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1984 J. Phys. A: Math. Gen. 17 L179

(http://iopscience.iop.org/0305-4470/17/4/005)

J. Phys. A: Math. Gen. 17 (1984) L179–L184. Printed in Great Britain

LETTER TO THE EDITOR

Wavevector scaling and the phase diagram of the chiral clock model

Phillip M Duxbury, Julia Yeomans and Paul D Beale
Department of Theoretical Physics, 1 Keble Road, Oxford, OX1 3NP, UK

Received 7 December 1983

Abstract. We use a finite-size renormalisation group to study the phase diagram of a spin model which exhibits modulated order, the two-dimensional, three-state, chiral clock model. In addition to the usual scaling of the correlation length, wavevector scaling is shown to provide useful information about the position of the Lifshitz point, and about the position and nature of the commensurate to incommensurate and commensurate to paramagnetic phase transitions.

Monolayers of atomic or molecular adsorbates on certain substrates, for example krypton on graphite (Chinn and Fain 1977), may exhibit a floating phase for certain ranges of coverage and temperature (for recent reviews see Selke *et al* 1983, Bak 1982). In the floating (or incommensurate) phase, the pair correlation function decays algebraically, and the characteristic wavevector of these correlations varies continuously with coverage and temperature (see for example Bak 1982, Villain 1980). In general, the floating phase lies between a low-temperature ordered (or commensurate) phase with constant correlations and a high-temperature paramagnetic phase in which the correlation function decays exponentially.

Recently, the finite-size renormalisation group (see Nightingale 1982 for a review) has been applied to two models which may exhibit a floating phase (Kinzel 1983, Shaub and Domany 1983). The results have not proved easy to interpret. Therefore in this letter we use this technique to study the two-dimensional, three-state chiral clock model, for which the existence of a floating phase is well established (see for example Ostlund 1981, Selke and Yeomans 1982).

In particular, we emphasise that not only the usual correlation length scaling, but also the scaling properties of the wavevector give valuable information about the model's critical behaviour. By using these methods of analysis, the phase diagram is determined and the position of the Lifshitz point is established. We comment on the scaling behaviour of the correlation length and wavevector and their associated exponents on the various phase boundaries.

The two-dimensional chiral clock model (Ostlund 1981, Huse 1981) is defined by the Hamiltonian

$$H = -J_0 \sum_{i,j} \{\cos[\tfrac{2}{3}\pi(n_{i,j} - n_{i,j+1})] + \cos[\tfrac{2}{3}\pi(n_{i,j} - n_{i+1,j+\Delta})]\} \tag{1}$$

where the coordinates (i, j) define a point on a square lattice. The spin variables $n_{i,j}$ take the values $0, 1, 2$. J_0 and Δ are interaction parameters and the sum is taken over nearest-neighbour sites. As Δ is increased, the competition between ferromagnetic and chiral order along the i direction increases. At finite temperatures this results in the occurrence of a phase with a non-zero wavevector, the floating phase. The phase diagram which results from our finite-size scaling analysis is shown in figure 1 for $0.0 \leqslant \Delta \leqslant 0.5$. Results for other values of Δ follow from symmetry arguments (Ostlund 1981).

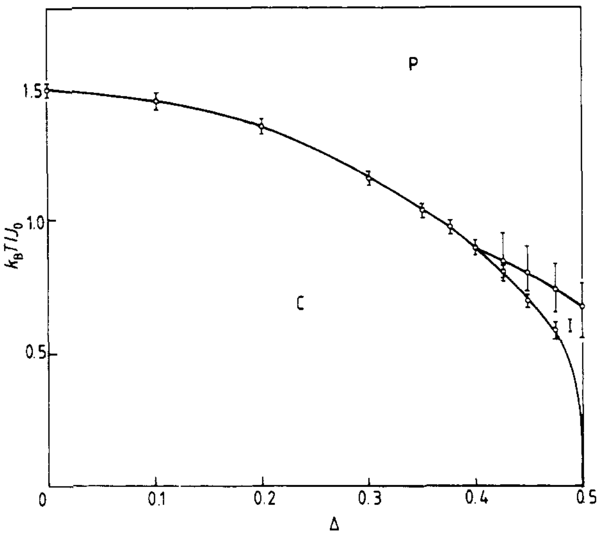

Figure 1. The phase diagram of the two-dimensional, three-state, chiral clock model, found from finite-size renormalisation group calculations. C, I and P denote the commensurate, incommensurate and paramagnetic phases respectively.

The Hamiltonian (1) has been the focus of considerable theoretical effort. Ostlund (1981) established the existence of the floating phase using free fermion analysis. Monte Carlo calculations (Selke and Yeomans 1982) suggest a Lifshitz point at $\Delta_L \simeq 0.40$–0.425, and the Monte Carlo renormalisation group has been applied at $\Delta = 0.50$ (Houlrik *et al* 1983). Hamiltonian series have been analysed by Howes (1982) and Centen *et al* (1982), and a Hamiltonian mass gap scaling analysis has been performed by Von Gehlen and Rittenberg (1983). Important analytical predictions using domain-wall arguments and general topological ideas have been presented by Garel and Pfeuty (1976), Pokrovsky and Talapov (1979), Schulz (1980), Huse *et al* (1983), Huse and Fisher (1982) and Haldane *et al* (1983).

Despite a broad agreement with the phase diagram of figure 1, several features remain controversial. In particular Haldane *et al* (1983), Schulz (1983) and Von Gehlen and Rittenberg (1983) suggest that the Lifshitz point occurs at $\Delta_L = 0.0$ while the other authors quoted above predict $\Delta_L \neq 0.0$. In addition Huse and Fisher (1982) have recently suggested that the critical boundary between $\Delta = 0.0$ and Δ_L should be in a new chiral universality class with

$$\delta q \times \xi \simeq \text{constant} \tag{2}$$

where $\delta q = q - q_0$, q_0 being the characteristic wavevector of the commensurate phase and q the wavevector of the system near the phase boundary just inside the paramagnetic phase. ξ is the correlation length. No new behaviour of the critical exponents along this line was found by Selke and Yeomans (1982) in their Monte Carlo study.

The recursion equations for the finite-size renormalisation group follow from assuming that the thermodynamic properties of an infinite strip of width N obey finite-size scaling exactly (Nightingale 1982). The fixed point is estimated from the solutions of

$$X_N(T_N^*) = X_{N-1}(T_N^*)[(N-1)/N]^\theta, \tag{3}$$

where in the case of correlation length scaling $X_N = 1/\xi_N$, and for wavevector scaling $X_N = \delta q_N$. θ is an exponent which allows for anisotropic scaling (Kinzel and Yeomans 1981, Barber 1983) and T_N^* is the estimate of the fixed point which in the limit $N \to \infty$ is expected to converge to the true critical temperature. Unbiased estimates of T_N^* and θ are found from the behaviour of the function (Shaub and Domany 1983)

$$Y_N(X_N) = \ln(X_{N-1}/X_N)/\ln[N/(N-1)]. \tag{4}$$

The critical exponents ν and $\bar{\beta}$, which characterise the correlation length and wavevector critical singularities respectively, are estimated from

$$\lambda = \frac{\ln\{(\partial X_N/\partial T)/(\partial X_{N-1}/\partial T)] \times [N/(N-1)]\}}{\ln[N/(N-1)]} \tag{5}$$

where $\lambda = 1/\nu$ for correlation length scaling and $\lambda = 1/\bar{\beta}$ for wavevector scaling.

The numerical procedure is to find the largest three eigenvalues of the transfer matrix of the chiral clock model using a direct iteration technique. The infinite direction of the strip is taken to lie along the direction of modulation to avoid discretisation of the wavevectors. The correlation length and wavevector are then given by

$$\xi^{-1} = \ln(\lambda_0/|\lambda_1|) \tag{6}$$

and

$$\delta q = \tan^{-1}(\mathrm{Im}(\lambda_1)/\mathrm{Re}(\lambda_1)) - q_0 \tag{7}$$

where λ_0 and λ_1 are the largest and the second largest eigenvalues of the transfer matrix. We have performed these calculations on strips of width up to eight sites using periodic boundary conditions.

The results for $Y_N(\delta q)$ and $Y_N(\xi)$ for $\Delta = 0.30$ are shown in figures 2(a) and 2(b) respectively. The wavevector and correlation length scale at the same temperature, indicating that $\delta q \to 0$ and $\xi \to \infty$ at the same temperature. This strongly suggests that

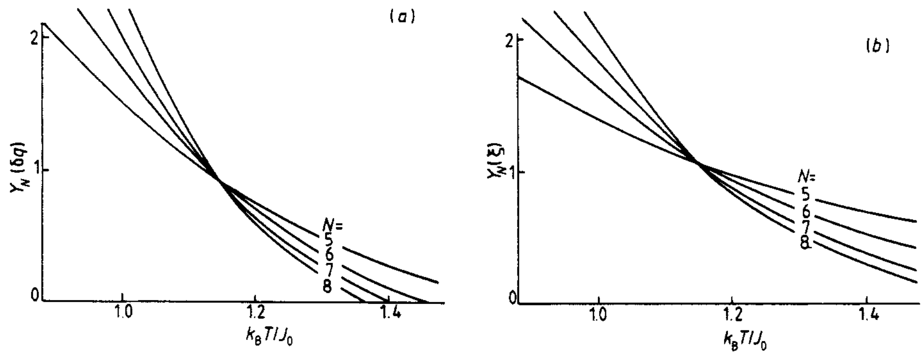

Figure 2. (a) The function $Y_N(\delta q) = \ln(\delta q_{N-1}/\delta q_N)/\ln[N/(N-1)]$ at $\Delta = 0.30$ for $N = 5, 6, 7, 8$. (b) The function $Y_N(\xi) = \ln(\xi_N/\xi_{N-1})/\ln[N/(N-1)]$ at $\Delta = 0.30$ for $N = 5, 6, 7, 8$

at this value of Δ there is a direct transition from a modulated paramagnetic phase to a normal ordered phase with constant modulation. From figure 2 we also note that the two anisotropy exponents are $\theta(\xi)\approx 1$ and $\theta(\delta q)\approx 1$ and hence $\xi\approx N$ and $\delta q\approx 1/N$. This is consistent with the chiral conjecture of Huse and Fisher (1982) given in (2).

The results for $Y_N(\delta q)$ and $Y_N(\xi)$ at $\Delta=0.45$, shown in figures 3(*a*) and 3(*b*), present a different picture. The correlation lengths scale at a higher temperature than that at which the wavevector vanishes. The point at which the correlation length scales then indicates a transition from a modulated paramagnetic phase to an ordered phase with non-zero wavevector. This, combined with the smooth (as opposed to steplike) behaviour of the finite-strip wavevectors inside this phase, suggest that it is a floating phase. The temperature at which the wavevectors vanish determines the transition to a normal ordered phase (the commensurate to incommensurate transition). It is worth noting that the correlation lengths (figure 3(*b*)) do not obviously scale with the size of the system at the commensurate to incommensurate phase boundary. A similar behaviour of $Y_N(\xi)$ found for a different model (Kinzel 1983) has been interpreted as a single anisotropic phase transition from the commensurate to the paramagnetic phase. Our previous knowledge of the phase diagram of the chiral clock model suggests that this is unlikely and that the behaviour of $Y_N(\xi)$ at the commensurate to incommensurate phase boundary should be attributed to finite size effects.

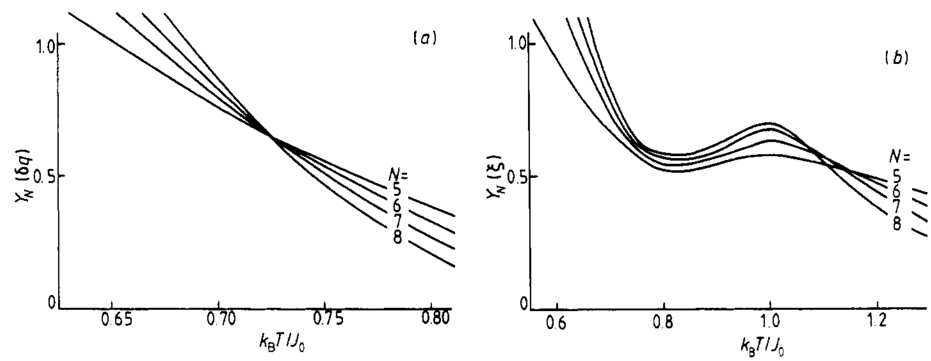

Figure 3. (*a*) The function $Y_N(\delta q)=\ln(\delta q_{N-1}/\delta q_N)/\ln[N/(N-1)]$ at $\Delta=0.45$ for $N=$ 5, 6, 7, 8. (*b*) The function $Y_N(\xi)=\ln(\xi_N/\xi_{N-1})/\ln[N/(N-1)]$ at $\Delta=0.45$ for $N=$ 5, 6, 7, 8.

We have carried out a similar analysis for a range of values of Δ between 0.00 and 0.50 giving the phase diagram shown in figure 1. In this figure, the commensurate to incommensurate phase boundary was located by wavevector scaling and the incommensurate to paramagnetic phase was located by correlation length scaling. A single commensurate to paramagnetic transition is implied when the correlation length and wavevector scale at the same temperature. The large error bars on the incommensurate to paramagnetic phase boundary reflect the slow convergence of the finite-size estimates along this line. The Lifshitz point was located at $\Delta_L=0.40\pm 0.03$ in good agreement with Selke and Yeomans (1982). We now discuss our results for the critical exponents calculated from evaluating (5) at the scaling points given by (4).

The anisotropy exponents $\theta(\delta q)$ and $\theta(\xi)$ are near 1 for $\Delta<\Delta_L$. For $\Delta=\Delta_L$ there is a sharp drop in $\theta(\xi)$ reflecting the anisotropic nature of the correlation length scaling at the Lifshitz point (Hornreich *et al* 1978). For $\Delta>\Delta_L$, $\theta(\xi)$ increases again and is not inconsistent with a return to isotropic scaling, although the convergence is slow. $\theta(\delta q)$ also becomes anisotropic near $\Delta = \Delta_L$ and decreases further as $\Delta \to 0.50$.

The correlation length exponent ν is found to equal 0.85 ± 0.05 (cf the Potts value $\nu = 0.833\ldots$) below the Lifshitz point, and hence gives no evidence for a change in universality class along this boundary. For $\Delta > \Delta_L$, ν becomes small, reflecting the desire of the scaled correlation lengths to become coincident as is expected for a massless phase.

The wavevector exponent $\bar{\beta}$ is equal to 0.80 ± 0.10 for $\Delta < \Delta_L$, which is consistent with the chiral scaling conjecture (2) (equation (2) would imply $\bar{\beta} = 0.833\ldots$). For $\Delta > \Delta_L$, $\bar{\beta}$ is near 1.0 but is poorly converged. Despite this poor convergence, the value of $\bar{\beta}$ found in this model for the commensurate to incommensurate transition, appears to be larger than the value 0.50 calculated by Pokrovsky and Talapov (1979) using domain-wall arguments.

Before concluding, it is worth making some comments about the techniques used in this letter. The combination of wavevector scaling and correlation length scaling has been used to locate a floating phase and a commensurate to paramagnetic phase transition. We note the further possibility that if the wavevector vanishes before the correlation length diverges (as the temperature is lowered), then the vanishing of the wavevector signals a disorder line. We have performed this analysis at $\kappa = 0.25$ in the two-dimensional ANNNI model and have found the disorder line to be at a temperature $T = 1.85 \pm 0.05$ (Duxbury *et al* 1984). We also note that while the commensurate to incommensurate to paramagnetic phase boundary are well located by our analysis, the floating to paramagnetic phase boundary is poorly located. This is not only due to the inherent difficulty in scaling correlation lengths at such transitions, but also to the proximity of the commensurate to incommensurate phase boundary. It is therefore necessary to refine the methods used in locating floating to paramagnetic phase transitions in two-dimensional systems of the sort studied here. Work in this direction, along with details of the analysis of the two-dimensional three-state chiral clock and the two-dimensional ANNNI model will be published elsewhere (Duxbury *et al* 1984).

To conclude, we have used the finite-size renormalisation group to study a rather simple model that exhibits modulated order, the two-dimensional three-state chiral clock model. It has been shown that wavevector scaling, in addition to correlation length scaling, provides an important tool in the study of such systems.

One of the authors (PMD) thanks Wolfgang Kinzel for several illuminating discussions, during which the idea of using wavevector scaling crystallised. Two of us (PMD and PDB) wish to thank the SERC for the award of postdoctoral fellowships.

References

Bak P 1982 *Rep. Prog. Phys.* **45** 587
Barber M N 1983 in *Phase Transitions and Critical Phenomena* ed C Domb and J Lebowitz vol 7, to be published
Centen P, Rittenberg V and Marcu M 1982 *Nucl. Phys.* B **205** 585
Chinn M D and Fain SC Jr 1977 *Phys. Rev. Lett.* **39** 146
Duxbury P M, Yeomans J M and Beale P D 1984 in preparation
Garel J and Pfeuty P 1976 *J. Phys. C: Solid State Phys.* **9** L245
Haldane F D M, Bak P and Bohr T 1983 *Phys. Rev.* B **28** 2743
Hornreich R M, Luban M and Shtrikman S 1978 *Phys. Rev. Lett.* **35** 1678

Houlrik J M, Knak Jensen S J and Bak P 1983 *Phys. Rev.* B **28** 2883
Howes S F 1982 *Phys. Rev.* B **27** 1762
Huse D A 1981 *Phys. Rev.* B **24** 5180
Huse D A and Fisher M E 1982 *Phys. Rev. Lett.* **49** 793
Huse D A, Szpilka A M and Fisher M E 1983 *Preprint*
Kinzel W 1983 *Phys. Rev. Lett.* **51** 996
Kinzel W and Yeomans J M 1981 *J. Phys. A: Math. Gen.* **14** L163
Nightingale M P 1982 *J. Appl. Phys.* **53** 7927
Ostlund S 1981 *Phys. Rev.* B **24** 398
Pokrovsky V L and Talapov A L 1979 *Phys. Rev. Lett.* **42** 65
Selke W and Yeomans J M 1982 *Z. Phys.* B **46** 311
Selke W, Binder K and Kinzel W 1983 *Surface Sci.* **125** 74
Shaub B and Domany E 1983 *Phys. Rev.* B **28** 2897
Schulz H J 1980 *Phys. Rev.* B **22** 5274
—— 1983 *Phys. Rev.* B **28** 2746
Von Gehlen G and Rittenberg V 1983 *Preprint*
Villain J 1980 in *Ordering in strongly fluctuating condensed matter* ed T Riste (New York: Plenum)