[4,11,12] indicate that there is no big dependence of Δ_L on K_n/K_t.

Two cases with $K_n = 10K_t$ and $K_n = 100K_t$ at $\Delta = 0.05$ have been studied. The results for the two cases are similar, so we only present in Table 2 the results for the case with $\Delta = 0.05$ and $K_n = 100K_t$, where the reduced critical wavevector

Table 2. Table of $\hat{q}_{\rm b}$, $\hat{q}_{\rm w}$ and $\hat{q}_{\rm n}$.

N	3	4	5	6	7
$\hat{q}_{\rm w}$	0.0463680	0.0402710	0.0353594	0.0320544	0.0291924
$\hat{q}_{\rm b}$	0.0362354	0.0314054	0.0276127	0.0250293	0.0228355
$\hat{q}_{\rm n}$	-0.00038	0.00069	0.00099		

is defined by $\hat{q} = 3q/(2\pi\Delta)$. Here, $\hat{q}_{\rm b}(N)$ is obtained by Bethe approximation and $\hat{q}_{\rm w}(N)$ by Weiss approximation, where N is the width of the finite strip, and $\hat{q}_{\rm c}(N)$ is obtained by Eq. (15) with $\delta N = 2$. These calculations for the wavevector need an accuracy of 10^{-8} for q. Higher accuracy will be needed for smaller Δ and our numerical values would not have been reliable enough then.

Although we only have three members in this new sequence $\{\hat{q}_{\rm n}(N)\}$ and we cannot make a very conclusive case, it looks very tempting to say that this sequence will converge to the true $\hat{q}_{\rm c}$ from below. Compared with previous results for Δ_L to be around 0.25 to 0.40,[4,11,12] we have $\Delta_L < 0.05$. Hence, we may conclude that even for a very small Δ the wavevector at the transition point is non-zero. This means that the transition should be from the paramagnetic to the incommensurate phase and that possibly no Lifshitz point exists at finite chirality at all.

4. Summary

In the above sections, we have used two different methods to approach the problem whether a Lifshitz point exists in the two-dimensional classical three-state chiral clock model at finite non-zero chirality. The first method gives more information about the general phase diagram, whereas the second method seems to more reliably determine the boundary of the disordered phase. However, both extrapolations together consistently indicate that most likely no Lifshitz point exists in this model at finite non-zero chirality. A study of somewhat wider strips on more powerful computers may take away all remaining doubt.

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