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Spin softening in models with competing interactions: A high-anisotropy expansion to all orders

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An expansion in inverse spin anisotropy, which enables us to study the behavior of discrete spin models as the spins soften, is developed. In particular we focus on models, such as the chiral clock model and the p-state clock model with competing first- and second-neighbor interactions, where there are special multiphase points at zero temperature at which an infinite number of ground states are degenerate. The expansion allows calculation of the ground state phase diagram near these points as the spin anisotropy, which constrains the spin to take discrete values, is reduced from infinity. Several different behaviors are found, from a single first-order phase boundary to infinite series of commensurate phases.

Competing interactions lead to many important physical phenomena.[1] Examples are charge-density waves, long-period phases in binary alloys, and ferrimagnetism in the rare earths.[2,3] Considerable understanding of these systems has been obtained by studying one-dimensional models which embody the competition. The most famous of these is the Frenkel-Kontorova model, atoms connected by springs lying in a periodic potential.[4] Several spin systems behave similarly, for example, the chiral X-Y model with p-fold spin anisotropy, D.[5–8] Here the value of the chirality selects a given wave vector which competes with the preferred spin directions defined by D.

These models have subtle and complicated ground states. Long-period commensurate and incommensurate phases are important and devil's staircase behavior, upsilon points, and symmetry-breaking second-order transitions are among the features observed.[9–11] If the interactions are convex the ground-state behavior is rather well understood.[12,13] For non-convex interactions, however, much less is known and most work has been numerical.[6] Spin systems, which generically fall into this category, have received less attention than Frenkel-Kontorova models.[11,14] An important aim is to understand which ground-state features can occur in these models and to ascertain whether any universal behavior arises.

To this end we have developed a new analytic approach which allows us to study the behavior of spin models in the limit where the pinning potential which results from the spin anisotropy, D, is large. This is an expansion in inverse spin anisotropy which can be carried to all orders where necessary. In the limit of infinite D the spins can take only discrete values and the ground state typically consists of a few short-period phases as a controlling parameter such as the chirality is varied. Interesting behavior can occur when the boundary between different ground states is infinitely degenerate, at so-called multiphase points.[15,16] Here, as D decreases from infinity and the spins are allowed to soften, we are able to demonstrate several different behaviors, ranging from a single first-order boundary to infinite series of commensurate phases.

The approach is described for the one-dimensional, classical X-Y model with competing first- and second-neighbor interactions and p-fold spin anisotropy

$$\mathscr{H}=\sum_i \{-J_1\cos(\theta_{i-1}-\theta_i)+J_2\cos(\theta_{i-2}-\theta_i) -D(\cos p\theta_i-1)/p^2\}. \quad (1)$$

J_1, J_2, and D are chosen to be positive and θ_i is an angle between 0 and 2π. For $D=0$ the ground state of the Hamiltonian (1) is ferromagnetic for $x\equiv J_2/J_1\leqslant 1/4$ and modulated with a wave vector $2\pi q=\cos^{-1}(1/4x)$ for $x>1/4$. At $D=\infty$ (1) becomes a p-state clock model and θ_i can take values $2\pi n_i/p$, $n_i=0,1,2,\ldots,p-1$. The ground state is now a sequence of short-period phases as x is varied. The boundaries between the different ground states can either be simple points where only a few distinct phases have the same energy or multiphase points where an infinite number of different states are degenerate.

A particular case of the latter which has very rich behavior is the boundary between states with wave vectors $1/p$ ($\{n_i\}=\ldots 012345\ldots$) and $3/(2p)$ ($\ldots 013467\ldots$) which occurs for all $p\geqslant 6$ at

$$x_0=\{\cos(2\pi/p)-\cos(4\pi/p)\}/\{2[\cos(4\pi/p)-\cos(6\pi/p)]\}. \quad (2)$$

Here all phases with $\delta n_i\equiv n_{i+1}-n_i=1,2$, with the proviso that $\delta n_i=\delta n_{i+1}=2$ is forbidden are degenerate for $D=0$.

To facilitate a description of the ground-state structures near this point it is helpful to define a wall as a position where $\delta n_i=2$ and a band as a sequence of spins between walls.[15,17] Then we label a state which is made up of a repeating sequence of bands $m_1,m_2,\ldots,m_n$ as $\langle m_1,m_2,\ldots,m_n\rangle$. With this definition the phases bordering the multiphase point at x_0 are $\langle\infty\rangle$ and $\langle 2\rangle$ and all phases consisting of bands of length $\geqslant 2$ are stable at the point itself.

The aim here is to investigate the stability of the phase diagram around x_0 as D decreases from infinity as an expansion in D^{-1}. Although we focus on the Hamiltonian (1) and a particular series of multiphase points the method is general and results for other models will be described later in the paper.

The expansion is possible because for D large the spins deviate from their clock positions by an angle analytic in D^{-1}. Writing

$$\theta_i = \theta_i^0 + \tilde{\theta}_i \tag{3}$$

and keeping only terms quadratic in $\tilde{\theta}_{i-1} - \tilde{\theta}_i$ and $\tilde{\theta}_{i-2} - \tilde{\theta}_i$ in the expansion of the Hamiltonian (1) gives

$$\tilde{\mathscr{H}} = \mathscr{H}|_{D=\infty} + J_1 c_{i,1}(\tilde{\theta}_{i-1} - \tilde{\theta}_i + s_{i,1}/c_{i,1})^2/2 - J_1 s_{i,1}^2/2c_{i,1} - J_2 c_{i,2}(\tilde{\theta}_{i-2} - \tilde{\theta}_i + s_{i,2}/c_{i,2})^2/2 + J_2 s_{i,2}^2/2c_{i,2} + D\tilde{\theta}_i^2/2, \tag{4}$$

where

$$s_{i,1} = \sin(\theta_{i-1}^0 - \theta_i^0), \quad c_{i,1} = \cos(\theta_{i-1}^0 - \theta_i^0),$$
$$s_{i,2} = \sin(\theta_{i-2}^0 - \theta_i^0), \quad c_{i,2} = \cos(\theta_{i-2}^0 - \theta_i^0). \tag{5}$$

The equilibrium values of the $\tilde{\theta}_i$ are given by minimizing the Hamiltonian (4). This leads to linear recursion relations

$$\tilde{\theta}_i = J_1\{c_{i,1}(\tilde{\theta}_{i-1} - \tilde{\theta}_i) + c_{i+1,1}(\tilde{\theta}_{i+1} - \tilde{\theta}_i) + s_{i,1} - s_{i+1,1}\}/D - J_2\{c_{i,2}(\tilde{\theta}_{i-2} - \tilde{\theta}_i) + c_{i+2,2}(\tilde{\theta}_{i+2} - \tilde{\theta}_i) + s_{i,2} - s_{i+2,2}\}/D. \tag{6}$$

If the full Hamiltonian (1) is used nonlinearities appear in the recursion relations (6). However, these do not affect the leading-order terms needed for the subsequent calculations.

Writing

$$\tilde{\theta}_i = \frac{\tilde{\theta}_i^1}{D} + \frac{\tilde{\theta}_i^2}{D^2} + \cdots + \frac{\tilde{\theta}_i^n}{D^n} + \cdots \tag{7}$$

Eq. (6) immediately gives

$$\tilde{\theta}_i^1 = J_1(s_{i,1} - s_{i+1,1}) - J_2(s_{i,2} - s_{i+2,2}), \tag{8}$$

$$\tilde{\theta}_i^n = J_1\{c_{i,1}(\tilde{\theta}_{i-1}^{n-1} - \tilde{\theta}_i^{n-1}) + c_{i+1,1}(\tilde{\theta}_{i+1}^{n-1} - \tilde{\theta}_i^{n-1})\} - J_2\{c_{i,2}(\tilde{\theta}_{i-2}^{n-1} - \tilde{\theta}_i^{n-1}) + c_{i+2,2}(\tilde{\theta}_{i+2}^{n-1} - \tilde{\theta}_i^{n-1})\}. \tag{9}$$

It follows from Eqs. (5) and (8) that the two spins in a 2-band, the edge spins of a 3-band, and the two spins nearest each edge of a band of length ≥ 4 have a deviation $\mathscr{O}(1/D)$. All other spins remain unmoved to this order. From Eq. (9) it is apparent that the next pairs of spins moving in from each edge of the band will have a deviation $\mathscr{O}(1/D^2)$, the next pairs $\mathscr{O}(1/D^3)$, and so forth.

We establish the stable phase sequences near x_0 by following an inductive argument originally due to Fisher and Selke[15] (see also, Refs. 18 and 19). Defining $E_{\langle\alpha\rangle}$ as the ground-state energy per spin of $\langle\alpha\rangle$ and $n_{\langle\alpha\rangle}$ as the number of spins per period, this can be summarized as follows: assume that $\mathscr{O}(1/D^n)$ two neighboring phases $\langle\alpha\rangle$ and $\langle\beta\rangle$ are stable and all phases comprised of α and β sequences are degenerate on the boundary between them. Then the first phase that can appear between them is $\langle\gamma\rangle \equiv \langle\alpha\beta\rangle$. If $\Delta E \equiv n_{\langle\alpha\beta\rangle}E_{\langle\alpha\beta\rangle} - n_{\langle\alpha\rangle}E_{\langle\alpha\rangle} - n_{\langle\beta\rangle}E_{\langle\beta\rangle} > 0$ the boundary remains stable to all orders. If $\Delta E < 0$ and $\mathscr{O}(1/D^m)$ with $m > n$, however, $\langle\alpha\beta\rangle$ appears as a stable phase on the $\langle\alpha\rangle{:}\langle\beta\rangle$ boundary over a region $\mathscr{O}(1/D^m)$ and the analysis must recommence about the new $\langle\alpha\rangle{:}\langle\alpha\beta\rangle$ and $\langle\alpha\beta\rangle{:}\langle\beta\rangle$ boundaries.

Hence the task is to calculate ΔE. Let $n_{\langle\alpha\rangle} = n_1$, $n_{\langle\gamma\rangle} = n$ and label the repeating spin sequences of $\langle\alpha\rangle$, $\langle\beta\rangle$, and $\langle\gamma\rangle$ as $(\alpha_1, \alpha_2, \ldots, \alpha_{n_1})$, $(\beta_{n_1+1}, \beta_{n_1+2}, \ldots, \beta_n)$, and $(\gamma_1, \gamma_2, \ldots, \gamma_n)$, respectively. It is lengthy but not difficult to show that

$$\Delta E = J_1 c_{1,1}\{(\alpha_0 - \beta_0)(\gamma_1 - \gamma_{n_1+1}) - (\alpha_1 - \beta_1)(\gamma_0 - \gamma_{n_1})\}/2 - J_2 c_{1,2}\{(\alpha_{-1} - \beta_{-1})(\gamma_1 - \gamma_{n_1+1}) - (\alpha_1 - \beta_1)(\gamma_{-1} - \gamma_{n_1-1})\}/2 - J_2 c_{2,2}\{(\alpha_0 - \beta_0)(\gamma_2 - \gamma_{n_1+2}) - (\alpha_2 - \beta_2)(\gamma_0 - \gamma_{n_1})\}/2. \tag{10}$$

This formula is exact for the quadratic Hamiltonian (4). Higher-order terms in the full Hamiltonian (1) appear as higher-order corrections.

The value of ΔE must obviously be independent of the choice of spin labeling. However, given an appropriate choice of labeling only the leading-order terms in the spin differences need to be calculated. This follows from noting that all possible states have an axis of symmetry. This lies either on or between spins depending on whether the number of spins in a period is even or odd. When states are combined there are two possibilities: (i) $n_{\langle\alpha\rangle}$ odd, $n_{\langle\beta\rangle}$ odd $\rightarrow$ $n_{\langle\gamma\rangle}$ even. For an odd state symmetry demands that one spin remains fixed ($\tilde{\theta} = 0$). Therefore we may choose $\alpha_0 = 0$, $\beta_0 = 0$. (ii) $n_{\langle\alpha\rangle}$ odd, $n_{\langle\beta\rangle}$ even $\rightarrow$ $n_{\langle\gamma\rangle}$ odd. We choose $\alpha_{(n_1+1)/2} = 0$ or equivalently $\gamma_1 - \gamma_{n_1+1} = \gamma_0 - \gamma_{n_1}$. This implies $(\alpha_1 - \beta_1) = -(\alpha_0 - \beta_0)$. (Consideration of how neighboring states are constructed shows that two adjacent even states are never generated.)

The spin differences can be calculated to leading order by replacing θ_i with $(\alpha_i - \beta_i)$ or the closely related $(\gamma_i - \gamma_{n_1+i})$ in Eqs. (8) and (9). Let $(\alpha_i - \beta_i)^1 = 0$, $i < n_0$. The choice of spin labeling detailed above maximizes n_0. Iteration of the recursion equations leads after an involved calculation which will be detailed elsewhere[20] to the following expressions for the energy differences for $n > 0$.

(i) $n_{\langle\gamma\rangle} = 1[\text{mod}4] \equiv 4n+1; n_0 = 2n-1$:

$$\Delta E = \{-J_{1,1}J_2^{2n}c_3^{2\tilde{n}_w}c_2^{2n-2-2\tilde{n}_w}(s_3 - s_2)^2 - 2J_{1,2}J_2^{2n-1}J_1 c_3^{n_w+\tilde{n}_w-1}c_2^{2n-3-n_w-\tilde{n}_w}(s_3 - s_2)^2[c_3c_1(n-1-x) + c_2^2 x] - 2J_{1,2}J_2^{2n-1}J_1 c_3^{n_w+\tilde{n}_w}c_2^{2n-2-n_w-\tilde{n}_w}(s_3 - s_2)(s_2 - s_1)\}/D^{2n}, \tag{11}$$

(ii) $n_{\langle\gamma\rangle}=2[\text{mod}4]\equiv 4n+2; n_0=2n-1$:

$$\Delta E=\{J_2^{2n+1}c_3^{2\tilde{n}_w}c_2^{2n-1-2\tilde{n}_w}(s_3-s_2)^2\}/D^{2n}, \tag{12}$$

(iii) $n_{\langle\gamma\rangle}=3[\text{mod}4]\equiv 4n+3; n_0=2n$:

$$\Delta E=\{2J_{1,2}J_2^{2n}J_1c_3^{n_w+\tilde{n}_w-1}c_2^{2n-2-n_w-\tilde{n}_w}(s_3-s_2)^2[c_3c_1(n-\tilde{x})+c_2^2\tilde{x}] + 2J_{1,2}J_2^{2n}J_1c_3^{n_w+\tilde{n}_w}c_2^{2n-1-n_w-\tilde{n}_w}(s_3-s_2)(s_2-s_1)\}/D^{2n+1}, \tag{13}$$

(iv) $n_{\langle\gamma\rangle}=4[\text{mod}4]\equiv 4n+4; n_0=2n$:

$$\Delta E=\{-J_2^{2n+2}c_3^{2\tilde{n}_w}c_2^{2n-2\tilde{n}_w}(s_3-s_2)^2\}/D^{2n+1}, \tag{14}$$

where $c_m=\cos(2\pi m/p)$, $s_m=\sin(2\pi m/p)$, $J_{1,1}=J_1\cos[2\pi(\alpha_1^0-\alpha_0^0)/p]$, $J_{1,2}=J_2\cos[2\pi(\alpha_1^0-\alpha_{-1}^0)/p]$, $J_{2,2}=J_2\cos[2\pi(\alpha_2^0-\alpha_0^0)/p]$, n_w and $\tilde{n}_w$ are the number of walls between n_0 and 2 and n_0 and 1, respectively, $x=\sum_{i=2,4,\ldots,(2n-2)}(\delta n_i-1)$ and $\tilde{x}=\sum_{i=1,3,\ldots,(2n-1)}(\delta n_i-1)$.

Different formulas are needed for for the phases $\langle m\rangle$ which border $\langle\infty\rangle$. (i) $\langle 4n\rangle+\langle\infty\rangle\rightarrow\langle 4n+1\rangle$:

$$\Delta E=-J_2^{2n-2}c_2^{2n-2}\{p_1^2[(2n-1)J_1c_1+J_2c_2] -2p_1p_2J_2c_2\}/D^{2n}, \tag{15}$$

(ii) $\langle 4n+1\rangle+\langle\infty\rangle\rightarrow\langle 4n+2\rangle$:

$$\Delta E=p_1^2J_2^{2n-1}c_2^{2n-1}/D^{2n}, \tag{16}$$

(iii) $\langle 4n+2\rangle+\langle\infty\rangle\rightarrow\langle 4n+3\rangle$:

$$\Delta E=J_2^{2n-1}c_2^{2n-1}\{p_1^2(2J_1nc_1+J_2c_2)-2J_2p_1p_2c_2\}/D^{2n+1}, \tag{17}$$

(iv) $\langle 4n+3\rangle+\langle\infty\rangle\rightarrow\langle 4n+4\rangle$:

$$\Delta E=-p_1^2J_2^{2n}c_2^{2n}/D^{2n+1}, \tag{18}$$

where $p_1=-J_2(s_3-s_2)$ and $p_2=J_1(s_2-s_1)-J_2(s_3-s_2)$.

Results for low-order phases, $n=0$, can be obtained directly from Eq. (4) and then the formulas (11)–(18) can be used to build up the phase diagram inductively. Although the energy differences ΔE are cumbersome it is not hard to establish their sign for different phase sequences and values of p. If ΔE is not too small the results can be checked numerically. This is done by minimizing the ground-state energy (1) with respect to the θ_i giving a set of coupled nonlinear equations which can be solved by iteration. Typically it is feasible to identifiy phases which appear $\mathcal{O}(1/D^7)$.

The results for the Hamiltonian (1) are strongly p dependent.

$p=6$: the $\langle 2\rangle$:$\langle 3\rangle$ boundary is stable. All energy differences are negative for phases which can be constructed by the iterative process of combining neighboring states which contain bands of length $\geqslant 3$. Hence all these phases spring from the multiphase point.

$p=7$: all phases lying between $\langle 223\rangle$ and $\langle\infty\rangle$ are stable. The $\langle 2\rangle$:$\langle 223\rangle$ boundary is not split.

$p=8$: many of the energy differences are zero. Hence the formalism breaks down. Numerical results show, however, that at least all phases expected to appear $\mathcal{O}(1/D^5)$ are stable.

$p=9$: no clear pattern emerges. $\mathcal{O}(1/D^5)$ the phase sequence is $\langle\infty\rangle$:$\langle 4\rangle$:$\langle 34\rangle$:$\langle 3\rangle$;$\langle 2333\rangle$;$\langle 233\rangle$;$\langle 23\rangle$;$\langle 23223\rangle$;$\langle 223\rangle$;$\langle 2223\rangle$;$\langle 2\rangle$, where : denotes a stable boundary and ; a boundary which may be split at higher orders of the expansion.

$p=10$: many of the energy differences are zero. Numerically we have been able to show that $\mathcal{O}(1/D^7)$ only the phases $\langle 2^k3\rangle$, $k=1,2,\ldots,5$ are stable between $\langle 2\rangle$ and $\langle 3\rangle$.

$p\geqslant 11$: the $\langle 2\rangle$:$\langle\infty\rangle$ boundary is stable and no new phases appear near x_0 and the transition is first order.

Results have also been obtained for several other models. The chiral X-Y model with p-fold anisotropy

$$\mathcal{H}=\sum_i \{-J\cos(\theta_{i-1}-\theta_i+\Delta)-D(\cos p\theta_i-1)/p^2\} \tag{19}$$

becomes the chiral clock model in the $D\rightarrow\infty$ limit. At the multiphase point at $\Delta=\pi/p$ between the ferromagnetic (. . . 000 . . .) and chiral (. . . 012 . . .) states

$$\Delta E=-\{4\sin^2(\pi/p)[J\cos(\pi/p)]^{n_{\langle\gamma\rangle}}\}/\{D^{n_{\langle\gamma\rangle}-1}\} \tag{20}$$

for a final phase $\langle\gamma\rangle$. This is always negative for $p\geqslant 3$ indicating, in agreement with Chou and Griffiths[6] that all phases are stable.

The Frenkel-Kontorova model with a piecewise parabolic potential

$$\mathcal{H}=\sum_i \{-J(\theta_{i-1}-\theta_i+\Delta)^2-D(\theta_i-\theta_i^0)^2\} \tag{21}$$

has a multiphase point at $\Delta=\pi/p$ between the ferromagnetic and chiral states. Here

$$\Delta E=-(8\pi^2J^{n_{\langle\gamma\rangle}})/(p^2D^{n_{\langle\gamma\rangle}-1}) \tag{22}$$

in agreement with the exact results of Aubry.[21]

The series expansion in inverse anisotropy outlined here provides a new tool to understand the crossover between discrete and continuous spin models particularly near $D=\infty$ where the narrowness of the phases renders numerical work difficult. Many interesting avenues remain to be explored. In particular it would be of interest to understand the behavior of models where the leading term in the energy differences vanishes and the recursion relations become nonlinear. Moreover it may be possible to recast the formalism in terms of interactions between domain walls[10,18,22] and hence attempt to classify the high-D behavior of systems with modulated structures. Finally the multiphase point considered here is a special case of the anti-integrable limits described by Aubry[16] which also exist in electronic models and systems of coupled anharmonic oscillators. Investigation of whether similar expansions exist for these models would be of considerable interest.

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