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Potts models with competing interactions

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Abstract. The mock ANNNI model is generalised in replacing the Ising spins by q-state Potts variables. Performing exact dedecoration transformations for general q and using Monte Carlo techniques in two dimensions for $q = 3$, a multitude of distinct spatially modulated long-range ordered phases, as well as phases with algebraic order, are found to spring from a multiphase point.

1. Introduction

Motivated by findings on the axial next-nearest-neighbour Ising (ANNNI) model (Fisher and Selke 1980), decorated Ising models with competing interactions have been introduced and studied by Huse *et al* (1981). These 'mock' ANNNI models are fully solvable in terms of properties of simple anisotropic nearest-neighbour (NN) Ising models with ferromagnetic couplings within layers and an effective, ferro- or antiferromagnetic, interlayer coupling. They have been found to exhibit behaviour quite similar to that of the true ANNNI models. In particular, they display multiphase points at zero temperature from which a multitude of distinct commensurate phases, characterised by a spatially modulated magnetisation, spring. However, no branching processes (Selke and Duxbury 1984) or incommensurate structures occur.

In this paper we replace the Ising spins of the mock ANNNI model by q-state Potts variables. It turns out that this simple generalisation has a rather drastic impact on half of the commensurate phases in two dimensions: if the effective interlayer coupling is antiferromagnetic, then long-range order is apparently destroyed and algebraic order of the Kosterlitz-Thouless type occurs. However, for ferromagnetic effective interlayer couplings, results on the Ising models carry over to the Potts case with only minor quantitative modifications.

The layout of this paper is as follows: in § 2 the mock axial next-nearest-neighbour Potts (or ANNNP) model is introduced and a dedecoration transformation is performed by which the model is mapped onto a NN anisotropic Potts model. This transformation is studied in the low-temperature regime in § 3 and explicit analytical expressions are obtained for the effective Potts coupling. In § 4 we present findings of a new Monte Carlo study on the correlation functions for the two-dimensional $q = 3$ metamagnetic NN Potts model (ferromagnetic intralayer and antiferromagnetic interlayer couplings). Some previous conjectures on the phase boundary of this metamagnetic model (Kinzel

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et al 1981, Truong 1984) are scrutinised. In § 5 we present results of numerical studies on the basis of the formulation and results of §§ 2-4. Phase diagrams of the two-dimensional mock ANNNP model are studied and the spatially modulated ordered phases are characterised.

2. The mock ANNNP models and the dedecoration transformation

The mock axial next-nearest-neighbour Potts (or ANNNP) models are q-state Potts models decorated in an uniaxial direction with spins coupled via competing interactions. The models are defined in full analogy to the mock ANNNI models (Huse *et al* 1981) by replacing Ising spins by Potts variables, with $q=2$ corresponding to the Ising case. In the most general case consider a d-dimensional hypercubic lattice with Potts spins $s_i=(1,2,\ldots,q)$. Within layers of $(d-1)$ dimensions the spins s_i interact with ferromagnetic nearest-neighbour couplings J_0. However, each spin s_i is coupled to its two nearest neighbours s_{i-1} and s_{i+1} in the two adjacent $(d-1)$-dimensional layers via a linear chain of n Potts spins σ_i, $i=1,2,\ldots,n$. The spins s_i are referred to as the nodal spins and σ_i the decorating or bond spins.

Along each chain the n decorating spins σ_i and the two nodal spins interact with ferromagnetic NN couplings $J_1>0$ and competing antiferromagnetic next-nearest-neighbour (NNN) couplings $J_2<0$, a situation illustrated in figure 1 for $d=2$. Note that we have chosen the NN couplings at the two ends of the chain to be $\frac{1}{2}J_1$, a choice which takes into account that the NN couplings at the ends of the chain are in competition with only one NNN coupling and which will facilitate our later consideration. The parameter controlling the competition is

$$\kappa=-J_2/J_1. \tag{1}$$

As each chain of n decorating spins is connected to the rest of the lattice through the two nodal spins only, we can perform an exact dedecoration transformation resulting in an effective NN coupling (independent of the dimension d)

$$J_{\text{eff}}(\kappa,T)=k_B T K_{\text{eff}}(\kappa,T) \tag{2}$$

between two NN nodal spins in adjacent $(d-1)$-dimensional layers. Thus, by so doing, we have reduced the mock ANNNP model to a NN Potts model. It follows that thermodynamic properties of the mock ANNNP model can be deduced from those of the NN models. For instance, in two dimensions, for $K_{\text{eff}}>0$, the phase boundary in the (κ, T) plane is known to be given by

$$[\exp(K_{\text{eff}})-1][\exp(K_0)-1]=q \tag{3}$$

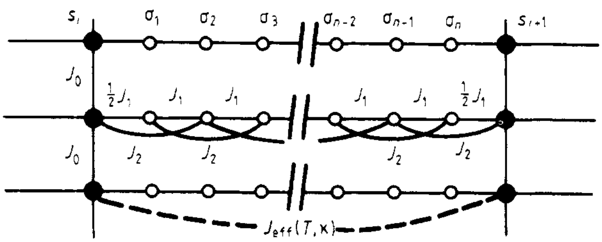

Figure 1. The two-dimensional mock ANNNP model. Full circles denote the nodal Potts spins, s_i, open circles the decorating spins, σ_i. The dedecoration transformation replaces the chain of n bond spins by an effective interaction between nodal spins.

where $K_0 = J_0/k_B T$ (see, e.g., Wu 1982). However, for $K_{\text{eff}} < 0$ the question has been raised (Truong 1984) on the validity of the phase boundary conjectured by Kinzel *et al* (1981). To improve the matter we present in § 4 results of a new Monte Carlo study on the phase boundary for the two-dimensional metamagnet NN model with $K_{\text{eff}} < 0$ and $q = 3$. In three (and higher) dimensions the anisotropic NN Potts model has not been studied in detail yet.

The dedecoration transformation can be carried out for general q and n by means of the transfer matrix method. However, straightforward generalisation of the transfer matrix method used by Huse *et al* (1981) requires the diagonalisation of a $q^2 \times q^2$ matrix which is not readily done for general q.

Here we use an alternate approach which requires the use of a 5×5 transfer matrix with q appearing as a parameter. This simplified approach makes it possible to carry out numerical calculations for general q without difficulty. In addition, it also leads to an exact formulation for identifying low-temperature properties.

The particular choice of the two end NN couplings $\frac{1}{2}J_1$ of a chain as shown in figure 1 permits us to build the chain of n decorating spins by combining $(n+1)$ building units as shown in figure 2. Let $Z_1(\sigma_1, \sigma_2, \sigma_3)$ denote the partition function of the unit shown. Then, the Boltzmann factor for a chain between two nodal spins s_i and s_{i+1} is

$$\begin{aligned} B(s_i, s_{i+1}) &= \sum_{\sigma_1, \ldots \sigma_n} Z_1(s_i, \sigma_1, \sigma_2) Z_1(\sigma_1, \sigma_2, \sigma_3) \ldots Z_1(\sigma_{n-1}, \sigma_n, s_{i+1}) \\ &= \sum_{\sigma_n} Z_n(s_i, \sigma_n, s_{i+1}) \end{aligned} \tag{4}$$

where we have introduced the general definition:

$$Z_{l+1}(s_i, \sigma_{l+1}, \sigma_{l+2}) = \sum_{\sigma_l} Z_l(s_i, \sigma_l, \sigma_{l+1}) Z_1(\sigma_l, \sigma_{l+1}, \sigma_{l+2}) \qquad l = 1, 2, \ldots, n-1 \tag{5}$$

with $\sigma_{n+1} = s_{i+1}$.

The evaluation of (4) is facilitated by writing

$$Z_l(\sigma_1, \sigma_2, \sigma_3) = A_l \delta_{12} + B_l \delta_{23} + C_l \delta_{13} + D_l \delta_{12} \delta_{23} + E_l \tag{6}$$

where δ_{ij} denotes the Kronecker symbol $\delta_{\sigma_i, \sigma_j}$. Then (5) can be written in a matrix form

$$\psi_{l+1} = \hat{T} \psi_l \qquad l = 1, 2, \ldots, n \tag{7}$$

where ψ is a column matrix whose transpose is given by

$$\tilde{\psi}_l = (A_l, B_l, C_l, D_l, E_l) \tag{8}$$

and $\hat{T}$ is the 5×5 matrix

$$\hat{T} = \begin{pmatrix} a & 0 & q+a+c & a+1 & 0 \\ a & a+c+d & 0 & 0 & qa+d \\ c & 0 & 0 & 0 & 0 \\ d & 0 & qa+d & a+c+d & 0 \\ 1 & a+1 & 0 & 0 & q+a+c \end{pmatrix} \tag{9}$$

where

$$\begin{aligned} &a = \exp(K_1/2) - 1 \qquad c = \exp(K_2) - 1 \\ &d = a^2(c+1) + 2ac. \end{aligned} \tag{10}$$

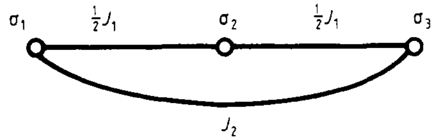

Figure 2. Building unit of a chain.

In fact, ψ_1 is readily determined from Z_1 and figure 2, yielding

$$\tilde{\psi}_1 = (a, a, c, d, 1). \tag{11}$$

Using (7) and (11), we can then compute Z_n by iteration. Finally we compute $B(s_i, s_{i+1})$ using (4), and K_{eff} using

$$\begin{aligned} \exp(K_{\text{eff}}) &= B(1,1)/B(1,2) \\ &= 1 + (qC_n + D_n)/(A_n + B_n + qE_n). \end{aligned} \tag{12}$$

We can also obtain correlation functions of the decorating spins. To illustrate, consider the expectation value of $F(\sigma_m)$ for arbitrary F:

$$\langle F(\sigma_m)\rangle = \sum_{\sigma_1,\ldots,\sigma_n} F(\sigma_m) Z_1(s_i, \sigma_1, \sigma_2) \ldots Z_1(\sigma_{n-1}, \sigma_n, s_{i+1})/B(s_i, s_{i+1}). \tag{13}$$

An analysis similar to that given above, details of which will be omitted, leads to the following expression:

$$\langle F(\sigma_m)\rangle_{s_i,s_{i+1}} = \Big(AF(s_i) + BF(s_{i+1}) + D\delta_{i,i+1}F(s_i) + (E + \delta_{i,i+1}C)\sum_\sigma F(\sigma)\Big)(B(s_i, s_{i+1}))^{-1} \tag{14}$$

where

$$\begin{aligned} A &= A_m(A_{n-m} + B_{n-m} + qE_{n-m}) + C_m B_{n-m} + D_m(B_{n-m} + E_{n-m}) \\ B &= B_m(A_{n-m} + C_{n-m} + D_{n-m}) + C_m C_{n-m} + E_m(qC_{n-m} + D_{n-m}) \\ C &= C_m A_{n-m} \\ D &= A_m(qC_{n-m} + D_{n-m}) + C_m D_{n-m} + D_m(A_{n-m} + C_{n-m} + D_{n-m}) \\ E &= B_m(B_{n-m} + E_{n-m}) + C_m E_{n-m} + E_m(A_{n-m} + B_{n-m} + qE_{n-m}). \end{aligned} \tag{15}$$

In particular, we find for the bond spin expectation values between two fully ordered nodal spins:

$$\begin{aligned} \langle \delta_{\sigma_m,1}\rangle_{1,1} &= (A + B + C + D + E)/[q(C + E) + A + B + D] \\ \langle \delta_{\sigma_m,1}\rangle_{1,2} &= (A + E)/(qE + A + B) \\ \langle \delta_{\sigma_m,2}\rangle_{1,2} &= (B + E)/(qE + A + B). \end{aligned} \tag{16}$$

3. Low-temperature phases

As in the case of the mock ANNNI model (Huse *et al* 1981), the point ($\kappa = \frac{1}{2}$, $T = 0$) is a multiphase point, and it is important to analyse the low-temperature properties near $\kappa = \frac{1}{2}$. For this purpose we consider $(\kappa - \frac{1}{2}) = \delta \to 0$, $T \to 0$, but

$$v = \exp(-\delta J_1/k_B T) = 2\cos\theta \tag{17}$$

fixed and finite. In this limit and to leading order we may replace (9) by

$$\hat{T} \rightarrow \begin{pmatrix} s & 0 & s & s & 0 \\ s & (v-1)s & 0 & 0 & (v+q-2)s \\ 0 & 0 & 0 & 0 & 0 \\ (v-2)s & 0 & (v+q-2)s & (v-1)s & 0 \\ 0 & s & 0 & 0 & s \end{pmatrix} \tag{18}$$

where $s = \exp(K_1/2) \rightarrow \infty$. Then to leading orders we may set, after making use of (7),

$$C_l = 0 \tag{19}$$

and use the following recursion relations for Ψ:

$$\begin{aligned} A_{l+1} &= s[A_l + D_l] \\ D_{l+1} &= s[(v-2)A_l + (v-1)D_l] \\ B_{l+1} &= s[A_l + (v-1)B_l + (v+q-2)E_l] \\ E_{l+1} &= s[B_l + E_l] \\ l &= 2, 3, \ldots, n. \end{aligned} \tag{20}$$

The recursion relations (20) can be solved by using the method of generating functions, leading to

$$\begin{aligned} A(z) &= \sum_{n=1}^{\infty} A_n z^n = \frac{z(1-z)}{1 - vz + z^2} \\ D(z) &= \sum_{n=1}^{\infty} D_n z^n = \frac{(v-2)z}{1 - vz + z^2} \\ B(z) &= \sum_{n=1} B_n z^n = \frac{z(1-z)[1 + zA(z)]}{1 - vz - (q-1)z^2} \\ E(z) &= \sum_{n=1} E_n z^n = \frac{z^2(1 + zA(z)]}{1 - vz - (q-1)z^2}. \end{aligned} \tag{21}$$

From (21) we obtain

$$\begin{aligned} A_l &= s^l \frac{\sin l\theta - \sin(l-1)\theta}{\sin\theta} \\ D_l &= (v-2)s^l \frac{\sin l\theta}{\sin\theta} \qquad l = 1, 2, 3, \ldots, n \end{aligned} \tag{22}$$

and

$$\begin{aligned} &E_1 = 0 \qquad E_2 = 1 \\ &E_l = a_{l-2} - (v-1)a_{l-3} \qquad l = 3, 4, \ldots, n \\ &B_1 = 1 \\ &B_l = E_{l+1} - E_l \qquad l = 2, 3, \ldots, n \end{aligned} \tag{23}$$

where

$$a_l = \frac{1}{q}\left(\frac{\alpha_+^{l+3} - \alpha_-^{l+3}}{\alpha_+ - \alpha_-} - \frac{\sin(l+3)\theta}{\sin\theta}\right)$$

$$\alpha_\pm = \tfrac{1}{2}\{v \pm [v^2 + 4(q-1)]^{1/2}\}.$$

These results are used in numerical calculations on the spatial modulation in the ordered phases, presented in § 5. In particular, the low-temperature asymptotes of the phase boundaries are given by $K_{\text{eff}} = 0$ (Huse *et al* 1981) or, using (12), (19) and (22), by $\sin n\theta = 0$ which is equivalent to

$$v = 2\cos(m\pi/n) \qquad m = 0, 1, \ldots, [n/2]. \tag{24}$$

Equation (24) shows that these asymptotes, which are the same as those found for the mock ANNNI model by Huse *et al* (1981), are independent of q. (Note that the $q = 2$ Potts interactions J_0 and J_1 are twice those of the usual Ising couplings.)

4. Monte Carlo study of the three-state metamagnetic Potts model

We consider the three-state metamagnetic NN Potts model on a square lattice (lattice constant a) with ferromagnetic interactions, $K_x = J_x/k_B T$, along one direction of the lattice, say, the x axis, and antiferromagnetic interactions, K_y, along the other axis. Obviously, K_x and K_y correspond to K_0 and K_{eff} in the mock ANNNP model. To determine the phase boundary of this model, we performed a Monte Carlo study computing, especially, the correlation function

$$C(\boldsymbol{r}) = \sum_X \langle \delta_{s_0, X} \delta_{s_r, X} \rangle \tag{25}$$

where the summation goes over the three states $X = 1, 2$ and 3; $\boldsymbol{r} = (x, y)$ denotes the distance from the origin, $\boldsymbol{0}$. While $C(\boldsymbol{r})$ decays monotonically along the x axis, there is an superimposed oscillatory behaviour with a periodicity of two lattice spacings along the y axis because of the antiferromagnetic interaction (see also Hoppe and Hirst 1985). In both cases the correlation lengths, $\xi_{x,y}$, can be extracted from the asymptotic form, for large $|\boldsymbol{r}|$,

$$C(\boldsymbol{r}) \sim \exp(-\xi/|\boldsymbol{r}|). \tag{26}$$

Results on the correlation lengths in the two directions for lattices of N columns and N rows, $N = 60$, are displayed in figure 3 for $J_x = -J_y$. Typically, runs of several 10^4

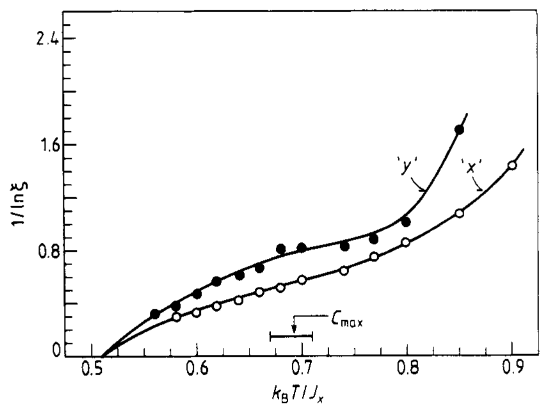

Figure 3. Correlation lengths for the NN three-state metamagnetic Potts model, with $J_x = -J_y$, plotted against temperature. 'y' denotes the correlation length, ξ_y, along the direction with antiferromagnetic couplings, 'x' the one along the direction with ferromagnetic NN interactions. For comparison the position of the maximum in the specific heat, $C_{\max}$, is shown. Systems of size 60×60 are used.

Monte Carlo steps per site were performed. Since full periodic boundary conditions have been imposed, finite-size effects are expected to be of minor importance for ξ_x (or ξ_y, which is, of course, smaller than ξ_x) no larger than about one-half of the linear lattice dimension. Indeed, we checked that by doing some runs for smaller systems ($N=20$ and 30). Our data are compatible with a phase transition of Kosterlitz-Thouless type at which the correlation length diverges as (Kosterlitz and Thouless 1973)

$$\xi \sim \exp[1/(T-T_c)^{1/2}] \tag{27}$$

i.e. $1/\ln \xi$ should vanish with a square root behaviour, see figure 3. Our estimate for the transition temperature, $k_B T/J_x = 0.51 \pm 0.03$, is in very good agreement with the estimates of Duxbury *et al* (1984) and Houlrik *et al* (1983) for the chiral clock model with the chirality parameter, Δ_c, equal to $\frac{1}{2}$. Indeed, the equivalence of the metamagnetic Potts model at $J_x = -J_y$ and the chiral clock model at $\Delta_c = 1/2$ has been noted before (Kinzel *et al* 1981, Selke and Yeomans 1982). In that context it should be mentioned that the Kosterlitz-Thouless type character of the phase transition was suggested first by Ostlund (1981) for the chiral clock model. A previous Monte Carlo study on that clock model (Selke and Yeomans 1982) presented supporting evidence, based mainly on the finite-size behaviour of the specific heat. Transfer matrix calculations for the Hamiltonian limit of the metamagnetic Potts model (Herrmann and Martin 1984) have provided additional evidence for such a transition.

Similar analyses for $J_y = -\alpha J_x$ ($\alpha = 0.3$ and 0.65) confirm the character of the transition and lead to the phase diagram depicted in figure 4. For comparison, results of two previous conjectures on the phase boundaries are included in the figure. Both conjectures, based on the Migdal-Kadanoff renormalisation group approximation (Kinzel *et al* 1981) or symmetry considerations (Truong 1984), are not exact. Nevertheless, for illustrative purposes we shall use the closed-form expression of Kinzel *et al* (1981) for the transition line

$$[1+\exp(K_x)][1-\exp(K_y)] = q \tag{28}$$

in the next section. With these findings on the metamagnetic three-state Potts model we continue to analyse the mock ANNNP model.

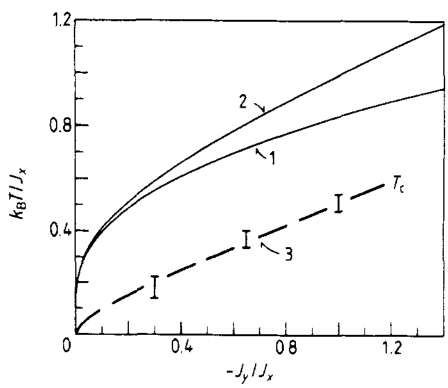

Figure 4. Phase boundary of the metamagnetic Potts model. 1 refers to the conjecture of Kinzel *et al* (1981), 2 to the one by Truong (1984), and 3 shows results of the present Monte Carlo study.

5. Phase diagram and spatially modulated phases

From (12), (3) and (28) (cf figure 4) it follows that the typical phase diagram of the two-dimensional mock ANNNP model consists of a series of loops springing from the multiphase point at $T=0$ and $\kappa=\frac{1}{2}$, which may be computed numerically, as illustrated in figure 5. For $q>2$ each loop encloses a usually ordered spatially modulated phase ($K_{\text{eff}}>0$) or a phase of algebraic order ($q=3$, $K_{\text{eff}}<0$; no detailed analysis of the metamagnetic NN Potts model for $q>3$ has been done so far). For $K_{\text{eff}}>0$ the phase boundary is of first ($q>4$) or second order ($q\leqslant 4$). The total number of loops is $[\frac{1}{2}n]$, where n is the number of decorating spins in between two nodal spins. Because of the alternation of the sign of K_{eff} in consecutive loops half of the loops are formed by the different types of phases. (To establish rigorously the existence of the loops with algebraic order for $q=3$ and general n the asymptotic behaviour of the phase boundary for small K_{eff}, $K_{\text{eff}}<0$ (see figure 4) needs to be known exactly. (28) would imply their existence.) In addition to the loops there is a transition line bounding a ferromagnetically ordered phase in the region $\kappa<\frac{1}{2}$, which is present for all n, while for odd n only there is another line bounding a (2, 2) antiphase state for $\kappa>\frac{1}{2}$. Each ordered phase for all $T>0$ is separated from its neighbours by a narrow disordered paramagnetic region. This behaviour is very similar to the one of the mock ANNNI model (Huse *et al* 1981).

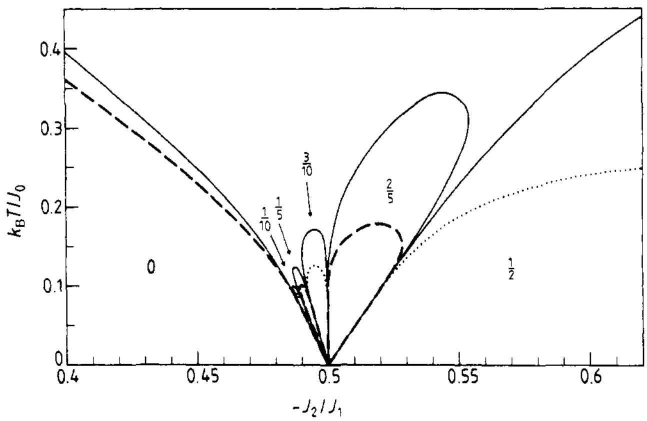

Figure 5. Phase diagram of the two-dimensional mock ANNNP model with $q=2$ (Ising) and $q=3$ for $J_1=5\ J_0$ and $n=9$. Full curves refer to $q=2$; bold broken curves are exact results (3) for $q=3$ and dotted curves are based on the approximate (28) for $q=3$. The long-range ordered phases are labelled by $\bar{q}a/\pi$ where $\bar{q}$ denotes the dominant wavenumber of the spatially modulated pattern.

The order characterising each phase with $K_{\text{eff}}>0$ is readily identified in the low-temperature limit near the multiphase point $(\kappa, T)=(\frac{1}{2}, 0)$, where the nodal spins become fully ordered (if $K_{\text{eff}}<0$ and in the case of algebraic order in two dimensions, the expectation values for the nodal spins are zero for all $T>0$). Fixing the nodal spins, the thermal averages for the decorating spins are given by (16) and (15), where, to leading orders of $\exp(K_1/2)$, we use (19), (22) and (23) in our calculations.

Numerical results for $q=3$ and $n=5, 9$ are displayed in figure 6. In full analogy to the mock ANNNI model the modulation of the spatial pattern is primarily with a wavelength $\lambda=2(n+1)a/m$ (or wavenumber $\bar{q}=2\pi/\lambda$), where $m=0, 2, 4, \ldots$. For

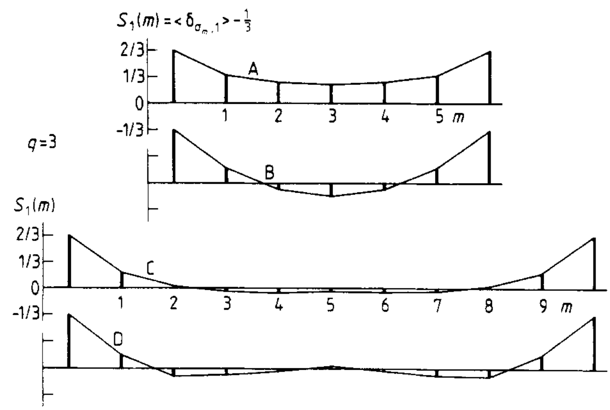

Figure 6. The pattern of the bond variables of the three-state mock ANNNP model with $n = 5$ and 9 in the low-temperature limit, $\exp(-2K_0) \ll 1$, for different values of $\Delta = (\kappa - \frac{1}{2})J_1/k_B T$, each corresponding to a distinct long-range ordered phase ($K_{\text{eff}} > 0$). The two nodal spins are set in state 1. A, $\Delta = 1$, $\bar{q}a = 0$, $n = 5$; B, $\Delta = 0$, $\bar{q}a = \pi/3$, $n = 5$; C, $\Delta = 0.5$, $\bar{q}a = \pi/5$, $n = 9$; C, $\Delta = -0.1$, $\bar{q}a = 2\pi/5$, $n = 9$.

$n = 5$ one may compare figure 6 to the corresponding one in Huse *et al* (1981) exemplifying the similarity of the mock Ising and Potts models for $K_{\text{eff}} > 0$. For $K_{\text{eff}} < 0$ we also expect a characteristic modulation in the correlation functions of the bond spins within each loop. Because of the apparently algebraic order in two dimensions for $q = 3$ the structure factor should exhibit power-law divergencies instead of Bragg peaks (Kosterlitz and Thouless 1973). However, no exact analytic results are available in this case.

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