Splitting the multiphase point

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Abstract

Models with competing interactions, for example the ANNNI model, can have special points at which the ground state is infinitely degenerate, so-called multiphase points. Small perturbations can lift this degeneracy and give rise to infinite sequences of long-period phases. This paper compares the effect of three possible perturbations, quantum fluctuations, thermal fluctuations and the softening of the spins from their quantised positions.
My aim in this paper is to summarise results showing that simple spin models with short-range interactions can have surprisingly complex phase diagrams, even at zero temperature. The models we shall consider are three-dimensional, with ferromagnetic interactions in two of the three dimensions. Along the third or axial direction there are competing interactions which lead to the possibility of many long-period structures becoming stable.

Arguably the paradigm of these systems is the axial next-nearest-neighbour Ising or ANNNI model (Elliott 1961, Yeomans 1988, Selke 1988,1992) which has ferromagnetic first-neighbour and antiferromagnetic second-neighbour interactions along the axial direction. The ANNNI model Hamiltonian is

\[
H_A = -J_0 \sum_{i,j} \sigma_{i,j} \sigma_{i,j'} - J_1 \sum_{i,j} \sigma_{i,j} \sigma_{i+1,j} + J_2 \sum_{i,j} \sigma_{i,j} \sigma_{i+2,j}.
\]

(1)

Here \(J_1\) and \(J_2\) are both positive, \(\sigma_{i,j} = \pm 1\) is the spin on site \((i, j)\), \(i\) labels planes along the axial direction, \(j\) labels sites within a plane and \(\langle j j' \rangle\) denotes a sum over nearest neighbours in a plane.

Defining \(\kappa = J_2/J_1\) the ground state of the ANNNI model can easily be seen by inspection to be ferromagnetic for \(\kappa < 1/2\) and an antiphase structure consisting of two planes with spins \(\sigma = 1\) followed by two planes of spins with \(\sigma = -1\) for \(\kappa > 1/2\). \(\kappa = 1/2\) is a multiphase point where the ground state is infinitely degenerate with all possible combinations of ferromagnetic and antiphase orderings having equal energy (Fisher and Selke 1980,1981).

The existence of such a degeneracy leads one to suspect that small perturbations could have a drastic effect on the phase diagram near the multiphase point. Candidates are thermal fluctuations, quantum fluctuations, or the softening of the spins from the two discrete Ising values. We shall compare and contrast the effect of the different perturbations. However, before considering each of these possibilities in turn, it is helpful to introduce the following notation (Fisher and Selke 1980,1981).

Of the phases degenerate at the multiphase point those that are periodic can be labelled by using \(\langle n_1, n_2, \ldots n_m \rangle\) to denote a state in which the spins form domains (of parallel planes) whose widths repeat periodically the sequence \(n_1, n_2, \ldots n_m\). For example the antiphase state...
is labelled \(\langle 2 \rangle\) and the phase in which consecutive planes have the ordering \(\ldots + ++ -- + + -- - - \ldots\) is \(\langle 2223 \rangle\) or \(\langle 2^33 \rangle\). The term \(p\)-band will be used to describe \(p\) consecutive planes of up (down) spins terminated by down (up) planes.

**THERMAL FLUCTUATIONS**

The phase diagram of the ANNNI model at finite temperatures near the multiphase point was worked out some time ago by Fisher and Selke (1980,1981) and refined by Fisher and Szpilka (1987b). They found that a sequence of phases \(\langle 2^k3 \rangle, \, k = 0, 1, 2 \ldots k_0\) with \(k_0 \to \infty\) as the temperature \(T \to 0\) spring from the multiphase point. Mixed phases \(\langle 2^k32^{k+1}3 \rangle\) (and possibly more complicated combinations of the basic sequences) are also stable at any finite temperature for sufficiently large \(k\). Fisher and Szpilka’s results are summarised in Figure 1.

The physics behind these results can be made transparent by considering the spin system as an array of interacting domain walls (Szpilka and Fisher 1986, Fisher and Szpilka 1987a). There is some freedom in the definition of a wall. For example they could be the boundaries between up and down bands but here it is more convenient to consider the three-bands as walls within a matrix of two-bands. At finite temperatures thermal wandering of the walls leads to interactions between them which can differentially stabilise the long-period phases.

The free energy of a given phase can be written in terms of a sequence of wall interaction free energies: \(F_w\), the free energy of an isolated wall; \(V_2(n)\), the interaction energy of two walls separated by \(n\) sites; and generally \(V_k(n_1, n_2, \ldots n_{k-1})\), the interaction energy of \(k\) walls with successive separations \(n_1, n_2, \ldots n_{k-1}\). In terms of these quantities one may write the total free energy of the system when there are walls at positions \(m_i\) as

\[
F = F_0 + n_w F_w + \sum_i V_2(m_{i+1} - m_i) + \sum_i V_3(m_{i+2} - m_{i+1}, m_{i+1} - m_i) \\
+ \sum_i V_4(m_{i+3} - m_{i+2}, m_{i+2} - m_{i+1}, m_{i+1} - m_i) + \ldots ,
\]

where \(F_0\) is the free energy with no walls present and \(n_w\) is the number of walls.
Successive approximations to the phase diagram follow from obtaining the two-wall interactions, the three-wall interactions and so forth. The stability of the phases in which the walls are equispaced follows from a consideration of the pair interactions. For a convex $V_2(n)$ all such phases are stable. Otherwise the stable phases can be identified via a graphical construction due to Fisher and Szpilka (1987a): if the extremal convex envelope of $V_2(n)$ versus $n$ is drawn, the points $[n, V_2(n)]$ which make up the envelope correspond to the stable phases in which the walls are a distance $n$ apart which we shall denote $\{n\}$. (Note that the notation $\{n\}$ only coincides with $\langle n \rangle$ for the case where the walls have been identified as the edges of ferromagnetic domains.)

The stability of the $\{n\} : \{n + 1\}$ boundaries depends on the three-wall interactions. The condition that the boundary correspond to a stable first-order transition is that $F_n < 0$ (Fisher and Szpilka 1987a), where

$$F_n \equiv V_3(n, n) - 2V_3(n, n + 1) + V_3(n + 1, n + 1).$$

(3)

If $F_n > 0$, $\{n, n + 1\}$ appears as a stable phase and there is the possibility that four-wall interactions can stabilise $\{n, n + 1\} \{\{n + 1, n + 1\}\}$ on the $\{n\} : \{n, n + 1\} \{\{n + 1\} : \{n, n + 1\}\}$ boundary and so on.

For the ANNNI model the wall–wall interactions were calculated by Fisher and Szpilka (1987b) using a low temperature series expansion. The calculations support the intuition that the graphs which give the leading order contribution to $V_2(n)$ are chains of second-neighbour flipped spins stretching between neighbouring walls. Similar chains joining second-neighbour walls are responsible for the three-wall interactions. There are however subtleties which must be addressed. For example disconnected graphs, which together span the distance between the walls, must be taken into account and care must be taken to subtract off the single wall energy and other background contributions.

The leading order result is that $V_2(n)$ is convex and $F_n < 0$ leading to the conclusion that there is an infinite phase sequence $\langle 2^k 3 \rangle$ and no mixed phases. However for large $k \sim \exp(4J_0/kT)$ Fisher and Szpilka (1987b) identified important correction terms. These
arise from diagrams when an extra spin is flipped within the chain: although they carry an extra Boltzmann weight the number of positions for the flipped spin increases with increasing $k$ and hence these diagrams can eventually affect the phase diagram. They result in a cut-off of the phase sequence and the appearance of mixed phases for any finite temperature. Other corrections which arise from additional flips outside the chain do not alter the structure of the phase diagram.

**QUANTUM FLUCTUATIONS**

It is of interest to ask whether quantum fluctuations lead to a similar splitting of the multiphase point of the ANNNI model. Obviously the Hamiltonian (1) is purely classical and cannot support quantum fluctuations. Therefore we consider instead Heisenberg spins which interact through the Hamiltonian

$$\mathcal{H} = -\frac{J_0}{S^2} \sum_{i(j,j')} S_{i,j} \cdot S_{i,j'} - \frac{J_1}{S^2} \sum_{i,j} S_{i,j} \cdot S_{i+1,j} + \frac{J_2}{S^2} \sum_{i,j} S_{i,j} \cdot S_{i+2,j} - \frac{D}{S^2} \sum_{i,j} (S_{i,j}^z)^2 - S^2) \quad (4)$$

where $S_{i,j}$ is a quantum spin of magnitude $S$. For $D = \infty$ the Hamiltonian (4) reduces to that of the ANNNI model. For classical spins $S = \infty$ the ground state (and therefore the multiphase point) is maintained for large $D$ and we shall work in this limit.

To study quantum fluctuations Harris, Micheletti and Yeomans (1995a,b) used the Dyson-Maleev transformation

$$S^z_i = \sigma_i (S - a_i^+ a_i) ,$$

$$S^+_i = \sqrt{2S} \left( \delta_{\sigma_i,1} \left[ 1 - \frac{a_i^+ a_i}{2S} \right] a_i + \delta_{\sigma_i,-1} a_i^+ \left[ 1 - \frac{a_i^+ a_i}{2S} \right] \right) ,$$

$$S^-_i = \sqrt{2S} \left( \delta_{\sigma_i,1} a_i^+ + \delta_{\sigma_i,-1} a_i \right) ,$$

where $\delta_{a,b}$ is unity if $a = b$ and is zero otherwise and $a_i^+$ ($a_i$) creates (destroys) a spin excitation at site $i$, to transform the Hamiltonian (4) into the bosonic form

$$\mathcal{H}(\{\sigma_i\}) = \mathcal{H}_A + \mathcal{H}_0 + V_|| + V_\perp + \mathcal{O}(S^{-2}) , \quad (6)$$

5
where

\[ \mathcal{H}_0 = \sum_{i,j} \left[ 2(D + 2J_0) + J_1 \sigma_{i,j}(\sigma_{i-1,j} + \sigma_{i+1,j}) - J_2 \sigma_{i,j}(\sigma_{i-2,j} + \sigma_{i+2,j}) \right] S^{-1} a_{i,j}^+ a_{i,j} \]  

(7)

with \( \tilde{D} = D + 2J_0 \) and \( V_{||} \) (\( V_\parallel \)) is the interaction between spins which are parallel (antiparallel)

\[ V_{||} = \frac{1}{S} \sum_{i,j} \left[ -J_1 X(i,i+1;j)(a_{i,j}^+ a_{i+1,j} + a_{i+1,j}^+ a_{i,j}) + J_2 X(i,i+2;j)(a_{i,j}^+ a_{i+2,j} + a_{i+2,j}^+ a_{i,j}) \right], \]  

(8)

\[ V_\parallel = \frac{1}{S} \sum_{i,j} \left[ -J_1 Y(i,i+1;j)(a_{i,j}^+ a_{i+1,j} + a_{i+1,j}^+ a_{i,j}) + J_2 Y(i,i+2;j)(a_{i,j}^+ a_{i+2,j} + a_{i+2,j}^+ a_{i,j}) \right], \]  

(9)

where \( X(i,i';j) \) [\( Y(i,i';j) \)] is unity if spins \((i,j)\) and \((i',j)\) are parallel [antiparallel] and is zero otherwise.

Just as for the case of thermal fluctuations it is helpful to think in terms of an array of walls whose interactions now result from quantum fluctuations. However, in contrast to finite temperatures, it is now most convenient to define a wall as a boundary between bands. The phases with equispaced walls which may be stabilised by the two-wall interaction are then \( \langle k \rangle \).

The form of the Hamiltonian (6) allows us to immediately identify the excitations responsible for mediating the wall–wall interactions by noting that fluctuations out of the classical ground state (the boson vacuum) can only be excited in pairs at the walls by the perturbation \( V_\parallel \). \( V_{||} \) is then able to propagate any excitation within the ferromagnetic domains.

Hence the lowest order contribution to the two-wall interactions will correspond to a pair of excitations at one wall, one of which moves to the neighbouring wall \textit{and back} and is then destroyed at the first wall in tandem with its original partner. Similarly the graphs responsible for the three-wall interactions correspond to a pair of excitations at the centre wall each of which moves to its neighbouring wall and back before being annihilated.

The contributions of these diagrams follow from standard non-degenerate perturbation theory. The small parameter is \( J/(D + 2J_0) \) (\( J \equiv J_1 \) or \( J_2 \)). The result is that to leading order the two-wall interaction is (Harris, Micheletti and Yeomans 1995b)
\[ V_2(n) = \frac{4J_2^n S^{-1}}{[4(D + 2J_0)]^{n-1}}, \quad n \text{ odd}, \]
\[ V_2(n) = \frac{J_2^n S^{-1}}{[4(D + 2J_0)]^n} (n^2J_1^2 - 4J_1J_2 + 8J_2^2), \quad n \text{ even}. \]

Hence to leading order \( V_2(n) \) is a convex function of \( n \) and all the phases \( \langle k \rangle \) are stable. \( F(n) \) defined by equation (3) can be shown to be negative and the \( \langle k \rangle : \langle k+1 \rangle \) phase boundaries are first order. Note that although this is qualitatively the same as the ANNNI behaviour, the quantitative nature of the phase sequence is entirely different.

Just as for the ANNNI model correction terms may be important for large \( k \sim [(D + 2J_0)/J]^{1/2} \). Firstly \( V_2(n) \) will suffer from strong even–odd oscillations and therefore transitions \( \langle k \rangle \rightarrow \langle k+2 \rangle \) will appear. Secondly perturbations which follow more complicated paths, although individually less important, may become dominant because of their greater statistical weights. A calculation attempting to take this into account indicates however that, unlike the ANNNI model, the phase sequence does not terminate at a finite value of \( k \) (Harris, Micheletti and Yeomans 1995b).

This difference can be understood as follows. In the present model in order for an excitation to sense the presence of a second wall, it has to travel from one wall to the other wall and return. Thus the interaction in the quantum case is proportional to the square of an oscillatory Green’s function, whereas in the ANNNI model the analogous function appears linearly.

**SPIN SOFTENING**

A third mechanism which might split the degeneracy at a multiphase point is the softening of the spins themselves (that is a non-infinite spin anisotropy \( D \) in the Hamiltonian (4)). There is no splitting for the ANNNI model because there is a finite energy barrier preventing spins from moving continuously from their positions at \( D = \infty \). However, for some value of \( D \) long-period commensurate or incommensurate phases must be stabilised as, for \( D = 0 \), the ground state of the Hamiltonian (4) is either ferromagnetic or incommensurate with a
wavevector that varies continuously with $\kappa$. Preliminary numerical results confirm that this is indeed the case (Micheletti, 1995).

However a more complete description of the same physics exists for a similar model (Seno, Yeomans, Harbord, Ko 1994) and it is this we prefer to consider here. This is the classical X-Y model with first- and second-neighbour competing interactions and a $p$-fold spin anisotropy $D$. Each classical XY spin vector lies in a plane perpendicular to the axial direction and has unit magnitude. The Hamiltonian is

$$H_{\text{XY}} = -J_0 \sum_{i,j} s_{i,j} \cdot s_{i,j'} - J_1 \sum_{i,j} s_{i,j} \cdot s_{i+1,j} + J_2 \sum_{i,j} s_{i,j} \cdot s_{i+2,j} + D \sum_{i,j} \left(1 - \cos(6\theta_{i,j})\right)$$  \hspace{1cm} (11)

where $\theta_{i,j}$ is the angle between the spin at site $(i, j)$ and a given axis. This model is relevant to an understanding of the ferrimagnetic ordering of rare-earths such as holmium where the spins are confined to the basal plane and subjected to a hexagonal spin anisotropy (Jensen and Mackintosh 1991).

The ground state of the Hamiltonian (11) is well understood in the two limits $D = 0$ and $D = \infty$. For $D = 0$ the ground state is ferromagnetic for $\kappa < \frac{1}{4}$. For $\kappa > \frac{1}{4}$ it exhibits helical order with a wavevector which is, in general, incommensurate with the underlying lattice. The magnitude of the wavevector is determined by the exchange energies through the relation $\cos q = (4\kappa)^{-1}$.

For $D = \infty$, however, the spin angles $\theta_{i,j}$ are constrained to take one of the discrete set of values $\pi k_{i,j}/3$, where $k_{i,j} = 0, 1, 2, 3, 4, 5$ will be used to label the different spin states. The Hamiltonian (11) then reduces to the 6-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 $\kappa$ is varied. For $\kappa < 1/3$ the ground state is ferromagnetic. For $\frac{1}{3} < \kappa < 1$ the order along the axial direction is helical with a sequence $k_i \equiv k_{i,j} = \ldots 01234501 \ldots$, with spins in adjacent planes differing by an angle $(\pi/3)$. For $\kappa > 1$ there are two degenerate states at zero temperature $\ldots 01340134 \ldots$ and $\ldots 00330033 \ldots$. Our aim is to describe the ground state of the Hamiltonian (11) as a function of $D$ and in particular the crossover between the two very different types of ordering at $D = 0$ and $D = \infty$.
For $D = \infty$ the ferromagnetic phase $\langle \infty \rangle$ and helical phase $\langle 1 \rangle$ coexist for $\kappa = 1/3$. However, this is not a multiphase point and there is a first-order transition between the phases for large $D$. Decreasing $D$ neither $\langle \infty \rangle$ nor $\langle 1 \rangle$ change their energy as the spins remain along an easy axis. Consequently the transition remains at $\kappa = 1/3$.

However, it is also necessary to consider two sets of phases which in the limit $D = \infty$ are very close in energy to the ferromagnetic and helical phases but which lower their energy as $D$ decreases. At $(\kappa = 1/4, D = \infty)$ all structures obtained by combining 1- and 2-bands are degenerate. At $(\kappa = 1/2, D = \infty)$ all phases comprising $m \geq 2$ bands are degenerate. As $D$ decreases sequences of periodic phases spring from the multiphase points. For large $D$, however, these are metastable because the phases $\langle \infty \rangle$ and $\langle 1 \rangle$ have lower energies. However, unlike $\langle \infty \rangle$ and $\langle 1 \rangle$ they can decrease their energy by a canting of the spins. For example in the phase $\langle 21 \rangle$ the two parallel spins move apart as $D$ is decreased reaching, for $D = 0$, the uniform arrangement with $q = 2\pi/9$. Therefore we have to consider the possibility of their appearing as stable phases for small $D$.

Following the energies of the hidden phase sequences numerically it is apparent that this is indeed the case (Seno, Yeomans, Harbord, Ko 1994). The results are shown in Figure 2a and are enlarged in Figure 2b. The phase diagram can be built up inductively with each phase being constructed from its neighbours (eg $\langle 12 \rangle + \langle 12^2 \rangle \rightarrow \langle 1212^2 \rangle$) as is usual for models of this type. Within numerical limitations all the expected states appear. Higher order phases are expected to occupy extremely small regions of the phase diagram and cannot be resolved numerically.

A different behaviour is seen near $\kappa = 1$ which is a multiphase point (see Figure 2). Here all states for which $|k_{i+1} - k_i| = 1$ or 2, with the proviso that two neighbouring jumps of 2, $|k_{i+2} - k_{i+1}| = |k_{i+1} - k_i| = 2$, are forbidden, are stable. We define a wall as lying between sites $i$ and $i+1$ if $|k_{i+1} - k_i| = 2$. The notation used above can still be employed to describe the stable states but we use square brackets to indicate that a band now contains helically coupled spins. For example $\ldots 01|345|12|450\ldots$, where walls are denoted by vertical lines, will be labelled $[23]$. 

\[9\]
A $1/D$ expansion (Seno and Yeomans 1994) shows that all phases which only contain bands of length $\geq 3$ and which obey the branching rules, spring from the multiphase point at $\kappa = 1$. To within the accuracy of the numerical calculation all phases containing 2- and 3-bands then appear between [2] and [3] as $D$ is decreased. It was possible to check for the existence of phases with periods of up to 100 lattice spacings.

The solid phase boundaries shown in Figure 2 follow the numerical results. As $D \to 0$ we also show by dotted lines the expected behaviour; that the phase widths decrease and a given phase touches the $D = 0$ axis at a single point corresponding to the appropriate value of $q$. Phases arising from the multiphase points at $\kappa = 1/4$, $\kappa = 1/2$, and $\kappa = 1$ touch the $D = 0$ axis for ranges of $\kappa$ from $1/2\sqrt{3} \to 1/2$, $1/4 \to 1/2\sqrt{3}$, and $1/2 \to \infty$ respectively. It is not possible to follow the low anisotropy behaviour numerically because an infinite number of phases would have to be considered.

An important question is whether incommensurate phases persist in the phase diagram for non-zero spin anisotropy. In the continuum limit the Hamiltonian (11) can be mapped onto the Frenkel-Kontorova model. Thus it is expected on the basis of previous work that, for small $D$, the devil’s staircase is incomplete with incommensurate phases appearing between the commensurate ones (Bak 1982).

In conclusion I should like to emphasise the immense richness of behaviour seen in these simple spin systems. The degeneracy of the multiphase point allows any perturbation to have a strong effect on the phase diagram. Although there are many qualitative similarities between the effect of different perturbations the quantitative results are strongly dependent on the details of the perturbation and the underlying model.

Finally I should point out that the models described here are of more than just theoretical interest. For example they have been used to model the ferrimagnetic order of the rare earths, mineral polytypism and antiphase domain ordering in binary alloys (Jensen and Mackintosh 1991, Loiseau, Van Tendeloo, Portier and Ducastelle 1985, Cheng, Heine and Jones 1990).
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FIGURE CAPTIONS

Figure 1: Schematic phase diagram of the ANNNI model at low temperatures. The mixed phases \( \langle 2^k 32^{k+1} 3 \rangle \) may be unstable to the appearance of higher-order mixed phases. The phase widths decrease exponentially with \( k \) and, for clarity, the widths of the higher-order phases have been exaggerated. (After Fisher and Szpilka 1987 b.)

Figure 2(a): Ground state phase diagram of the XY model with competing axial interactions and 6-fold spin anisotropy \( D \). Bold lines depict the numerical results; the dotted boundaries show the expected behaviour of the phase boundaries as \( D \to 0 \).

Figure 2(b): An enlargement of Figure 2(a) for \( 1/4 < J_2/J_1 < 1/2 \) and small \( D \). (After Seno, Yeomans, Harbord and Ko 1994.)