

Modulated structures stabilized by spin softening: An expansion in inverse spin anisotropy

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We develop an analytic approach which allows us to study the behavior of spin models with competing interactions and p -fold spin anisotropy D in the limit where the pinning potential which results from D is large. This is an expansion in inverse spin anisotropy which must be carried out to all orders where necessary. Interesting behavior occurs near where the boundary between different ground states is infinitely degenerate for infinite D . Here as D decreases and the spins are allowed to soften, we are able to demonstrate the existence of several different behaviors ranging from a single first-order boundary to infinite series of commensurate phases. The method is illustrated by considering the soft chiral clock model and the soft clock model with first- and second-neighbor competing interactions. In the latter case the results are strongly dependent on the value of p .

I. INTRODUCTION

There are many examples of long-period phases in nature. These include the ferrimagnetic phases of the rare earths, long-period atomic ordering in binary alloys, and polytypism, the possibility of many different forms of long wavelength structural order in some minerals.

The underlying physical mechanism responsible for the formation of long-period structures is often the existence of competing interactions. Therefore it is of interest to understand the properties of model systems with such competition. Perhaps the simplest of these is the axial next-nearest-neighbor Ising (ANNNI) model, a ferromagnetic Ising model with second-neighbor antiferromagnetic interactions along one lattice axis. Despite its simplicity the ANNNI model has a very rich phase structure with infinite sequences of commensurate and incommensurate phases at finite temperatures.^{1,2}

If continuous spins are considered similar structures can occur even in the ground state. Banerjee and Taylor³ performed numerical work on the chiral X - Y model with $p =$ two-fold spin anisotropy D and showed that long-period phases are stable. Chou and Griffiths⁴ later proved that an infinite number of commensurate phases appear as ground states for $p \geq 3$. Numerical work has also shown that the X - Y model with first- and second-neighbor competing interactions and $p =$ six-fold spin anisotropy has a highly complicated ground-state phase diagram.⁵

Note that a common feature of these models is the spin anisotropy D . As D is increased from zero to infinity the spins are confined to increasingly deep potential wells and the model crosses over from a continuous to a discrete spin limit. For example, the X - Y model with p -fold spin anisotropy becomes a p -state clock model for $D = \infty$.

For infinite spin anisotropy the ground state typically

comprises a few short-period phases. The boundaries between the phases can either correspond to a first-order transition where only the neighboring phases are stable or a multiphase point at which an infinite number of phases are degenerate.⁶ As D decreases from infinity the states at the multiphase point can either remain degenerate with the point becoming a multiphase line or their energy can be differentiated as the spins soften. In the latter case some or all of the degenerate phases may become ground states in their own right and typically a fan of phases springs from the multiphase point. Indeed we shall see that in many respects D^{-1} behaves in a way akin to temperature with the spin softening playing the part of entropic fluctuations.

The large D region of the phase diagram is difficult to explore numerically because the phase sequences can be very complicated and the widths of the stable phases small. Therefore our aim in this paper is to describe an analytic technique which is useful in helping to understand the ground state of models with competing interactions for large spin anisotropy D . This is an expansion in $1/D$ taken to all orders where necessary. A short paper has summarized some of the results of the calculations.⁷ Here our aim is to describe the technical details of the expansion.

In Sec. II of the paper we explain the approach in some detail for the chiral X - Y model with p -fold spin anisotropy. In II A the model is defined and our notation introduced. The energy differences which are central to the argument are defined in II B and their dependence on the deviation of the spins from their positions at $D = \infty$ is calculated. II C describes the convenient labeling of the spin states which allows a calculation of the energy differences to leading order presented in II D. From these we are able to show, in agreement with Chou and Griffiths,⁴ that all possible phases are stable near the multiphase

point for $p \geq 3$. In Sec. II E the widths of the long-period phases are calculated.

The calculation is repeated in Sec. III for the X - Y model with first- and second-neighbor competing interactions and p -fold spin anisotropy. This is an involved calculation because of the existence of the second-neighbor interactions. Previous numerical results for this model for $p = 6$ were unable to probe the large D limit.⁵ We find that the behavior near the multiphase points is complicated and highly dependent on p .

The results are summarized and discussed in Sec. IV.

II. THE CHIRAL XY MODEL

A. Definitions and notation

The approach is most easily explained by considering its application to the chiral XY model with p -fold spin anisotropy. This is described by the Hamiltonian

$$\mathcal{H} = \sum_i \{-J \cos(\theta_{i-1} - \theta_i + \Delta) - D(\cos p\theta_i - 1)/p^2\} \quad (1)$$

where the θ_i are angular variables which can take values between 0 and 2π lying on the sites i of a one-dimensional lattice.

Note that the Hamiltonian (1) is invariant under the transformation

$$\Delta \rightarrow \Delta' = \Delta + 2\pi m/p, \quad (2)$$

for any integer m given the reidentification

$$\theta_i \Rightarrow \theta'_i = (\theta_i + 2\pi m i/p) \quad (3)$$

and therefore we may restrict our attention to $0 \leq \Delta < 2\pi/p$. Moreover the system is invariant under

$$\begin{aligned} \Delta &\Rightarrow \Delta' = 2\pi/p - \Delta, \\ \theta_j &\Rightarrow \theta'_j = (-\theta_j + 2\pi j/p). \end{aligned} \quad (4)$$

Thus the phase boundaries for $\Delta > \pi/p$ are related to those for $\Delta < \pi/p$ by reflection in the line $\Delta = \pi/p$. However, the phases themselves must be identified differently within the two regimes according to (4).

For $D = \infty$ the spins are restricted to discrete values $2\pi n_i/p$ where $n_i = 0, 1, \dots, p-1$ and the Hamiltonian (1) becomes that of the p -state chiral clock model. The ground state is well known in this limit. For $0 \leq \Delta \leq \pi/p$ it is ferromagnetic whereas for $\pi/p \leq \Delta \leq 2\pi/p$, $n_{i+1} = n_i + 1$, the increase in the chirality Δ favoring a twist in the spin ordering. At $\Delta = \pi/p$ itself the ground state is infinitely degenerate, with any phase for which $n_{i+1} - n_i = 0$ or 1 for all i having equal energy. Such a point is often termed a multiphase point. It is expected on the basis of previous work that as D decreases from infinity the degeneracy will be lifted. Our aim is to explore the phase structure through an expansion in D^{-1} . We consider $p \geq 3$.

To this end we require a notation capable of distinguishing the different phases stable at the multiphase point. Typically a stable ground state will consist of a sequence of bands where $n_{i-1} - n_i = 0$ separated by walls with $n_{i-1} - n_i = 1$. $[\ell_1, \ell_2, \dots, \ell_m]$ will be used to describe a phase where the repeating sequence consists of m bands of length $\ell_1, \ell_2, \dots, \ell_m$. It may be helpful to list some examples for $p = 6$

$$\begin{aligned} [12] & \dots | 0 | 11 | 2 | 33 | \dots \\ [23^2] & \dots | 00 | 111 | 222 | 33 | 444 | 555 | \dots \\ [1] & \dots | 0 | 1 | 2 | 3 | 4 | 5 | \dots \\ [\infty] & \dots 000000 \dots, \end{aligned} \quad (5)$$

where a vertical line is used to denote a wall. In the subsequent text we shall use the term l band to describe a band of length l spins. For example $[23^2]$ consists of a 2 band followed by two 3 bands.

B. The energy differences

The goal is to establish which of the infinite number of phases degenerate at the multiphase point remain stable for finite D . This is done by using an expansion in inverse spin anisotropy, D^{-1} . The difficulty is that in order to check the stability of all commensurate phases certain terms must be calculated at all orders in D^{-1} .

However, the relevant terms can be identified and the phase diagram constructed inductively using an argument first developed by Fisher and Selke to study the phase diagram of the axial nearest-neighbor Ising model using a low temperature expansion.⁶ We summarize their argument here.

Consider two phases $[\alpha]$ and $[\beta]$ which share a common boundary at a given order of a series expansion. Fisher and Selke showed that the first phase which can appear between them as the expansion is taken to higher orders is $[\gamma] = [\alpha\beta]$. To check whether this phase does indeed appear the important energy difference is

$$\Delta E \equiv n_{[\gamma]} E_{[\gamma]} - n_{[\alpha]} E_{[\alpha]} - n_{[\beta]} E_{[\beta]}, \quad (6)$$

where $E_{[\alpha]}, E_{[\beta]}, E_{[\gamma]}$ are the ground-state energies per spin and $n_{[\alpha]}, n_{[\beta]}, n_{[\gamma]}$, the number of spins per period of $[\alpha], [\beta]$ and $[\gamma]$, respectively.

There are three possibilities:

(i) $\Delta E > 0$ and the boundary between $[\alpha]$ and $[\beta]$ remains stable to all orders.

(ii) $\Delta E < 0$ and $[\alpha\beta]$ appears as a stable phase in the vicinity of the $[\alpha] : [\beta]$ boundary. The analysis must recommence about the new $[\alpha] : [\alpha\beta]$ and $[\alpha\beta] : [\beta]$ boundaries.

(iii) $\Delta E = 0$ and $[\gamma]$ remains degenerate on the $[\alpha] : [\beta]$ boundary to all orders.

To explore the phase structure our goal is to calculate ΔE and investigate its sign. To this end we write

$$\theta_i = \theta_i^0 + \tilde{\theta}_i, \quad (7)$$

where θ_i^0 is the value of the spin θ_i for $D = \infty$, and

expand the Hamiltonian (1) to quadratic order in the $\{\tilde{\theta}_i\}$.

$$\begin{aligned} \tilde{\mathcal{H}} = \mathcal{H}|_{D=\infty} + \sum_i \{ & Jc_i^\theta (\tilde{\theta}_{i-1} - \tilde{\theta}_i + s_i^\theta/c_i^\theta)^2/2 \\ & + D\tilde{\theta}_i^2/2 - J(s_i^\theta)^2/(2c_i^\theta) \}, \end{aligned} \quad (8)$$

where

$$c_i^\theta = \cos(\theta_{i-1}^0 - \theta_i^0 + \Delta), \quad s_i^\theta = \sin(\theta_{i-1}^0 - \theta_i^0 + \Delta). \quad (9)$$

We shall henceforth work with the quadratic approximation (8) to the chiral XY model. To leading order this gives the same results for the energy differences as the full Hamiltonian (1).

In equilibrium the energy of each phase must be minimal. Differentiating (8) with respect to the θ_i leads to the relation

$$\begin{aligned} D\tilde{\theta}_i = J(c_i^\theta \tilde{\theta}_{i-1} - c_i^\theta \tilde{\theta}_i - c_{i+1}^\theta \tilde{\theta}_i + c_{i+1}^\theta \tilde{\theta}_{i+1} \\ + s_i^\theta - s_{i+1}^\theta), \end{aligned} \quad (10)$$

which we shall need below.

For the quadratic Hamiltonian $\tilde{\mathcal{H}}$ the energy differences can be calculated exactly. Let $n_{[\alpha]} = n_1$ and $n_{[\gamma]} = n$ and label the spins within the phases $[\alpha]$, $[\beta]$ and $[\gamma]$ by $\alpha_i, \beta_i, \gamma_i$, respectively. Then, using (8) the energy of each phase relative to its value at $D = \infty$ is

$$\begin{aligned} n_1 E_{[\alpha]} = \sum_{i=1}^{n_1} \{ & Jc_i^\alpha (\tilde{\alpha}_{i-1} - \tilde{\alpha}_i + s_i^\alpha/c_i^\alpha)^2/2 \\ & + D\tilde{\alpha}_i^2/2 - J(s_i^\alpha)^2/(2c_i^\alpha) \}, \end{aligned}$$

$$\begin{aligned} (n - n_1) E_{[\beta]} = \sum_{i=n_1+1}^n \{ & Jc_i^\beta (\tilde{\beta}_{i-1} - \tilde{\beta}_i + s_i^\beta/c_i^\beta)^2/2 \\ & + D\tilde{\beta}_i^2/2 - J(s_i^\beta)^2/(2c_i^\beta) \}, \end{aligned}$$

$$\begin{aligned} n E_{[\gamma]} = \sum_{i=1}^n \{ & Jc_i^\gamma (\tilde{\gamma}_{i-1} - \tilde{\gamma}_i + s_i^\gamma/c_i^\gamma)^2/2 \\ & + D\tilde{\gamma}_i^2/2 - J(s_i^\gamma)^2/(2c_i^\gamma) \}. \end{aligned} \quad (11)$$

Because $[\gamma] \equiv [\alpha\beta]$ we can choose to label the spins in such a way that

$$\begin{aligned} \gamma_i^0 = \alpha_i^0, \quad 1 \leq i \leq n_1, \\ \gamma_i^0 = \beta_i^0, \quad n_1 + 1 \leq i \leq n \end{aligned} \quad (12)$$

and take

$$\begin{aligned} c_i^\alpha = c_i^\gamma, \quad s_i^\alpha = s_i^\gamma, \quad 1 \leq i \leq n_1; \\ c_i^\beta = c_i^\gamma, \quad s_i^\beta = s_i^\gamma, \quad n_1 + 1 \leq i \leq n. \end{aligned} \quad (13)$$

This means that we may drop the α, β, γ superscripts on the $\{c_i\}$ and $\{s_i\}$ and the final terms in (11) drop out when the energy difference is calculated

$$\begin{aligned} \Delta E = \sum_{i=1}^{n_1} [& J\{c_i(\tilde{\gamma}_{i-1} - \tilde{\gamma}_i + s_i/c_i)^2 - c_i(\tilde{\alpha}_{i-1} - \tilde{\alpha}_i + s_i/c_i)^2\}/2 + D(\tilde{\gamma}_i^2 - \tilde{\alpha}_i^2)/2] \\ & + \sum_{i=n_1+1}^n [J\{c_i(\tilde{\gamma}_{i-1} - \tilde{\gamma}_i + s_i/c_i)^2 - c_i(\tilde{\beta}_{i-1} - \tilde{\beta}_i + s_i/c_i)^2\}/2 + D(\tilde{\gamma}_i^2 - \tilde{\beta}_i^2)/2]. \end{aligned} \quad (14)$$

This expression can be simplified considerably using (10). Recalling the periodicity of the ground-state phases which ensures

$$\tilde{\alpha}_i = \tilde{\alpha}_{n_1+i}, \quad \tilde{\beta}_i = \tilde{\beta}_{n-n_1+i}, \quad \tilde{\gamma}_i = \tilde{\gamma}_{n+i}, \quad \forall i \quad (15)$$

leads after some algebra to

$$\begin{aligned} \Delta E = Jc_1 \{ & (\tilde{\alpha}_{n_1} - \tilde{\beta}_n)(\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}) \\ & - (\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_n - \tilde{\gamma}_{n_1}) \} / 2. \end{aligned} \quad (16)$$

Note that ΔE depends only on the difference between a small number of spins. It is this which facilitates its calculation. The expression (16) is exact for the quadratic Hamiltonian (8) but only correct to leading order for the full Hamiltonian (1). However, this will be sufficient for the calculations presented below.

C. Labeling the spins

The energy differences we are trying to calculate are independent of the labeling of the spins given that the conditions (13) hold. In general differences such as $\tilde{\alpha}_{n_1} - \tilde{\beta}_n$ in the energy difference (16) will be polynomials in

D^{-1} . Low order terms will cancel when the difference in (16) is taken, in such a way that the final result becomes independent of the labeling. However, computationally the problem is simplified by a careful choice of spin labels which allow the leading order contribution to ΔE to be obtained directly.

We first point out that every commensurate ground state of the Hamiltonian (1) has two points of mirror symmetry in each period evenly spaced along the chain.⁸ It is possible to distinguish two cases. For states of odd period half the symmetry points are located on lattice sites and the other half between lattice sites. By symmetry the spins located on the lattice sites corresponding to mirror symmetry points do not deviate from their $D = \infty$ position for finite D ($\tilde{\theta} = 0$). For states of even period the symmetry points are located either all between or all on lattice sites. For states formed by the branching process $[\alpha] + [\beta] \Rightarrow [\alpha\beta]$ only the former can occur.

As the branching process $[\alpha] + [\beta] \Rightarrow [\gamma] \equiv [\alpha\beta]$ proceeds states are made up in two ways: (i) odd + odd \Rightarrow even, (ii) odd + even \Rightarrow odd. (A moment's reflection shows that even + even \Rightarrow even never occurs because, as the ground states are formed inductively, no neighboring even phases ever appear.)

Our aim is to choose the origin for the labeling of the spins in such a way that the formula (16) for the energy difference is simplified. It is necessary to consider each of the two cases (i) and (ii) separately.

(i) *odd + odd* \Rightarrow *even*.

We recall the notation $[\alpha] + [\beta] \Rightarrow [\gamma]$ with $[\alpha]$ and $[\beta]$ having n_1 and n spins, respectively, in each period. A

convenient choice of labeling is

$$\tilde{\alpha}_{n_1} = 0; \quad \tilde{\beta}_n = 0. \quad (17)$$

It will be useful later to write the spin deviations within a period of each phase in a way that explicitly displays the symmetry

$$\begin{aligned} \{\tilde{\alpha}_i\} &\equiv \{\tilde{\alpha}_1, \tilde{\alpha}_2, \dots, \tilde{\alpha}_{(n_1-1)/2}, \tilde{\alpha}_{(n_1+1)/2}, \dots, \tilde{\alpha}_{n_1-2}, \tilde{\alpha}_{n_1-1}, \tilde{\alpha}_{n_1}\} \\ &= \{\tilde{\alpha}_1, \tilde{\alpha}_2, \dots, \tilde{\alpha}_{(n_1-1)/2}, -\tilde{\alpha}_{(n_1-1)/2}, \dots, -\tilde{\alpha}_2, -\tilde{\alpha}_1, 0\}, \end{aligned} \quad (18)$$

$$\begin{aligned} \{\tilde{\beta}_i\} &\equiv \{\tilde{\beta}_{n_1+1}, \tilde{\beta}_{n_1+2}, \dots, \tilde{\beta}_{(n+n_1-1)/2}, \tilde{\beta}_{(n+n_1+1)/2}, \dots, \tilde{\beta}_{n-2}, \tilde{\beta}_{n-1}, \tilde{\beta}_n\} \\ &= \{\tilde{\beta}_{n_1+1}, \tilde{\beta}_{n_1+2}, \dots, \tilde{\beta}_{(n+n_1-1)/2}, -\tilde{\beta}_{(n+n_1-1)/2}, \dots, -\tilde{\beta}_{n+2}, -\tilde{\beta}_{n+1}, 0\}. \end{aligned} \quad (19)$$

$\langle\alpha\rangle$ and $\langle\beta\rangle$ combine to give an even state $\langle\gamma\rangle$ with symmetry points between $i = (n_1 - 1)/2$, $i = (n_1 + 1)/2$ and $i = (n + n_1 - 1)/2$, $i = (n + n_1 + 1)/2$.

$$\begin{aligned} \{\tilde{\gamma}_i\} &\equiv \{\tilde{\gamma}_1, \tilde{\gamma}_2, \dots, \tilde{\gamma}_{(n_1-1)/2}, \tilde{\gamma}_{(n_1+1)/2}, \dots, \tilde{\gamma}_{n_1-1}, \tilde{\gamma}_{n_1}, \tilde{\gamma}_{n_1+1}, \tilde{\gamma}_{n_1+2}, \dots, \tilde{\gamma}_{(n+n_1-1)/2}, \tilde{\gamma}_{(n+n_1+1)/2}, \dots, \tilde{\gamma}_{n-1}, \tilde{\gamma}_n\} \\ &= \{\tilde{\gamma}_1, \tilde{\gamma}_2, \dots, \tilde{\gamma}_{(n_1-1)/2}, -\tilde{\gamma}_{(n_1-1)/2}, \dots, -\tilde{\gamma}_2, -\tilde{\gamma}_1, -\tilde{\gamma}_n, -\tilde{\gamma}_{n-1}, \dots, -\tilde{\gamma}_{(n+n_1+1)/2}, \tilde{\gamma}_{(n+n_1+1)/2}, \dots, \tilde{\gamma}_{n-1}, \tilde{\gamma}_n\}. \end{aligned} \quad (20)$$

Because $\tilde{\alpha}_{n_1} - \tilde{\beta}_n = 0$, (16) simplifies immediately to

$$\Delta E = -Jc_1(\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_n - \tilde{\gamma}_{n_1})/2. \quad (21)$$

(ii) *odd + even* \Rightarrow *odd*.

We take $[\alpha]$ odd and $[\beta]$ even. Choosing $\alpha_{(n_1+1)/2} = 0$,

$$\{\tilde{\alpha}_i\} = \{\tilde{\alpha}_1, \tilde{\alpha}_2, \dots, \tilde{\alpha}_{(n_1-1)/2}, 0, -\tilde{\alpha}_{(n_1-1)/2}, \dots, -\tilde{\alpha}_2, -\tilde{\alpha}_1\}. \quad (22)$$

A consistent choice of labeling for $[\beta]$ which results in the correct final state is to take the mirror symmetry points to lie between spins $i = 0$ and $i = 1$ and between $i = (n - n_1)/2$ and $i = (n - n_1)/2 + 1$. Hence we may write

$$\begin{aligned} \{\tilde{\beta}_i\} &= \{\tilde{\beta}_{n_1+1}, \tilde{\beta}_{n_1+2}, \dots, \tilde{\beta}_{(n+n_1)/2}, \\ &\quad -\tilde{\beta}_{(n+n_1)/2}, \dots, -\tilde{\beta}_{n_1+2}, -\tilde{\beta}_{n_1+1}\}. \end{aligned} \quad (23)$$

It is immediately apparent from (22) and (23) that

$$\tilde{\alpha}_{n_1} - \tilde{\beta}_n = -(\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1}). \quad (24)$$

Using $[\alpha]$ and $[\beta]$ to construct $[\gamma]$ will preserve a point of mirror symmetry at $i = (n_1 + 1)/2$. Hence

$$\begin{aligned} \{\tilde{\gamma}_i\} &= \{\tilde{\gamma}_1, \tilde{\gamma}_2, \dots, \tilde{\gamma}_{(n_1-1)/2}, 0, -\tilde{\gamma}_{(n_1-1)/2}, \dots, \\ &\quad -\tilde{\gamma}_2, -\tilde{\gamma}_1, -\tilde{\gamma}_n, -\tilde{\gamma}_{n-1}, \dots, \\ &\quad -\tilde{\gamma}_{(n+n_1)/2}, \tilde{\gamma}_{(n+n_1)/2}, \dots, \tilde{\gamma}_{n-1}, \tilde{\gamma}_n\}, \end{aligned} \quad (25)$$

from which it follows that

$$\tilde{\gamma}_n - \tilde{\gamma}_{n_1} = -(\tilde{\gamma}_{n_1+1} - \tilde{\gamma}_1). \quad (26)$$

Using (24) and (26) the energy difference (16) simplifies to

$$\Delta E = -Jc_1(\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_n - \tilde{\gamma}_{n_1}). \quad (27)$$

D. Recursion equations

The next step is the calculation of the spin deviations in formulas (21) and (27). To do this we start from

Eq. (10) which followed from minimizing the ground-state energy. Let

$$\tilde{\theta}_i = \frac{\theta_i^1}{D} + \frac{\theta_i^2}{D^2}. \quad (28)$$

Substituting into (10) and equating like powers of D^{-1} gives

$$\theta_i^1 = J(s_i - s_{i+1}), \quad (29)$$

$$\begin{aligned} \theta_i^n &= J(c_i \theta_{i-1}^{n-1} - c_i \theta_i^{n-1} - c_{i+1} \theta_i^{n-1} + c_{i+1} \theta_{i+1}^{n-1}), \\ n &> 1. \end{aligned} \quad (30)$$

Again it is necessary to consider separately the combination of states with different symmetries.

(i) *odd + odd* \rightarrow *even*. Note first that $\alpha_i^1 - \beta_{n_1+i}^1$ depends only on the $\{s_i^\alpha\}$ and $\{s_i^\beta\}$, that is, only on the value of the spins for $D = \infty$. Let

$$\alpha_i^1 - \beta_{n_1+i}^1 = 0, \quad i < n_0, \quad (31)$$

$$\alpha_i^1 - \beta_{n_1+i}^1 = a_0, \quad i = n_0. \quad (32)$$

Then a consequence of the spin labeling and symmetry summarized by Eqs. (18) and (19) is that

$$\alpha_{-i}^1 - \beta_{n_1-i}^1 = 0, \quad i < n_0, \quad (33)$$

$$\alpha_{-i}^1 - \beta_{n_1-i}^1 = -a_0, \quad i = n_0. \quad (34)$$

It is apparent from the recursion equations (30) that after one step of the iteration the spin differences $\tilde{\alpha}_i - \tilde{\beta}_{n_1+i}$ and $\tilde{\alpha}_{-i} - \tilde{\beta}_{n_1-i}$ with $i = (n_0 - 1)$ will attain a nonzero value; after a second step these differences with $i = n_0 - 2$ will become nonzero and so on. Therefore iterating $(n_0 - 1)$ times gives the leading order result

$$\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1} = J^{n_0-1} \cos(\pi/p)^{n_0-1} a_0 / D^{n_0}. \quad (35)$$

Note that we have assumed that $c_i = \cos(\pi/p) \forall i$. This is true to leading order near $\Delta = \pi/p$.

It is also appropriate to mention here that further iteration of the linear equations will generate corrections to (35) which are correct for the quadratic Hamiltonian (8) but not for the full chiral clock model (1). However, these terms are not necessary for our argument.

As a consequence of the conditions (13) and because $[\gamma] = [\alpha\beta]$ it must also hold that

$$\gamma_i^1 - \gamma_{n_1+i}^1 = 0, \quad -n_0 < i < n_0, \quad (36)$$

$$\gamma_i^1 - \gamma_{n_1+i}^1 = a_0, \quad i = \pm n_0. \quad (37)$$

Iterating n_0 times using (30) gives

$$\tilde{\gamma}_n - \tilde{\gamma}_{n_1} = 2J^{n_0} \cos(\pi/p)^{n_0} a_0 / D^{n_0+1}, \quad (38)$$

where the factor 2 appears because terms which iterate both from the right and left along the chain contribute to this order. Hence the energy difference (21) is

$$\Delta E = -J^{2n_0} \cos(\pi/p)^{2n_0} a_0^2 / D^{2n_0+1}. \quad (39)$$

(ii) *odd + even* \Rightarrow *odd*. We assume as before that (31) and (32) hold. It follows immediately from considering (22) and (23) that

$$\alpha_i^1 - \beta_{n_1+i}^1 = 0, \quad -(n_0 - 1) < i < n_0, \quad (40)$$

$$\alpha_{n_0}^1 - \beta_{n_1+n_0}^1 = a_0, \quad \alpha_{-(n_0-1)}^1 - \beta_{n_1-(n_0-1)}^1 = -a_0. \quad (41)$$

Similarly

$$\gamma_i^1 - \gamma_{n_1+i}^1 = 0, \quad -(n_0 - 1) < i < n_0, \quad (42)$$

$$\gamma_i^1 - \gamma_{n_1+i}^1 = a_0, \quad i = n_0, -(n_0 - 1). \quad (43)$$

Iterating $(n_0 - 1)$ times,

$$\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1} = J^{n_0-1} \cos(\pi/p)^{n_0-1} a_0 / D^{n_0} \quad (44)$$

from terms iterating from the right and

$$\tilde{\gamma}_n - \tilde{\gamma}_{n_1} = J^{n_0-1} \cos(\pi/p)^{n_0-1} a_0 / D^{n_0} \quad (45)$$

from terms iterating from the left. Using (27) the energy difference is

$$\Delta E = -J^{2n_0-1} \cos(\pi/p)^{2n_0-1} a_0^2 / D^{2n_0}. \quad (46)$$

Both of the energy differences (39) and (46) are negative. Hence for $p \geq 3$ all phases appear for large D near the multiphase point in agreement with the conclusions of Chou and Griffiths.⁴

Noting that $s_i = \pm \sin(\pi/p) \forall i$ it is apparent by inspection that $a_0^2 = 4J^2 \sin^2(\pi/p)$. We prove in Appendix A that $n_0 = [(n_{[\gamma]} + 1)/2] - 1$ where $[n]$ is the integer part of n . Therefore for all combinations of phases

$$\Delta E = -J^{n_{[\gamma]}-2} \cos(\pi/p)^{n_{[\gamma]}-2} a_0^2 / D^{n_{[\gamma]}-1}. \quad (47)$$

Correction terms $\mathcal{O}(1/D^{n_{[\gamma]}})$ will arise from contributions to the energy difference (16) and the recursion equations (10) from nonharmonic terms in the Hamiltonian (1). There will also be correction terms within the harmonic approximation (8) itself arising from further iteration of the recursion equations (10).

E. Phase widths

An advantage of the formalism presented above is that it allows a calculation of the widths of the long-period phases. We define $\Delta_{\alpha\gamma}$, $\Delta_{\beta\gamma}$, and $\Delta_{\alpha\beta}$ by

$$E_{[\alpha]}(\Delta_{\alpha\gamma}) = E_{[\gamma]}(\Delta_{\alpha\gamma}), \quad (48)$$

$$E_{[\beta]}(\Delta_{\beta\gamma}) = E_{[\gamma]}(\Delta_{\beta\gamma}), \quad (49)$$

$$E_{[\alpha]}(\Delta_{\alpha\beta}) = E_{[\beta]}(\Delta_{\alpha\beta}). \quad (50)$$

For a stable phase $[\gamma]$ $\Delta_{\alpha\beta}$ will lie between $\Delta_{\alpha\gamma}$ and $\Delta_{\beta\gamma}$ and if the phase $[\gamma]$ is not too wide a Taylor expansion gives

$$E_{[\alpha]}(\Delta_{\alpha\gamma}) = E_{[\alpha]}(\Delta_{\alpha\beta}) + E'_{[\alpha]}(\Delta_{\alpha\gamma} - \Delta_{\alpha\beta}), \quad (51)$$

$$E_{[\gamma]}(\Delta_{\alpha\gamma}) = E_{[\gamma]}(\Delta_{\alpha\beta}) + E'_{[\gamma]}(\Delta_{\alpha\gamma} - \Delta_{\alpha\beta}), \quad (52)$$

where ' denotes a derivative with respect to Δ .

Subtracting (52) from (51) and using (48) gives

$$(E'_{[\alpha]} - E'_{[\gamma]})(\Delta_{\alpha\gamma} - \Delta_{\alpha\beta}) = E_{[\gamma]}(\Delta_{\alpha\beta}) - E_{[\alpha]}(\Delta_{\alpha\beta}) \quad (53)$$

$$= E_{[\gamma]}(\Delta_{\alpha\beta}) - \frac{n_{[\alpha]}}{n_{[\gamma]}} E_{[\alpha]}(\Delta_{\alpha\beta}) - \frac{n_{[\beta]}}{n_{[\gamma]}} E_{[\beta]}(\Delta_{\alpha\beta}) \quad (54)$$

$$\equiv \frac{\Delta E}{n_{[\gamma]}}, \quad (55)$$

where in the penultimate step we have used (50) and in the final step the definition of ΔE , Eq.(6). Writing down a similar expression for $\Delta_{\beta\gamma} - \Delta_{\alpha\beta}$ and combining it with (55) gives an expression for the width of the phase $[\gamma]$

$$W_{[\gamma]} \equiv (\Delta_{\beta\gamma} - \Delta_{\alpha\gamma}) = \Delta E \{ (E'_{[\beta]} - E'_{[\gamma]})^{-1} - (E'_{[\alpha]} - E'_{[\gamma]})^{-1} \} / n_{[\gamma]}. \quad (56)$$

For $D = \infty$ the energy per spin of a ground-state phase at the multiphase point $[\alpha]$, say, is

$$E_{[\alpha]} = -J \{ l_{[\alpha]} \cos \Delta + (1 - l_{[\alpha]}) \cos(-2\pi/p + \Delta) \}, \quad (57)$$

where $l_{[\alpha]}$ is the fraction of nearest-neighbor ferromagnetic bonds. Differentiating the expression (57) and similar formulas for $[\beta]$ and $[\gamma]$ and substituting into (56)

gives to leading order

$$W_{[\gamma]} = \frac{\Delta E(l_{[\alpha]} - l_{[\beta]})}{2Jn_{[\gamma]} \sin(\pi/p)(l_{[\beta]} - l_{[\gamma]})(l_{[\alpha]} - l_{[\gamma]})}. \quad (58)$$

It is not hard to show inductively that

$$\begin{aligned} l_{[\beta]} - l_{[\alpha]} &= (n_{[\alpha]}n_{[\beta]})^{-1}, & l_{[\beta]} - l_{[\gamma]} &= (n_{[\beta]}n_{[\gamma]})^{-1}, \\ l_{[\alpha]} - l_{[\gamma]} &= (n_{[\alpha]}n_{[\gamma]})^{-1}. \end{aligned} \quad (59)$$

Therefore using (47) we finally obtain

$$W_{[\gamma]} = -2J^{n_{[\gamma]}-1} \cos(\pi/p)^{n_{[\gamma]}-2} \sin(\pi/p)n_{[\gamma]}/D^{n_{[\gamma]}-1}. \quad (60)$$

III. XY MODEL WITH COMPETING FIRST- AND SECOND-NEIGHBOR INTERACTIONS AND p -FOLD SPIN ANISOTROPY

A. Definitions and notation

In the second part of the paper we extend the formalism developed earlier to obtain new results for a more complex spin model. This is the XY model with competing first- and second-neighbor interactions and p -fold spin anisotropy. Each classical XY spin vector lies in a plane perpendicular to the z axis and has unit length. The Hamiltonian can be written

$$\mathcal{H} = \sum_i \left[-J_1 \cos(\theta_{i-1} - \theta_i) + J_2 \cos(\theta_{i-2} - \theta_i) - D(\cos(p\theta_i) - 1)/p^2 \right], \quad (61)$$

where θ_i is the angle between the spin located at site i and, say, the x axis. Competition is introduced along the z direction by taking the first- and second-neighbor interactions to be ferromagnetic and antiferromagnetic, respectively ($J_1 > 0, J_2 > 0$). $x = J_2/J_1$ will prove an important variable in the description of the phase diagram.

The parameter $D > 0$ models a p -fold spin anisotropy in the (x, y) plane. The ground state in the two limits $D = 0$ and $D = \infty$ is well understood. For $D = 0$ it is ferromagnetic for $x < 1/4$. For $x > 1/4$ it exhibits helical order with a wave vector $\vec{q} = q\hat{z}$ which is, in general, incommensurate with the underlying lattice. The magnitude of the wave vector is determined by the exchange energies through the relation $\cos q = (4x)^{-1}$.

For $D = \infty$, however, the spin angles θ_i are constrained to take one of the discrete set of values $2\pi n_i/p$, $n_i = 0, 1, \dots, p-1$. The Hamiltonian (61) then reduces to a p -state clock model with competing interactions. The ground state now has a very different character: only a few short-period commensurate phases are stable as x is varied. Boundaries between the different ground states can either be simple first-order transitions with only the neighboring phases being stable or multiphase points at which an infinite number of phases have the same energy.

To fully describe the ground states and the phases degenerate at the multiphase points it is necessary to extend the notation introduced in Sec. II A. Note that at multiphase points such as $x = 1$ for $p = 6$ all phases with $n_i - n_{i-1} = 1, 2$, with the proviso that $n_{i+1} - n_i = n_i - n_{i-1} = 2$ is not allowed, are stable. Hence the natural definition of a wall is as lying between spins i and $i-1$ for which $n_i - n_{i-1} = 2$. The term band is used as before to describe the sequence of spins between two walls. The phases stable at the multiphase point can then be more easily described as those containing only bands of lengths ≥ 2 .

A given state will be labeled by $\langle \ell_1, \ell_2, \dots, \ell_m \rangle$ where the repeating sequence comprises bands of length $\ell_1, \ell_2, \dots, \ell_m$. It may be helpful to list some examples for $p = 6$:

$$\begin{aligned} \langle 2 \rangle & \dots | 01 | 34 | 01 | \dots \\ \langle 23 \rangle & \dots | 01 | 345 | 12 | 450 | \dots \\ \langle 3^2 4 \rangle & \dots | 012 | 450 | 2345 | 123 | 501 | 3450 | \dots \\ \langle \infty \rangle & \dots 01234 \dots \end{aligned} \quad (62)$$

Compare the notation using square brackets $[\ell_1, \ell_2, \dots, \ell_m]$ introduced in Sec. II A where the walls correspond to $n_i - n_{i-1} = 1$ in a background matrix of $n_i - n_{i-1} = 0$. This will also be needed here.

We are now in a position to describe the ground states of the Hamiltonian (61) for all values of p and $D = \infty$. The results which were obtained by comparing the energies of the possible ground states and checked using the Floria-Griffiths algorithm⁹ to ensure no states were missed are summarized in Fig. 1.

(i) For $p = 2$ and 3, $[\infty]$ is stable for $x < 1/2$ and $[2]$

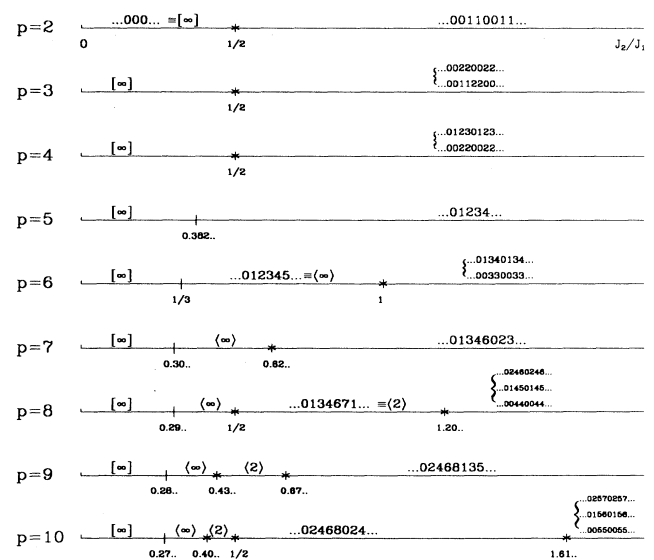


FIG. 1. Ground states of the p -state clock model with ferromagnetic first-neighbor interactions J_1 and antiferromagnetic second-neighbor interactions J_2 . The phases are labeled by the spin sequences $\dots n_{i-2}n_{i-1}n_i n_{i+1}n_{i+2} \dots$. A vertical line represents a first-order boundary and a star a multiphase point.

for $x > 1/2$. $x = 1/2$ is a multiphase point.

(ii) For $p = 4$, $[\infty]$ is stable for $x < 1/2$ and $\langle \infty \rangle \equiv [1]$ (together with the phase ...002200 ...) for $x > 1/2$. Again $x = 1/2$ is a multiphase point.

(iii) For $p = 5$ for $x < x_0^{(5)} = \{1 + \cos(2\pi/5)\}^{-1}/2$, $[\infty]$ is stable. For $x > x_0$, $\langle \infty \rangle$ is stable. x_0 is not a multiphase point.

(iv) For $p \geq 6$ there is a common trend for small x . For $x < x_1^{(p)} = \{1 + \cos(2\pi/p)\}^{-1}/2$, $[\infty]$ is stable. For $x_1^{(p)} < x < x_0^{(p)} = \{\cos(2\pi/p) - \cos(6\pi/p)\}/2\{\cos(4\pi/p) - \cos(6\pi/p)\}$, the phase $\langle \infty \rangle$ appears. For $x > x_0^{(p)}$, $\langle 2 \rangle$ is stable. (For $p = 6$ the state ...003300 ... is degenerate with $\langle 2 \rangle$.) For $p = 6$ and 7 the phases listed above provide all the ground states. For $p \geq 8$ other phases are stable for higher values of x , but these phases will not concern us here. At the points $x_1^{(p)}$ the phases $[\infty]$ and $\langle \infty \rangle$ coexist but no other phases are stable and there is

a first order transition. $x_0^{(p)}$, however, is a multiphase point where all phases comprising bands of length ≥ 2 are degenerate.

Our aim is to apply an expansion in D^{-1} to understand the phase structure in the vicinity of the multiphase points $x_0^{(p)}$. We proceed in the same way as in Sec. II. The results are listed in Sec. III F. A brief account of this work has appeared elsewhere.⁷

B. The energy differences

Our approach follows that described in Sec. II B for the chiral clock model. The first step as before is to expand the Hamiltonian (61) to second order in the $\tilde{\theta}_i$, the deviations of the spins from their positions at $D = \infty$, which were defined by Eq. (7). This gives

$$\begin{aligned} \tilde{\mathcal{H}} = \mathcal{H} |_{D=\infty} + \sum_i \{ & J_{i,[1]}^\theta (\tilde{\theta}_{i-1} - \tilde{\theta}_i + \Delta_{i,[1]}^\theta)^2 - J_1 (s_{i,[1]}^\theta)^2 / c_{i,[1]}^\theta \\ & + J_2 (s_{i,[2]}^\theta)^2 / c_{i,[2]}^\theta - J_{i,[2]}^\theta (\tilde{\theta}_{i-2} - \tilde{\theta}_i + \Delta_{i,[2]}^\theta)^2 + D \tilde{\theta}_i^2 \} / 2, \end{aligned} \quad (63)$$

where

$$\begin{aligned} s_{i,[m]}^\theta &= \sin(\theta_{i-[m]}^0 - \theta_i^0), & c_{i,[m]}^\theta &= \cos(\theta_{i-[m]}^0 - \theta_i^0), \\ \Delta_{i,[m]}^\theta &= s_{i,[m]}^\theta / c_{i,[m]}^\theta, & J_{i,[m]}^\theta &= J_m c_{i,[m]}^\theta. \end{aligned} \quad (64)$$

Minimizing (63) with respect to $\tilde{\theta}_i$ leads to the equation

$$\begin{aligned} D \tilde{\theta}_i &= J_{i,[1]} (\tilde{\theta}_{i-1} - \tilde{\theta}_i + \Delta_{i,[1]}^\theta) - J_{i+1,[1]} (\tilde{\theta}_i - \tilde{\theta}_{i+1} + \Delta_{i+1,[1]}^\theta) \\ &\quad - J_{i,[2]} (\tilde{\theta}_{i-2} - \tilde{\theta}_i + \Delta_{i,[2]}^\theta) + J_{i+2,[2]} (\tilde{\theta}_i - \tilde{\theta}_{i+2} + \Delta_{i+2,[2]}^\theta). \end{aligned} \quad (65)$$

It is possible to calculate the energy difference ΔE , defined by (6), exactly for the quadratic Hamiltonian (63). As before we consider the branching process $[\alpha] + [\beta] \Rightarrow [\alpha\beta] \equiv [\gamma]$, let $n_{[\alpha]} = n_1$ and $n_{[\gamma]} = n$ and identify the spins within the phases $[\alpha]$, $[\beta]$, and $[\gamma]$ by α_i , β_i , and γ_i , respectively. We choose to label the spins such that

$$\begin{aligned} \gamma_i^0 &= \alpha_i^0, & 1 \leq i \leq n_1, \\ \gamma_i^0 &= \beta_i^0, & n_i + 1 \leq i \leq n, \end{aligned} \quad (66)$$

from which it follows that

$$\begin{aligned} \Delta_{i,[m]}^\alpha &= \Delta_{i,[m]}^\gamma, & J_{i,[m]}^\alpha &= J_{i,[m]}^\gamma, & 1 \leq i \leq n_1, \\ \Delta_{i,[m]}^\beta &= \Delta_{i,[m]}^\gamma, & J_{i,[m]}^\beta &= J_{i,[m]}^\gamma, & n_i + 1 \leq i \leq n. \end{aligned} \quad (67)$$

The energy difference (6) may now be written

$$\begin{aligned} 2\Delta E &= \sum_{i=1}^{n_1} \{ [J_{i,[1]} (\tilde{\gamma}_{i-1} - \tilde{\gamma}_i + \tilde{\Delta}_{i,[1]})^2 - J_{i,[1]} (\tilde{\alpha}_{i-1} - \tilde{\alpha}_i + \Delta_{i,[2]})^2] \\ &\quad - [J_{i,[2]} (\tilde{\gamma}_{i-2} - \tilde{\gamma}_i + \Delta_{i,[2]})^2 - J_{i,[2]} (\tilde{\alpha}_{i-2} - \tilde{\alpha}_i + \Delta_{i,[2]})^2] + D(\tilde{\gamma}_i^2 - \tilde{\alpha}_i^2) \} \\ &\quad + \sum_{i=n_i+1}^n \{ [J_{i,[1]} (\tilde{\gamma}_{i-1} - \tilde{\gamma}_i + \Delta_{i,[1]})^2 - J_{i,[1]} (\tilde{\beta}_{i-1} - \tilde{\beta}_i + \Delta_{i,[1]})^2] \\ &\quad - [J_{i,[2]} (\tilde{\gamma}_{i-2} - \tilde{\gamma}_i + \Delta_{i,[2]})^2 - J_{i,[2]} (\tilde{\beta}_{i-2} - \tilde{\beta}_i + \Delta_{i,[2]})^2] + D(\tilde{\gamma}_i^2 - \tilde{\beta}_i^2) \}. \end{aligned} \quad (68)$$

Using Eq. (65) this can be simplified to give

$$\begin{aligned}
2\Delta E = & J_{1,[1]}\{(\tilde{\alpha}_{n_1} - \tilde{\beta}_n)(\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}) - (\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_n - \tilde{\gamma}_{n_1})\} \\
& - J_{1,[2]}\{(\tilde{\alpha}_{n_1-1} - \tilde{\beta}_{n-1})(\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}) - (\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_{n-1} - \tilde{\gamma}_{n_1-1})\} \\
& - J_{2,[2]}\{(\tilde{\alpha}_{n_1} - \tilde{\beta}_n)(\tilde{\gamma}_2 - \tilde{\gamma}_{n_1+2}) - (\tilde{\alpha}_2 - \tilde{\beta}_{n_1+2})(\tilde{\gamma}_n - \tilde{\gamma}_{n_1})\}. \tag{69}
\end{aligned}$$

Again the energy difference depends only on the difference of the spin deviations on a few sites. Given a careful labeling of the states these can be calculated to leading order and their signs determined.

C. Labeling the spins

We label the spins in a way identical to that described in Sec. II C. This simplifies the formula for the energy difference ΔE as follows:

(i) *odd + odd* \Rightarrow *even*. With the choice (17) it can be read off immediately from (18), (19), and (20) that

$$\begin{aligned}
\tilde{\alpha}_{n_1} - \tilde{\beta}_n &= 0, \\
\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1} &= -(\tilde{\alpha}_{n_1-1} - \tilde{\beta}_{n-1}), \\
(\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}) &= (\tilde{\gamma}_n - \tilde{\gamma}_{n_1}), \tag{70}
\end{aligned}$$

and hence from (69),

$$\begin{aligned}
2\Delta E = & -J_{1,[1]}(\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_n - \tilde{\gamma}_{n_1}) + J_{1,[2]}(\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_{n-1} - \tilde{\gamma}_{n_1-1} + \tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}) \\
& + J_{2,[2]}(\tilde{\alpha}_2 - \tilde{\beta}_{n_1+2})(\tilde{\gamma}_n - \tilde{\gamma}_{n_1}). \tag{71}
\end{aligned}$$

(ii) *odd + even* \Rightarrow *odd*. Using (22), (23), and (25),

$$\begin{aligned}
\tilde{\alpha}_{n_1-1} - \tilde{\beta}_{n-1} &= -(\tilde{\alpha}_2 - \tilde{\beta}_{n_1+2}), \\
\tilde{\alpha}_{n_1} - \tilde{\beta}_n &= -(\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1}), \\
(\tilde{\gamma}_{n-1} - \tilde{\gamma}_{n_1-1}) &= -(\tilde{\gamma}_{n_1+2} - \tilde{\gamma}_2), \\
(\tilde{\gamma}_n - \tilde{\gamma}_{n_1}) &= -(\tilde{\gamma}_{n_1+1} - \tilde{\gamma}_1). \tag{72}
\end{aligned}$$

Therefore,

$$\begin{aligned}
2\Delta E = & 2J_{1,[1]}(\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}) + J_{1,[2]}(\tilde{\alpha}_2 - \tilde{\beta}_{n_1+2})(\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}) + (\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_2 - \tilde{\gamma}_{n_1+2}) \\
& + J_{2,[2]}(\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1})(\tilde{\gamma}_2 - \tilde{\gamma}_{n_1+2}) + (\tilde{\alpha}_2 - \tilde{\beta}_{n_1+2})(\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}). \tag{73}
\end{aligned}$$

D. Recursion equations

We follow Sec. IID in using recursion equations to derive the leading order terms in the energy differences (71) and (73). Substituting (28) into the energy minimization Eqs. (65) gives

$$\begin{aligned}
\theta_i^1 &= J_1(s_{i,[1]} - s_{i+1,[1]}) - J_2(s_{i,[2]} - s_{i+2,[2]}), \tag{74} \\
\theta_i^n &= J_{i,[1]}(\theta_{i-1}^{n-1} - \theta_i^{n-1}) - J_{i+1,[1]}(\theta_i^{n-1} - \theta_{i+1}^{n-1}) \\
& - J_{i,[2]}(\theta_{i-2}^{n-1} - \theta_i^{n-1}) + J_{i+2,[2]}(\theta_i^{n-1} - \theta_{i+2}^{n-1}). \tag{75}
\end{aligned}$$

For the model with second-neighbor interactions it is necessary to consider four different cases when calculating the energy differences.

(i) *odd + odd* \Rightarrow *even; even starting position*. Let

$$\begin{aligned}
\alpha_i^1 - \beta_{n_1+i}^1 &= 0, \quad -2n_0 < i < 2n_0, \\
\alpha_{2n_0}^1 - \beta_{n_1+2n_0}^1 &= a_0, \quad \alpha_{-2n_0}^1 - \beta_{n_1-2n_0}^1 = -a_0, \tag{76}
\end{aligned}$$

that is, i is even when $\alpha_i^1 - \beta_{n_1+i}^1$ is first nonzero. We consider $n_0 \geq 1$ throughout. This implies

$$\begin{aligned}
\gamma_i^1 - \gamma_{n_1+i}^1 &= 0, \quad -2n_0 < i < 2n_0, \\
\gamma_i^1 - \gamma_{n_1+i}^1 &= a_0, \quad i = \pm 2n_0. \tag{77}
\end{aligned}$$

The recursion equations (75) show that the spin deviations $\tilde{\alpha}_i - \tilde{\beta}_{n_1+i}$ for $i = \pm(2n_0 - 1)$ and $i = \pm(2n_0 - 2)$ will be $\mathcal{O}(1/D^2)$; for $i = \pm(2n_0 - 3)$ and $i = \pm(2n_0 - 4)$ will be $\mathcal{O}(1/D^3)$, and so forth. Hence

$$\begin{aligned}
\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1} &\sim \mathcal{O}(1/D^{n_0+1}), \quad \tilde{\gamma}_n - \tilde{\gamma}_{n_1} \sim \mathcal{O}(1/D^{n_0+1}), \\
\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1} &\sim \mathcal{O}(1/D^{n_0+1}), \quad \tilde{\alpha}_2 - \tilde{\beta}_{n_1+2} \sim \mathcal{O}(1/D^{n_0}) \tag{78}
\end{aligned}$$

and the leading order term in the energy difference (71) is

$$2\Delta E = J_{2,[2]}(\tilde{\alpha}_2 - \tilde{\beta}_{n_1+2})(\tilde{\gamma}_n - \tilde{\gamma}_{n_1}). \tag{79}$$

From the recursion equations (75) iterating $(n_0 - 1)$ times

$$\begin{aligned}
\tilde{\alpha}_2 - \tilde{\beta}_{n_1+2} &= \{a_0(-J_2)^{n_0-1} c_{2c}^{n_w[2n_0,2]} \\
& \times c_{2i}^{n_0-1-n_w[2n_0,2]}\} / D^{n_0}, \tag{80}
\end{aligned}$$

where $n_w(i, j)$ is the number of walls between i and j and

$$\cos(\alpha_{i-2}^0 - \alpha_i^0) \equiv c_{2c} = \cos(6\pi/p), \quad (81)$$

if the iteration step jumps across a wall and

$$\cos(\alpha_{i-2}^0 - \alpha_i^0) \equiv c_{2i} = \cos(4\pi/p), \quad (82)$$

if it does not.

Similarly, iterating n_0 times and collecting equal terms from the left and right,

$$\tilde{\gamma}_n - \tilde{\gamma}_{n_1} = \{2a_0(-J_2)^{n_0} c_{2c}^{n_w[2n_0,0]} c_{2i}^{n_0 - n_w[2n_0,0]}\} / D^{n_0+1}. \quad (83)$$

Substituting (80) and (83) into (79) gives

$$\Delta E = \{J_{2,[2]} a_0^2 (-J_2)^{2n_0-1} c_{2c}^{n_w[2n_0,2] + n_w[2n_0,0]} \times c_{2i}^{2n_0 - n_w[2n_0,2] - n_w[2n_0,0] - 1}\} / D^{2n_0+1}. \quad (84)$$

$\tilde{\alpha}_n = 0$. Therefore the band containing $i = n$ of the state $\langle \alpha \rangle$ must be of odd length. 1 bands are forbidden. If the band is of length 3, $J_{2,[2]} = J_2 c_{2c}$ and $n_w[2n_0, 0] = n_w[2n_0, 2] + 1$. If it is of length ≥ 5 , $J_{2,[2]} = J_2 c_{2i}$ and $n_w[2n_0, 0] = n_w[2n_0, 2]$. In both cases,

$$\Delta E_0 = -\{a_0^2 (J_2)^{2n_0} c_{2c}^{2n_w[2n_0,0]} c_{2i}^{2n_0 - 2n_w[2n_0,0]}\} / D^{2n_0+1}, \quad (85)$$

where the relevance of the subscript on ΔE will become apparent later.

(ii) *odd + odd \Rightarrow even; odd starting position.* Let

$$\begin{aligned} \alpha_i^1 - \beta_{n_1+i}^1 &= 0, & -(2n_0 - 1) < i < (2n_0 - 1), \\ \alpha_{2n_0-1}^1 - \beta_{n_1+2n_0-1}^1 &= a_0, \\ \alpha_{-(2n_0-1)}^1 - \beta_{n_1-(2n_0-1)}^1 &= -a_0, \end{aligned} \quad (86)$$

where we now consider i odd for $\alpha_i^1 - \beta_{n_1+i}^1$ first nonzero. This implies

$$\begin{aligned} \gamma_i^1 - \gamma_{n_1+i}^1 &= 0, & -(2n_0 - 1) < i < (2n_0 - 1), \\ \gamma_i^1 - \gamma_{n_1+i}^1 &= a_0, & i = \pm(2n_0 - 1). \end{aligned} \quad (87)$$

Iterating the recursion equations (75) shows that

$$\begin{aligned} \tilde{\alpha}_1 - \tilde{\beta}_{n_1+1} &\sim \mathcal{O}(1/D^{n_0}), & \tilde{\gamma}_n - \tilde{\gamma}_{n_1} &\sim \mathcal{O}(1/D^{n_0+1}), \\ \tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1} &\sim \mathcal{O}(1/D^{n_0}), & \tilde{\alpha}_2 - \tilde{\beta}_{n_1+2} &\sim \mathcal{O}(1/D^{n_0}), \end{aligned} \quad (88)$$

and hence the leading order term in the energy difference (71) is

$$2\Delta E = J_{1,[2]} (\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1}) (\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1} + \tilde{\gamma}_{n-1} - \tilde{\gamma}_{n_1-1}). \quad (89)$$

From the recursion equations (75) iterating $(n_0 - 1)$ times,

$$\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1} = \tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1} = \tilde{\gamma}_{n-1} - \tilde{\gamma}_{n_1-1} = \{a_0(-J_2)^{n_0-1} c_{2c}^{n_w[2n_0-1,1]} c_{2i}^{n_0-1 - n_w[2n_0-1,1]}\} / D^{n_0}. \quad (90)$$

$J_{1,[2]} = J_2 c_{2i}$ as the band containing the spin $i = n$ must be of length ≥ 3 . Therefore,

$$\Delta E_2 = \{a_0^2 (J_2)^{2n_0-1} c_{2c}^{2n_w[2n_0-1,1]} c_{2i}^{2n_0-1 - 2n_w[2n_0-1,1]}\} / D^{2n_0}. \quad (91)$$

(iii) *odd + even \Rightarrow odd; even starting position.* Let

$$\begin{aligned} \alpha_i^1 - \beta_{n_1+i}^1 &= 0, & -(2n_0 - 1) < i < 2n_0, \\ \alpha_{2n_0}^1 - \beta_{n_1+2n_0}^1 &= a_0, & \alpha_{-(2n_0-1)}^1 - \beta_{n_1-(2n_0-1)}^1 &= -a_0, \\ \alpha_{2n_0+1}^1 - \beta_{n_1+2n_0+1}^1 &= a_1, & \alpha_{-2n_0}^1 - \beta_{n_1-2n_0}^1 &= -a_1 \end{aligned} \quad (92)$$

and similarly for the $\gamma_i^1 - \gamma_{n_1+i}^1$. Noting from the recursion equations (75) that

$$\begin{aligned} \tilde{\alpha}_1 - \tilde{\beta}_{n_1+1} &\sim \mathcal{O}(1/D^{n_0+1}), & \tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1} &\sim \mathcal{O}(1/D^{n_0+1}), \\ \tilde{\gamma}_2 - \tilde{\gamma}_{n_1+2} &\sim \mathcal{O}(1/D^{n_0}), & \tilde{\alpha}_2 - \tilde{\beta}_{n_1+2} &\sim \mathcal{O}(1/D^{n_0}), \end{aligned} \quad (93)$$

and that whatever the arrangement of walls symmetry implies $J_{1,[2]} = J_{2,[2]}$ the energy difference (73) becomes

$$\Delta E = J_{1,[2]} \{(\tilde{\alpha}_2 - \tilde{\beta}_{n_1+2}) (\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}) + (\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1}) (\tilde{\gamma}_2 - \tilde{\gamma}_{n_1+2})\}. \quad (94)$$

Iterating the recursion equations (75) $(n_0 - 1)$ times

$$\tilde{\alpha}_2 - \tilde{\beta}_{n_1+2} = \tilde{\gamma}_2 - \tilde{\gamma}_{n_1+2} = \{a_0(-J_2)^{n_0-1} c_{2c}^{n_w[2n_0,2]} c_{2i}^{n_0-1 - n_w[2n_0,2]}\} / D^{n_0}. \quad (95)$$

Calculation of $\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1}$ is slightly more involved as iterating n_0 times contributions can arise either from hops from $i = 2n_0$ which include a J_1 term or from hops from $i = 2n_0 + 1$ which include only J_2 terms,

$$\begin{aligned} \tilde{\alpha}_1 - \tilde{\beta}_{n_1+1} = & \{a_0(-J_2)^{n_0-1} J_1 c_{2c}^{n_w[2n_0,1]-1} c_{2i}^{n_0-n_w[2n_0,1]-1} (c_{2c} c_{1i}(n_0 - \tilde{n}_0) + c_{2i} c_{1c} \tilde{n}_0) \\ & + a_1(-J_2)^{n_0} c_{2c}^{n_w[2n_0+1,1]} c_{2i}^{n_0-n_w[2n_0+1,1]} \\ & - a_0(-J_2)^{n_0} c_{2c}^{n_w[-(2n_0-1),1]} c_{2i}^{n_0-n_w[-(2n_0-1),1]} \} / D^{n_0+1}, \end{aligned} \quad (96)$$

where \tilde{n}_0 is the number of paths in which the J_1 hop crosses a wall between $2n_0$ and 1, $c_{1c} = \cos(4\pi/p)$, and $c_{1i} = \cos(2\pi/p)$. The expression for $\tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1}$ is similar but the last term, as it corresponds to iteration from the left, contributes with opposite sign. Therefore the energy difference (73) is

$$\begin{aligned} \Delta E_3 = & \{2J_{1,[2]} a_0^2 (J_2)^{2n_0-2} J_1 c_{2c}^{n_w[2n_0,2]+n_w[2n_0,1]-1} c_{2i}^{2n_0-2-n_w[2n_0,2]-n_w[2n_0,1]} (c_{2c} c_{1i}(n_0 - \tilde{n}_0) + c_{2i} c_{1c} \tilde{n}_0) \\ & - 2J_{1,[2]} a_0 a_1 (J_2)^{2n_0-1} c_{2c}^{n_w[2n_0,2]+n_w[2n_0+1,1]} c_{2i}^{2n_0-1-n_w[2n_0,2]-n_w[2n_0+1,1]} \} / D^{2n_0+1}. \end{aligned} \quad (97)$$

(iv) *odd + even* \Rightarrow *odd; odd starting position*. Let

$$\begin{aligned} \alpha_i^1 - \beta_{n_1+i}^1 &= 0, & -(2n_0 - 2) < i < 2n_0 - 1, \\ \alpha_{2n_0-1}^1 - \beta_{n_1+2n_0-1}^1 &= a_0, & \alpha_{-(2n_0-2)}^1 - \beta_{n_1-(2n_0-2)}^1 = -a_0, \\ \alpha_{2n_0}^1 - \beta_{n_1+2n_0}^1 &= a_1, & \alpha_{-(2n_0-1)}^1 - \beta_{n_1-(2n_0-1)}^1 = -a_1, \end{aligned} \quad (98)$$

and similarly for the $\gamma_i^1 - \gamma_{n_1+i}^1$. Iterating Eqs. (75) ($n_0 - 1$) times

$$\tilde{\alpha}_1 - \tilde{\beta}_{n_1+1} = \tilde{\gamma}_1 - \tilde{\gamma}_{n_1+1} = \{a_0(-J_2)^{n_0-1} c_{2c}^{n_w[2n_0-1,1]} c_{2i}^{n_0-1-n_w[2n_0-1,1]} \} / D^{n_0}, \quad (99)$$

$$\begin{aligned} \tilde{\alpha}_2 - \tilde{\beta}_{n_1+2} &= \tilde{\gamma}_2 - \tilde{\gamma}_{n_1+2} \\ &= \{a_0(-J_2)^{n_0-2} J_1 c_{2c}^{n_w[2n_0-1,2]-1} c_{2i}^{n_0-n_w[2n_0-1,2]-2} (c_{2c} c_{1i}(n_0 - 1 - n'_0) + c_{2i} c_{1c} n'_0) \\ &\quad + a_1(-J_2)^{n_0-1} c_{2c}^{n_w[2n_0,2]} c_{2i}^{n_0-1-n_w[2n_0,2]} \} / D^{n_0} \end{aligned} \quad (100)$$

where n'_0 is the number of paths in which the J_1 hop crosses a wall between $2n_0 - 1$ and 2. Using these formulas the energy difference (73) is

$$\begin{aligned} \Delta E_1 = & \{-J_{1,[1]} a_0^2 (J_2)^{2n_0-2} c_{2c}^{2n_w[2n_0-1,1]} c_{2i}^{2n_0-2-2n_w[2n_0-1,1]} \\ & - 2J_{1,[2]} a_0^2 (J_2)^{2n_0-3} J_1 c_{2c}^{n_w[2n_0-1,2]+n_w[2n_0-1,1]-1} c_{2i}^{2n_0-3-n_w[2n_0-1,2]-n_w[2n_0-1,1]} (c_{2c} c_{1i}(n_0 - 1 - n'_0) + c_{2i} c_{1c} n'_0) \\ & + 2J_{1,[2]} a_0 a_1 (J_2)^{2n_0-2} c_{2c}^{n_w[2n_0-1,1]+n_w[2n_0,2]} c_{2i}^{2n_0-2-n_w[2n_0-1,1]-n_w[2n_0,2]} \} / D^{2n_0}. \end{aligned} \quad (101)$$

E. Phases bounding $\langle \infty \rangle$

The formulas for the energy differences calculated in the preceding section may no longer hold when one of the initial phases is $\langle \infty \rangle = \dots 0123\dots$. Therefore this case is now treated separately. As the phase diagram is constructed recursively the phases which will appear on the $\langle \infty \rangle$ boundary are $\langle m \rangle$, $m = 3, 4, 5, \dots$. Hence the energy differences we wish to calculate are

$$\Delta E^{\langle \infty \rangle} = (m+1)E_{\langle m+1 \rangle} - mE_{\langle m \rangle} - E_{\langle \infty \rangle}. \quad (102)$$

In the $\langle \infty \rangle$ phase the spins remain in their clock positions as D is reduced from ∞ .

We must again consider four possibilities.

(i) $\langle 4n+3 \rangle + \langle \infty \rangle \Rightarrow \langle 4n+4 \rangle$. We consider $n \geq 1$ throughout. Choose $\langle \beta \rangle = \langle \infty \rangle$. Then $\tilde{\beta} = 0$ and $n_1 = n - 1$. The initial conditions are

$$\alpha_i^1 = 0, \quad -2n < i < 2n, \quad (103)$$

$$\alpha_{2n}^1 = -\alpha_{-2n}^1 = a_0, \quad (104)$$

$$\gamma_i^1 = 0, \quad -(2n+1) < i < 2n, \quad (105)$$

$$\gamma_{2n}^1 = -\gamma_{-(2n+1)}^1 = a_0. \quad (106)$$

Noting that $\gamma_{n_1} = -\gamma_n$ the calculation follows that described in Sec. III D(i). The energy difference is given by Eq. (85) with $n_w[2n, 0] = 0$,

$$\Delta E_0^{\langle \infty \rangle} = -\{a_0^2 (J_2)^{2n} c_{2i}^{2n}\} / D^{2n+1}. \quad (107)$$

(ii) $\langle 4n+1 \rangle + \langle \infty \rangle \Rightarrow \langle 4n+2 \rangle$. Again choose $\langle \beta \rangle = \langle \infty \rangle$. The initial conditions are now

$$\alpha_i^1 = 0, \quad -(2n-1) < i < 2n-1, \quad (108)$$

$$\alpha_{2n-1}^1 = -\alpha_{-(2n-1)}^1 = a_0, \quad (109)$$

$$\gamma_i^1 = 0, \quad -2n < i < 2n-1, \quad (110)$$

$$\gamma_{2n-1}^1 = -\gamma_{-2n}^1 = a_0. \quad (111)$$

Recalling that $n_1 = n - 1$,

$$\begin{aligned} \tilde{\gamma}_1 \sim \tilde{\gamma}_{n_1-1} \sim \tilde{\alpha}_1 \sim \tilde{\alpha}_2 \sim \mathcal{O}(1/D^{n-1}), \\ \tilde{\gamma}_{n-1} \sim \tilde{\gamma}_{n_1} \sim \tilde{\gamma}_n \sim \tilde{\gamma}_{n_1+1} \sim \mathcal{O}(1/D^n), \end{aligned} \quad (112)$$

and that the symmetry of $\langle \gamma \rangle$ implies

$$\tilde{\gamma}_1 = -\tilde{\gamma}_{n_1-1}, \quad (113)$$

the leading term in the energy difference (71) is

$$\Delta E = 2J_{1,[2]}\tilde{\alpha}_1\tilde{\gamma}_1. \quad (114)$$

Iterating the recursion equations (75) ($n-1$) times to obtain $\tilde{\alpha}_1$ and $\tilde{\gamma}_1$ gives a result

$$\Delta E_2^{<\infty>} = \{a_0^2(J_2)^{2n-1}c_{2i}^{2n-1}\}/D^{2n}. \quad (115)$$

(iii) $\langle 4n+2 \rangle + \langle \infty \rangle \Rightarrow \langle 4n+3 \rangle$. To use the energy difference formula (60) $\langle \beta \rangle$ must be even. Therefore we choose $\langle \alpha \rangle = \langle \infty \rangle$ implying $n_1 = 1$ and $\tilde{\alpha}_i = 0 \forall i$. The initial conditions are

$$\begin{aligned} \beta_{n_1+i}^1 &= 0, & -(2n-1) < i < 2n, \\ \beta_{n_1+2n}^1 &= -\beta_{n_1-(2n-1)}^1 = a_0 & \beta_{n_1+2n+1}^1 &= -\beta_{n_1-2n}^1 = a_1 \\ \gamma_i^1 &= 0, & -(2n-1) < i < (2n+1), \\ \gamma_{2n+1}^1 &= -\gamma_{-(2n-1)}^1 = a_0, & \gamma_{2n+2}^1 &= -\gamma_{-2n}^1 = a_1. \end{aligned} \quad (116)$$

Using the symmetry properties of $\langle \beta \rangle$ and $\langle \gamma \rangle$,

$$\tilde{\beta}_{n_1+i} = -\tilde{\beta}_{n_1-i+1}, \quad \tilde{\gamma}_i = -\tilde{\gamma}_{-i+2} \quad (117)$$

and noting that

$$\tilde{\beta}_3 \sim \tilde{\gamma}_3 \sim \mathcal{O}(1/D^{n-1}), \quad \tilde{\beta}_2 \sim \tilde{\gamma}_2 \sim \mathcal{O}(1/D^n), \quad (118)$$

the leading order contribution to the energy difference (73) is

$$2\Delta E = (J_{1,[2]} + J_{2,[2]})(\tilde{\beta}_3\tilde{\gamma}_2 + \tilde{\beta}_2\tilde{\gamma}_3). \quad (119)$$

Iterating the recursion equations (75) to obtain the spin deviations the final result is

$$\begin{aligned} \Delta E_3^{(\infty)} &= J_2^{2n-1}c_{2i}^{2n-1}\{a_0^2(2J_1nc_{1i} + J_2c_{2i}) \\ &\quad - 2a_0a_1J_2c_{2i}\}/D^{2n+1}. \end{aligned} \quad (120)$$

(iv) $\langle 4n \rangle + \langle \infty \rangle \Rightarrow \langle 4n+1 \rangle$. Choosing $\langle \alpha \rangle = \langle \infty \rangle$ the initial conditions are

$$\begin{aligned} \beta_{n_1+i}^1 &= 0, & -(2n-2) < i < 2n-1, \\ \beta_{n_1+2n-1}^1 &= -\beta_{n_1-(2n-2)}^1 = a_0, \\ \beta_{n_1+2n}^1 &= -\beta_{n_1-(2n-1)}^1 = a_1 \\ \gamma_i^1 &= 0, & -(2n-2) < i < 2n, \\ \gamma_{2n}^1 &= -\gamma_{-(2n-2)}^1 = a_0, & \gamma_{2n+1}^1 &= -\gamma_{-(2n-1)}^1 = a_1. \end{aligned} \quad (121)$$

Using the symmetry properties (117) the leading order contribution to the energy difference (73) is

$$\begin{aligned} 2\Delta E &= 2J_{1,[1]}\tilde{\beta}_2\tilde{\gamma}_2 + (J_{1,[2]} + J_{2,[2]})(\tilde{\beta}_3\tilde{\gamma}_2 \\ &\quad + \tilde{\beta}_2\tilde{\gamma}_3 - \tilde{\beta}_2\tilde{\gamma}_2). \end{aligned} \quad (122)$$

Using the recursion equations (75) we obtain

$$\begin{aligned} \Delta E_1^{(\infty)} &= -J_2^{2n-2}c_{2i}^{2n-2}\{a_0^2(J_1c_{1i}(2n-1) + J_2c_{2i}) \\ &\quad - 2a_0a_1J_2c_{2i}\}/D^{2n}. \end{aligned} \quad (123)$$

There will be correction terms to the formulas for the energy differences which arise both from nonharmonic terms in the Hamiltonian (61) and from further iteration of the recursion equation (75). These will be more dangerous than for the chiral XY model as they may carry an additional factor n_0^2/D where the n_0^2 comes from, say, dividing a J_2 step into two J_1 steps and placing them at any position along the chain. Therefore for large n_0 these terms could dominate, possibly changing the sign of the ΔE and the sequence of phases could terminate for any finite D . Analytic calculation of the correction terms would be prohibitively difficult. However, numerical results show no sign of deviations from the leading behavior for $n_{[\gamma]}=15$. A similar mechanism has been described for the ANNNI model at finite temperatures.¹⁰

To apply the formulas for the energy differences it is necessary to ascertain which ΔE_k and $\Delta E_k^{(\infty)}$, $k = 1, 2, 3, 4$ should be used at each step of the iteration procedure. By checking low order examples or by an inductive argument similar to that given in Appendix A one finds that ΔE_k and $\Delta E_k^{(\infty)}$ are relevant for a final phase with $n_{[\gamma]} = k \pmod{4}$.

The values of a_0 and a_1 ,

$$\begin{aligned} a_0 &= J_2\{\sin(6\pi/p) - \sin(4\pi/p)\}/D, \\ a_1 &= -J_1\{\sin(4\pi/p) - \sin(2\pi/p)\}/D, \end{aligned} \quad (124)$$

follow immediately from (75).

F. The sequence of phases

The stability of the short-period phases is most easily checked by an explicit evaluation of their energy using the Hamiltonian (63). Phases which appear $\mathcal{O}(1/D)$ and $\mathcal{O}(1/D^2)$ are shown schematically in Fig. 2. Stable boundaries are denoted by a vertical line; boundaries at which an infinite number of phases still coexist $\mathcal{O}(1/D^2)$ by a star. By using the energy differences derived above it is possible to calculate which of these phases are in fact stable when higher order terms in $1/D$ are considered. The results depend sensitively on p and so we consider each value in turn.

$p = 6$. For $p = 6$ the calculation of terms $\mathcal{O}(1/D^2)$ establishes that the $\langle 2 \rangle : \langle 3 \rangle$ boundary is stable. However, all other boundaries are multiphase lines and therefore any phase which contains only bands of lengths ≥ 3 may appear in the phase diagram. To understand which of these phases are stable we need the signs of the energy differences.

The energy differences are simplified by noting that for $p = 6$, $a_1 = 0$. To obtain the sign of ΔE_1 given by Eq. (101) two cases must be considered. If there is a wall on the axis of symmetry (i.e., between α_0 and α_1) then, recalling that all bands are of length at least 3, $J_{1,[1]} = J_1c_{1c}$, $J_{1,[2]} = J_2c_{2c}$, and $n_w[2n_0 - 1, 2] = n_w[2n_0 - 1, 1]$. Putting in values for c_{2c} , etc., gives

$$\Delta E_1 = 3J_1J_2^{2n_0}(\frac{1}{2})^{\{2n_0-2n_w-1\}}(\frac{5}{4} - n_0 + 3n_0'/2)/D^{2n_0}. \quad (125)$$

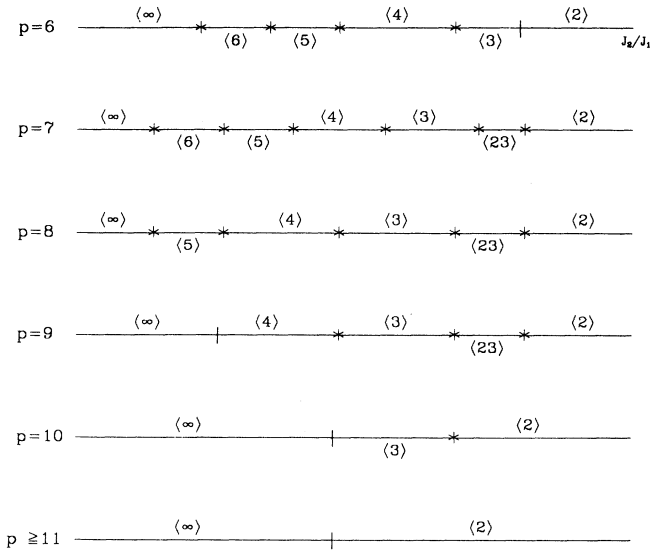


FIG. 2. Phase diagram of the soft clock model with competing interactions near the multiphase point $x_0^{(p)}$ showing the phases that are stabilized by terms in the energy $\mathcal{O}(1/D)$ (labeled above the line) and $\mathcal{O}(1/D^2)$ (labeled below the line). Examples of the notation used to describe the states are given in Eq. (62). A vertical line represents a first-order boundary and a star a multiphase line at which an infinite number of phases remain degenerate to this order.

If there is no wall on the axis of symmetry, $J_{1,[1]} = J_1 c_{1i}$, $J_{1,[2]} = J_2 c_{2i}$, and $n_w[2n_0 - 1, 2] = n_w[2n_0 - 1, 1]$. Therefore,

$$\Delta E_1 = 3J_1 J_2^{2n_0} \left(\frac{1}{2}\right)^{\{2n_0 - 2n_w + 1\}} (1 - 2n_0 + 3n'_0) / D^{2n_0}, \quad (126)$$

which is negative. Using similar arguments, or by inspection, all the other energy differences are found to be negative.¹¹ Therefore, all phases which contain only

$$\langle \infty \rangle : \langle 4 \rangle : \langle 34 \rangle : \langle 3 \rangle ; \langle 2333 \rangle ; \langle 233 \rangle ; \langle 23 \rangle ; \langle 23223 \rangle ; \langle 223 \rangle ; \langle 2223 \rangle : \langle 2 \rangle, \quad (127)$$

where $:$ denotes a stable boundary and $;$ a boundary which may be split at higher orders of the expansion.

$p = 10$. For $p = 10$, $a_0 = 0$, which means that the leading order terms in the energy differences are zero and the series analysis breaks down. Numerically we have been able to show that the only stable phases are $\langle 2^k 3 \rangle$ appearing between $\langle 2 \rangle$ and $\langle 3 \rangle$. The existence of these phases has been checked for $k \leq 5$ by expanding the energies $\mathcal{O}(1/D^6)$.

$p = 11$. A calculation $\mathcal{O}(1/D)$ shows that the $\langle 2 \rangle : \langle \infty \rangle$ boundary is stable; no new phases appear near x_0 and the transition is first order.

IV. DISCUSSION

Models with competing interactions may have ground states which include special points, so-called multiphase

bands of lengths ≥ 3 appear in the phase diagram.

$p = 7$. For $p = 7$ it can be shown, using arguments similar to those presented for $p = 6$, that all the energy differences are negative for large enough n_0 . The cases where n_0 is small and n'_0 and \tilde{n}_0 are close in value to n_0 must be checked independently. One finds that all the relevant cases are negative except ΔE_1 for $n_0 = 2$, $n'_0 = 1$. This determines the stability of $\langle 2^3 3 \rangle$. Therefore for $p = 7$ the $\langle 2 \rangle : \langle 223 \rangle$ boundary is not split. All phases lying between $\langle 223 \rangle$ and $\langle \infty \rangle$ are, however, stable.

$p = 8$. The energy differences ΔE_0 , ΔE_1 , ΔE_2 , and ΔE_3 given by Eqs. (85), (101), (91), and (97) are zero. Therefore higher order terms which are prohibitively difficult to calculate are needed to establish the signs of the energy differences.

However, it is possible to obtain an expansion of the energies of the low order phases numerically directly from the Hamiltonian (61). [The quadratic approximation (63) to the Hamiltonian may not be sufficient to pick up the correct leading behavior in this case.] Comparing these energies one finds that at least all phases expected to appear $\mathcal{O}(1/D^5)$ ($n_{\langle \gamma \rangle} \leq 12$) are stable.

$p = 9$. For $p = 9$ the situation is complicated and no clear pattern of phases emerges. Results $\mathcal{O}(1/D^2)$ indicate that only phases which are made up of bands of lengths ≤ 4 can appear. One finds by inspection $\Delta E_0 < 0$ [Eq. (85)]; $\Delta E_2 > 0$ [Eq. (91)]. For large enough n_0 , if there is a wall on the axis of symmetry, $\Delta E_3 < 0$ and $\Delta E_1 > 0$ from Eqs. (97) and (101), whereas if there is no wall on the axis of symmetry, $\Delta E_3 > 0$ and $\Delta E_1 < 0$. However, for low values of n_0 , where \tilde{n}_0 and n'_0 are close in value to n_0 these conclusions may not hold and each case must be treated independently. In particular for $\langle 23 \rangle + \langle 2 \rangle \Rightarrow \langle 223 \rangle$, which corresponds to the case ΔE_3 with no wall on the axis of symmetry and for $\langle 2^2 3 \rangle + \langle 2 \rangle \Rightarrow \langle 2^3 3 \rangle$, which corresponds to the case ΔE_1 with a wall on the axis of symmetry, the energy differences are negative.

Hence $\mathcal{O}(1/D^5)$ the phase sequence is

points,⁶ where the ground state is infinitely degenerate. At these points one might expect that small perturbations can have a drastic effect. One possible such perturbation is to allow the spins to soften; others are temperature¹⁰ or quantum fluctuations.¹²

The aim of this paper has been to study the first of these possibilities. We have considered continuous spin models with a p -fold spin anisotropy D which in the $D \rightarrow \infty$ limit exhibit a multiphase point. An expansion in $1/D$ is described which allows us to calculate the form of the phase diagram near the multiphase points as the spins soften.

The first model we considered was the chiral XY model with p -fold spin anisotropy, which for large D can be thought of as a soft chiral clock model. This model provided a useful illustration of the technique. We showed in agreement with Chou and Griffiths⁴ that for $p \geq 3$ all phases formed by combining adjacent structures are sta-

ble near the multiphase point and obtained leading order expressions for the widths of the phases.

We then described results for the more complicated situation of the XY model with first- and second-neighbor interactions for large D . Here the situation is very complex with the behavior near the multiphase point being strongly dependent on the value of p . For $6 \leq p \leq 10$ infinite sequences of phases are stable, but their quantitative form is different for different p . For $p \geq 11$ the phase boundary emanating from the multiphase point is first order.

We note that not only does the symmetry of the anisotropy have a nonuniversal effect on the nature of the phase diagram but also that the physical form of the perturbation is important. For example, for the ANNNI model itself temperature leads to a phase sequence $[2^k 3]$, $k = 0, 1, 2, \dots$,^{6,10} quantum fluctuations result in a phase sequence $[k]$, $k = 2, 3, 4, \dots$,¹² whereas when the spins soften there is a single first-order transition.

The models described here have a complex mathematical structure but also interesting applications to real systems. For example, rare-earth magnetism has been modeled by an XY model with competing interactions and six-fold spin anisotropy.¹³ Modulated structures in UNi_2Si_2 have been described using a model expected to behave in a similar way to those considered here.¹⁴

Finally we comment on some further possible uses for the technique introduced in this paper. Bassler, Sasaki, and Griffiths¹⁵ have described an epsilon point, a checkerboard structure of long-period phases which is in some sense a two-dimensional version of the sequences of phases we have been concerned with here. Sasaki¹⁶ found some evidence for the existence of such a point in a spin model by performing an expansion in $1/D$ to order $1/D^2$. An expansion taken to all orders will give firmer proof of where such points can be found.¹⁷ A similar technique can be used to investigate interface unbinding where spin softening can allow an interface to unbind from a surface through a series of layering transitions.¹⁸

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APPENDIX A

We aim here to show how n_0 defined by Eqs. (31) and (40) is related to $n_{[\gamma]}$, the length of the final phase in the

process $[\alpha] + [\beta] \Rightarrow [\gamma]$.

Consider two odd phases $[\alpha]$ and $[\beta]$. Let $n_0 \equiv n_0([\alpha\beta])$ for $[\alpha] + [\beta] \Rightarrow [\alpha\beta]$. Using the labeling scheme defined in Sec. II C(i),

$$[\alpha] = (\{\alpha\}, -\{\alpha\}, 0), \quad (\text{A1})$$

where we use $\{\alpha\}$ as shorthand for $\{\alpha_1, \alpha_2, \dots, \alpha_{(n_1-1)/2}\}$ [see equation (18)]. Similarly,

$$[\beta] = (\{\beta\}, -\{\beta\}, 0). \quad (\text{A2})$$

The resulting even phase is

$$[\alpha\beta] = (\{\alpha\}, -\{\alpha\}, 0, \{\beta\}, -\{\beta\}, 0). \quad (\text{A3})$$

Consider now the process $[\alpha\beta] + [\beta] \Rightarrow [\alpha^2\beta]$. Now an even and odd state are combined and therefore the labeling scheme defined in Sec. II C(ii) is appropriate. From (A2) and (A3),

$$[\alpha\beta] = (-\{\beta\}, 0, \{\alpha\}, -\{\alpha\}, 0, \{\beta\}),$$

$$[\beta] = (-\{\beta\}, 0, \{\beta\}). \quad (\text{A4})$$

By inspection of (A4) it is apparent that

$$n_0([\alpha\beta^2]) = n_0([\alpha\beta]) + (n_{[\beta]} + 1)/2, \quad (\text{A5})$$

that is, adding an odd state $[\beta]$ to an even state increases n_0 by $(n_{[\beta]} + 1)/2$.

A similar argument shows that for $[\alpha]$ odd and $[\beta]$ even,

$$n_0([\alpha\beta^2]) = n_0([\alpha\beta]) + (n_{[\beta]})/2, \quad (\text{A6})$$

$$n_0([\alpha^2\beta]) = n_0([\alpha\beta]) + (n_{[\alpha]} - 1)/2, \quad (\text{A7})$$

that is, adding an even (odd) state $[\beta]$ ($[\alpha]$) to an odd state $[\alpha\beta]$ increases n_0 by $n_{[\beta]}/2$ ($\{n_{[\alpha]} - 1\}/2$).

It is not hard to check that the conditions (A5), (A6), and (A7) are consistent with

$$n_0 = \{n_{[\gamma]} - (2m + 1)\}/2, \quad n_{[\gamma]} \text{ odd},$$

$$n_0 = \{n_{[\gamma]} - (2m + 2)\}/2, \quad n_{[\gamma]} \text{ even}, \quad (\text{A8})$$

for any integer m . By inspection $n_0([23]) = 2$. Therefore, $m = 0$ and

$$n_0 = \left\lceil \frac{n_{[\gamma]} + 1}{2} \right\rceil - 1, \quad (\text{A9})$$

where $[n]$ is the integer part of n .

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