LETTER TO THE EDITOR

Critical behaviour of modulated phases in the chiral clock model

M Siegert and H U Everts

Institut für Theoretische Physik, Universität Hannover, Appelstrasse 2, 3000 Hannover, Federal Republic of Germany

Abstract. The critical properties of the modulated phases in the uniaxial chiral clock model in three dimensions are investigated by a renormalisation group (RG) calculation and a Monte Carlo study. From the RG calculation it follows that the model belongs to the XY universality class, i.e. that it scales isotropically at criticality in spite of its spatial anisotropy. Using the scaling properties of the fourth cumulant of the order parameter we devise a method by which one can discriminate between isotropic and anisotropic scaling quite generally in a numerical simulation. Our numerical results confirm the predictions of the RG calculation.

In attempts to explain modulated phases in solids, two models have been studied extensively: the anisotropic next-nearest-neighbour Ising (ANNNI) model (Elliot 1961) and the three-state chiral clock (CC3) model (Ostlund 1981, Huse 1981). While at low temperatures the basic features of these models are well understood (Selke and Duxbury 1984, Fisher and Szpilka 1987, Szpilka and Fisher 1987, Siegert and Everts 1987) the situation is less clear near the critical temperature. In particular, for the CC3 model it is not known to which universality class the phase transition between modulated phases and the disordered state belongs. Figure 1 displays schematically the phase diagram of the CC3 model. Because of the spatial anisotropy of the interaction it is not clear *a priori* that the model scales isotropically at the critical temperature, i.e. it is not inconceivable that the correlation lengths $\xi_\parallel$ and $\xi_\perp$, respectively parallel and
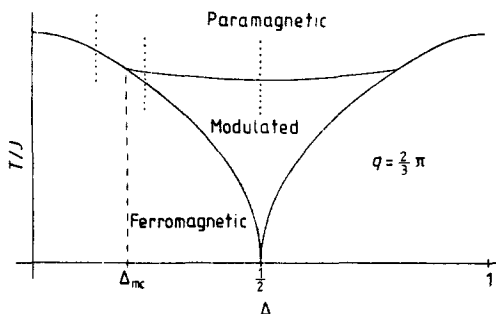

Figure 1. Schematic phase diagram of the CC3 model. The phase transition between the paramagnetic and the modulated phases is of second order; all other transition curves correspond to first-order transitions. The dotted lines indicate the Δ values where Monte Carlo simulations were carried out.

perpendicular to the axial direction of the model, diverge with different exponents: $\xi_\parallel \sim t^{-\nu_\parallel}$, $\xi_\perp \sim t^{-\nu_\perp}$. In this article we present a renormalisation group calculation and a Monte Carlo study of the critical properties of the CC3 model in three dimensions.

The three-state chiral clock model on a d-dimensional layered lattice is defined by the Hamiltonian

$$H = -J_0 \sum_\alpha \sum_{\langle i,j \rangle} S_{i\alpha} S_{j\alpha} - J \sum_\alpha \sum_i S_{i\alpha} R(\Delta) S_{i\alpha+1} \qquad J_0, J > 0. \tag{1}$$

The subscript α labels the $(d-1)$-dimensional layers and i, j count the lattice sites within a layer, $\langle i,j \rangle$ denotes a nearest-neighbour pair. The allowed spin states are $S_{i\alpha} = (\cos \frac{2}{3}\pi n_{i\alpha}, \sin \frac{2}{3}\pi n_{i\alpha})$, $n_{i\alpha} = 0, 1, 2$. The matrix $\hat{R}(\Delta)$ rotates the spins through the angle $\frac{2}{3}\pi\Delta$. The phase diagram of the CC3 model is symmetric to $\Delta = \frac{1}{2}$; the corresponding phases are related by the symmetry operation

$$\Delta \to 1 - \Delta \Rightarrow q \to \tfrac{2}{3}\pi - q \tag{2}$$

where q is the wavenumber of the modulation. Within our numerical simulations we always set $J_0 = J$. To construct a Ginzburg-Landau-Wilson (GLW) functional we start from a generalisation of the mean-field free energy:

$$-\beta F = \frac{1}{2} \sum_{\langle r,r' \rangle} S(r) \hat{K}(r' - r) S(r') - \sum_r V(S(r)). \tag{3}$$

The first term resembles the Hamiltonian (1) and the potential $V(S(r))$ is an expansion of the mean-field entropy (Siegert and Everts 1985):

$$V(S(r)) = S^2(r) - \tfrac{1}{3}S_1(r)(S_1^2(r) - 3S_2^2(r)) + \tfrac{1}{2}(S^2(r))^2 + \ldots \tag{4}$$

the third-order term reflects the three-state Potts symmetry of the model. The steps leading from equation (3) to the GLW functional are the same as in the Landau expansion of the mean-field free energy (Siegert and Everts 1985). We introduce the complex order parameter $\mu(r) = S_1(r) + iS_2(r)$ and adopt the ansatz $\mu(r) = A(r)\exp(iq_0 r_\parallel) + B(r)\exp(-2iq_0 r_\parallel)$. Here, q_0 denotes the wavenumber of the modulated phase, $r_\parallel$ is the axial component of the position vector r and the amplitudes $A(r)$, $B(r)$ are assumed to be slowly varying functions. In mean-field theory this ansatz suffices to calculate the free energy correctly up to sixth order in $A(B = \mathcal{O}(A^2))$, thus no higher harmonics are needed. The second harmonic with amplitude B must be included, since it contributes in fourth order. Neglecting rapidly oscillating terms such as $A^3(r)\exp(3iq_0 r_\parallel)$, taking the continuum limit and changing to the wavenumber representation,

$$A(r) = \int \frac{d^d q}{(2\pi)^d} A(q) \exp(iq \cdot r),$$

etc, we arrive at the GLW Lagrangian

$$\begin{aligned}
\mathcal{L} = \int \frac{d^d q}{(2\pi)^d} &\{[\tfrac{1}{2}K_0(2(d-1) - q_\perp^2) + K \cos(\tfrac{2}{3}\pi\Delta - q_0)(1 - \tfrac{1}{2}q_\parallel^2) - 1]A(q)A^*(-q) \\
&+ [\tfrac{1}{2}K_0(2(d-1) - q_\perp^2) + K \cos(\tfrac{2}{3}\pi\Delta + 2q_0)(1 - \tfrac{1}{2}q_\parallel^2) - 1]B(q)B^*(-q)\} \\
&+ \frac{1}{2} \int \frac{d^d q\, d^d q'}{(2\pi)^{2d}} \{A(q)A(q')B(-q-q') + \text{cc}\} \\
&- \frac{1}{2} \int \frac{d^d q\, d^d q'\, d^d q''}{(2\pi)^{3d}} \{A(q)A(q')A^*(q'')A^*(-q-q'-q'') \\
&+ 4A(q)A^*(q')B(q'')B^*(-q-q'-q'')
\end{aligned}$$

$$+ B(q)B(q')B^*(q'')B^*(-q-q'-q'')\}$$

$$K_0 = J_0/T \qquad K = J/T \qquad q = (q_\perp, q_\parallel).$$

$A^*(q)$, $B^*(q)$ are the Fourier transforms of the complex conjugates of $A(r)$, $B(r)$. Introducing the real fields $\sigma(r)$, $\tau(r)$, $A(r) = \sigma_1(r) + i\sigma_2(r)$, $B(r) = \tau_1(r) + i\tau_2(r)$ we obtain the following generalised GLW Lagrangian:

$$\mathcal{L} = -\int \frac{d^d q}{(2\pi)^d} \{\tfrac{1}{2}(r_\sigma + q_\perp^2 + \kappa_\sigma q_\parallel^2)\sigma(q)\sigma(-q) + \tfrac{1}{2}[r_\tau + \eta(q_\perp^2 + \kappa_\tau q_\parallel^2)]\tau(q)\tau(-q)\}$$

$$+ p\int \frac{d^d q\, d^d q'}{(2\pi)^{2d}} \{(\sigma_1(q)\sigma_1(q') - \sigma_2(q)\sigma_2(q'))\tau_1(-q-q')$$

$$- 2\sigma_1(q)\sigma_2(q')\tau_2(-q-q')\}$$

$$- \int \frac{d^d q\, d^d q'\, d^d q''}{(2\pi)^{3d}} \{\tfrac{1}{2}u_1(\sigma(q)\sigma(q'))(\sigma(q'')\sigma(-q-q'-q''))$$

$$+ u_2(\sigma(q)\sigma(q'))(\tau(q'')\tau(-q-q'-q''))$$

$$+ \tfrac{1}{2}u_3(\tau(q)\tau(q'))(\tau(q'')\tau(-q-q'-q''))\} \tag{5}$$

$$r_\sigma = (2/K_0)[1 - (d-1)K_0 - K\cos(\tfrac{2}{3}\pi\Delta - q_0)]$$

$$r_\tau = (2/K_0)[1 - (d-1)K_0 - K\cos(\tfrac{2}{3}\pi\Delta + 2q_0)]$$

$$\kappa_\sigma = (K/K_0)\cos(\tfrac{2}{3}\pi - q_0) \qquad \kappa_\tau = (K/K_0)\cos(\tfrac{2}{3}\pi + 2q_0).$$

The new parameters η, p, u_1, u_2, u_3 are allowed to deviate from their mean-field values under renormalisation. Since $r_\sigma < r_\tau$ the critical temperature is given as in mean-field theory (Siegert and Everts 1985) by $r_\sigma = 0$, $q_0 = \tfrac{2}{3}\pi\Delta$. The renormalisation group transformation for the functional (5) is performed in the same manner as for a metamagnet (Nelson and Fisher 1975). Firstly, we rescale the momentum variable $q_\parallel$ to eliminate the anisotropy in the propagator of the σ field. The effect is to replace κ_τ by $\kappa_\tau/\kappa_\sigma =: \kappa$ and setting $\kappa_\sigma = 1$. After integrating over the outer momentum shell, rescaling the momentum by a factor b and the fields σ and τ by factors c_σ and c_τ respectively, one finds that, in order to obtain a Gaussian fixed point with $r_\sigma = 0$, $r_\tau > 0$, the fields have to be rescaled differently, i.e. $c_\sigma = b^{1+d/2}$, $c_\tau = b^{d/2}$. Then the parameters η, u_2, u_3 turn out to be irrelevant. Thus the anisotropy of the propagator of the τ field drops out so that the scaling of the correlation lengths is indeed isotropic: $\nu_\parallel = \nu_\perp = \nu$. One arrives at a reduced functional

$$\mathcal{L}' = -\int \frac{d^d q}{(2\pi)^d} [\tfrac{1}{2}(r_\sigma + q^2)\sigma(q)\sigma(-q) + \tfrac{1}{2}r_\tau\tau(q)\tau(-q)]$$

$$+ p\int \frac{d^d q\, d^d q'}{(2\pi)^{2d}} [(\sigma_1(q)\sigma_1(q') - \sigma_2(q)\sigma_2(q'))\tau_1(-q-q')$$

$$- 2\sigma_1(q)\sigma_2(q')\tau_2(-q-q')]$$

$$- \frac{u_1}{2}\int \frac{d^d q\, d^d q'\, d^d q''}{(2\pi)^{3d}} (\sigma(q)\sigma(q'))(\sigma(q'')\sigma(-q-q'-q'')) \tag{6}$$

which contains the τ field only quadratically. Thus in the functional integral $\int \Pi_q \mathcal{D}\tau(q)\, e^{-\mathcal{L}'} =: e^{-\mathcal{L}''}$ the τ field can be integrated out, yielding a Lagrangian

$$\mathcal{L}'' = \mathcal{L}_{XY} = -\int \frac{d^d q}{(2\pi)^d} \tfrac{1}{2}(r_\sigma + q^2)\sigma(q)\sigma(-q)$$

$$-\int \frac{d^d q\, d^d q'\, d^d q''}{(2\pi)^{3d}} \frac{u}{2} (\sigma(q)\sigma(q'))(\sigma(q'')\sigma(-q-q'-q'')) \tag{7}$$

with $u = u_1 - p^2/r_\tau$. From the Lagrangian (7) it follows that the phase transition of the modulated phases of the CC3 model belongs to the universality class of the three-dimensional XY model with critical exponents $\nu \approx 0.670$, $\gamma \approx 1.317$, $\alpha \approx -0.01$ (Le Guillon and Zinn-Justin 1980, Albert 1982).

In the following we demonstrate how these results can be obtained by a Monte Carlo study. Since we shall employ finite-size extrapolations, we briefly review the finite-size scaling theory for anisotropic systems (see also Binder and Wang 1989). The starting point is the homogenity relation for the free energy

$$F = b^{-(2-\alpha)} f(bt, b^{-\nu_\perp} L_\perp, b^{-\nu_\parallel} L_\parallel) \tag{8}$$

where b is an arbitrary scaling factor, $t = T/T_c - 1$ is the reduced temperature and α is the specific heat exponent. In the present context $L_\parallel$ is the length of the system along the chiral axis and $L_\perp$ is the linear dimension of the ferromagnetic layers perpendicular to this axis. $\nu_\parallel$, $\nu_\perp$ are the possibly different exponents of the correlation length $\xi_\parallel$, $\xi_\perp$ in these two directions. The derivatives of the free energy, such as the susceptibility or the specific heat, obey analogous scaling relations:

$$k_B T \chi = b^\gamma \bar{\chi}(bt, b^{-1}L_\perp^{1/\nu_\perp}, b^{-1}L_\parallel^{1/\nu_\parallel}). \tag{9}$$

Setting $b = L_\perp^{1/\nu_\perp}$ and defining $z = L_\parallel^{1/\nu_\parallel}/L_\perp^{1/\nu_\perp}$, one sees that $\bar{\chi}$ depends only on $L_\perp^{1/\nu_\perp} t$ and z

$$k_B T \chi = L_\perp^{\gamma/\nu_\perp} \bar{\chi}(L_\perp^{1/\nu_\perp} t, 1, z). \tag{10}$$

The shift $\varepsilon = 1 - T_c(L_\perp, L_\parallel)/T_c$, defined as the reduced temperature at the maximum of the susceptibility, i.e. $k_B T_c \chi_{max} = L_\perp^{\gamma/\nu_\perp} \bar{\chi}(L_\perp^{1/\nu_\perp}\varepsilon, 1, z)$, is given by $\partial \chi/\partial t|_{t=\varepsilon} = 0$. This yields

$$\varepsilon = L_\perp^{-1/\nu_\perp} \tau(z). \tag{11}$$

In general, equation (11) cannot be used to extract the exponent $\nu_\perp$ (or equivalently $\nu_\parallel$) from finite-size results as z itself depends on $\nu_\perp$ and $\nu_\parallel$ and the function $\tau(z)$ is not known. One possibility is to take the anisotropic limit $L_\perp \gg L_\parallel \gg 1$ (or $L_\parallel \gg L_\perp \gg 1$) where one can approximate $\tau(z)$ by a constant. This method has been tested for the Ising model by Binder and Wang (1989) with the result that very large systems are required and the accuracy is very poor.

A function which has proved to be very useful in Monte Carlo simulations is the reduced fourth-order cumulant $u = 1 - \langle M^4 \rangle/(3\langle M^2 \rangle^2)$ of the order parameter M, since this is a pure scaling function (Binder 1981, 1985, Binder and Wang 1989):

$$u(t, L_\perp, L_\parallel) = \bar{u}(L_\perp^{1/\nu} t, z) \tag{12}$$

which at $T = T_c$ depends only on z:

$$u(0, L_\perp, L_\parallel) = \bar{u}(0, z) =: g(z). \tag{13}$$

If scaling is isotropic ($\nu_\perp = \nu_\parallel = \nu$) then u is simply a function of the aspect ratio $s = L_\parallel/L_\perp$, $u(T = T_c) = \tilde{g}(s)$. In this case the graphs of $u(T)$ for different values of $L_\perp$

but fixed value of s must intersect in the same point when $T = T_c$. Obviously, this is not the case if $\nu_\perp \neq \nu_\parallel$. Monte Carlo results for $u(T)$ can thus be used to discriminate between isotropic and anisotropic scaling.

In the simulation of the CC3 model we employed the standard Metropolis algorithm. Generally 4×10^5 Monte Carlo steps were used in the averaging procedure. As an order parameter we choose the first harmonic of the magnetisation

$$\langle M \rangle = \frac{1}{L_\parallel} \left\langle \sum_{\alpha=1}^{L_\parallel} (M_{1\alpha} \cos q_0\alpha + M_{2\alpha} \sin q_0\alpha) \right\rangle \tag{14}$$

where $M_\alpha = \Sigma_i S_{i\alpha}/L_\perp^2$ is the magnetisation of the αth layer. Most calculations are done for $\Delta = \frac{1}{2}$ since for this value of Δ the wavenumber of the stable modulated phase is known to be $q_0 = \frac{2}{6}\pi$ owing to the symmetry relation (2). Note that for $\Delta = \frac{1}{2}$ the model is equivalent to a metamagnetic Potts model with antiferromagnetic interactions in the axial direction and ferromagnetic interactions perpendicular to this direction. Figure 2 shows plots of the fourth cumulant $u(T)$ for two different values $s = 1$ and $s = 2$ of the aspect ratio. The two clearly distinguishable intersection points are located at exactly the same termperature, $T_c/J = 2.287 \pm 0.002$. On account of the very high precision, the method discriminates very sensitively between isotropic and anisotropic scaling.

Knowing that scaling is isotropic for the CC3 model, one can now proceed to extrapolate the critical exponents from finite-size results in the usual fashion:

$$k_B T_c \chi = L_\perp^{\gamma/\nu} \tilde{\chi}(L_\perp^{1/\nu} t, s) \tag{15a}$$

$$\varepsilon = L_\perp^{-1/\nu} \tilde{\tau}(s). \tag{15b}$$
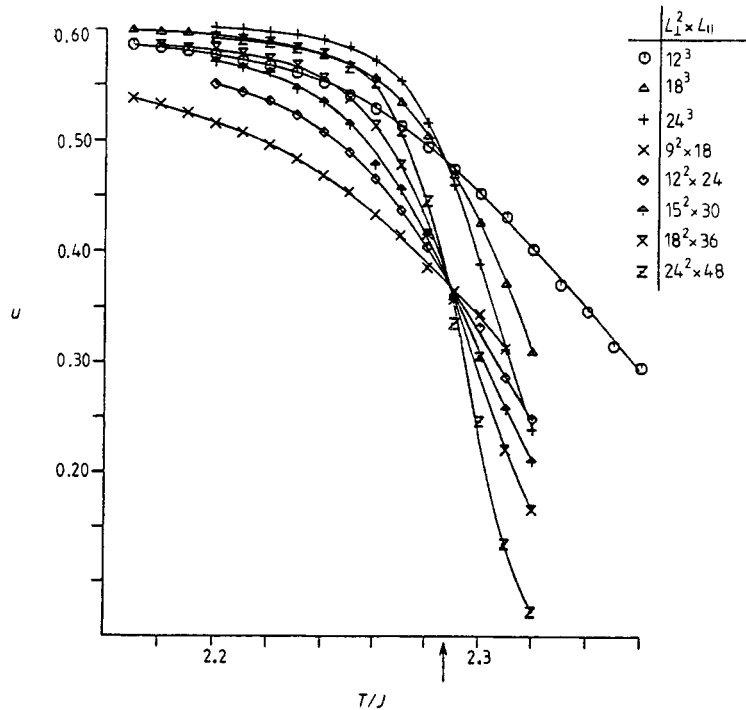

Figure 2. Monte Carlo results for the fourth-order cumulant u, $\Delta = 0.5$. The arrow indicates the critical temperature T_c.

To determine the exponent ν from the shift ε, the value of $\tilde{\tau}(s)$ in equation (15b) is of crucial importance. Figure 3 shows Monte Carlo data for the specific heat and for the susceptibility (determined from the fluctuations of the energy and the order parameter) for $s = 1$ and $s = 2$. While, for $s = 1$ the shift is nearly zero and the data are useless for the determination of ν, there is a pronounced shift for $s = 2$. From these data we obtain the results $\nu = \frac{2}{3} \pm 0.02$, $\alpha = 0.0 \pm 0.06$, $\gamma = 1.28 \pm 0.04$.

We conclude with a brief description of our Monte Carlo results for $\Delta \neq \frac{1}{2}$. At $\Delta = 0.3$ the phase transition between the ferromagnetic and disordered states is clearly of first order. The maxima of the specific heat and the susceptibility diverge proportional to the volume L^3 (we choose $s = 1$). For values of Δ slightly larger than Δ_{mc}, the value
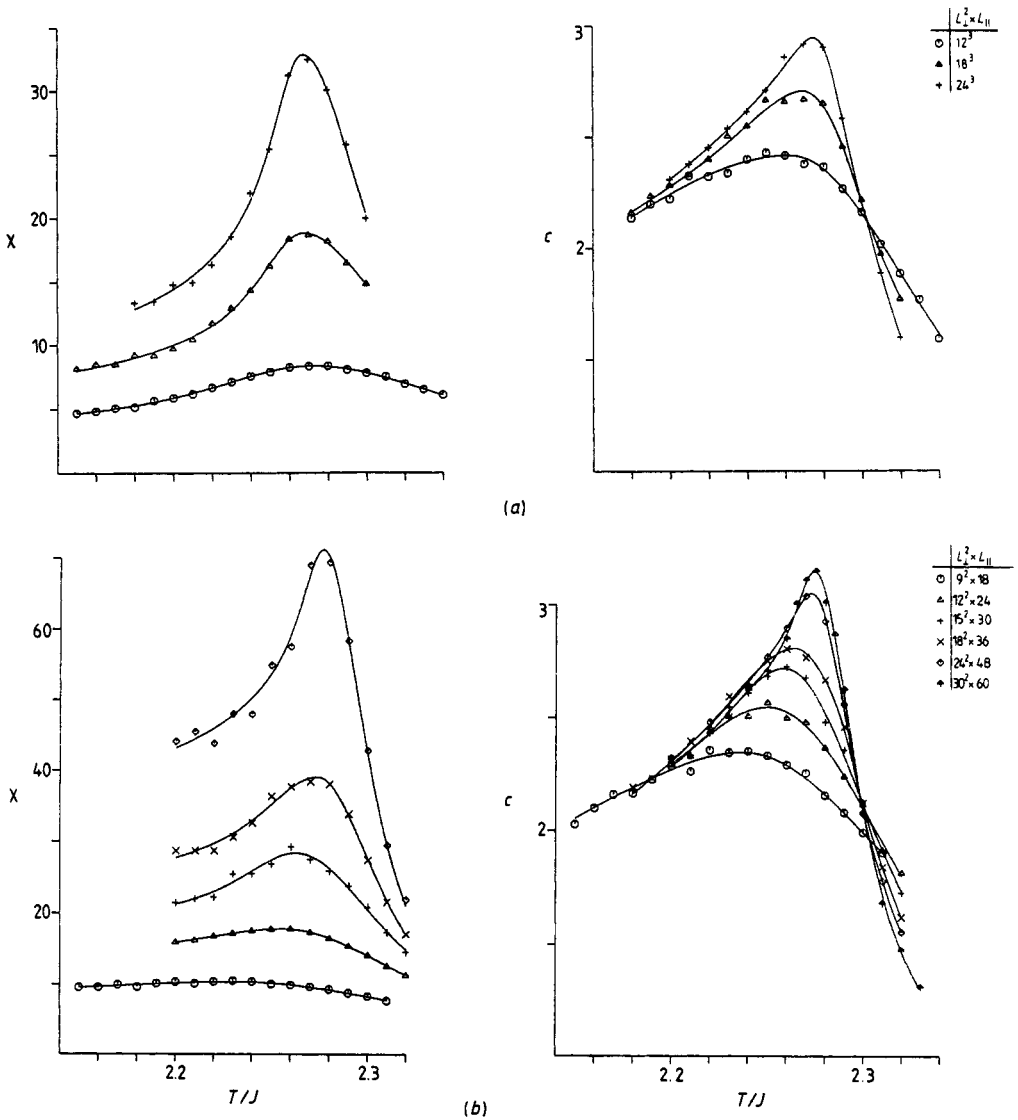

(a)

(b)

Figure 3. Monte Carlo results for the susceptibility χ and the specific heat c, $\Delta = 0.5$, (a) for aspect ratios $s = 1$, (b) for $s = 2$.

at the multicritical point, where ferromagnetic, disordered and modulated phases coexist, it is difficult to resolve the peaks originating from the ferromagnetic–modulated transition and the modulated–disordered transition. The former is a first-order transition and exhibits strong hysteresis effects, thus the latter transition can only be studied within relatively short simulations (we use 2×10^5 Monte Carlo steps), so that no transition from the modulated configuration to the metastable ferromagnetic state occurs. The wavenumber q_0 of the stable modulated phase is determined by studying small lattices with $L_\perp = 12$, $L_\parallel = 10, 11, \ldots, 15$. At $\Delta = 0.36$ we find $q_0 \simeq \frac{2}{12}\pi$ and from the susceptibility data for system sizes $L_\perp = L_\parallel = n \times 12$, $n = 1, 2, 3$, we obtain the exponent $\gamma/\nu = 1.95$. This is surprisingly close to the XY value as one expects relatively large errors due to the proximity of the transition to the ferromagnetic state. The value of γ/ν is clearly distinct from 3, which would obtain if the transition were of first order. Thus we find no indication for a first-order transition from modulated phases to the disordered state in contrast to the mean-field theory (Öttinger 1983, Siegert and Everts 1985), but in agreement with the Bethe approximation (Siegert and Everts 1987).

References

Albert D Z 1982 *Phys. Rev.* B **25** 4810
Binder K 1981 *Z. Phys.* B **43** 119
—— 1985 *J. Comput. Phys.* **59** 1
Binder K and Wang J-S 1989 *J. Stat. Phys.* **55** 87
Elliot R J 1961 *Phys. Rev.* **124** 346
Fisher M E and Szpilka A M 1987 *Phys. Rev.* B **36** 5343
Huse D A 1981 *Phys. Rev.* B **24** 5180
Le Guillon J C and Zinn-Justin J 1977 *Phys. Rev. Lett.* **39** 95
Nelson D R and Fisher M E 1975 *Phys. Rev.* B **11** 1030
Ostlund S 1981 *Phys. Rev.* B **24** 398
Ottinger H C 1983 *J. Phys. C: Solid State Phys.* **16** L597
Selke W and Duxbury P M 1984 *Z. Phys.* B **57** 49
Siegert M and Everts H U 1985 *Z. Phys.* B **60** 265
—— 1987 *Z. Phys.* B **66** 227
Szpilka A M and Fisher M E 1987 *Phys. Rev.* B **36** 5363