Quantum Fluctuations in the ANNNI Model

A. B. Harris,1,2 C. Micheletti,1 and J. M. Yeomans1

(1) Theoretical Physics, Oxford University, 1 Keble Rd. Oxford OX1 3NP, UK
(2) Department of Physics, University of Pennsylvania, Philadelphia, PA 19104-6396
(January 5, 2017)

Abstract

We obtain the ANNNI model from a Heisenberg model with large single-ion anisotropy energy, $D$, as might be relevant for helical spin systems. We treat quantum fluctuations to lowest order in $1/S$ at zero temperature within an expansion in $J/D$, where $J$ is an exchange energy. The transition from the state with periodicity $p = 4$ to the uniform state ($p = \infty$) occurs via an infinite sequence of first order transitions in which $p$ increases monotonically.

PACS numbers: 75.30.Et, 71.70.Ej, 75.30.Gw
Systems with long-period modulated structures are surprisingly common in nature. Examples include helical phases in the rare-earths and their compounds[1], polytypism[2], and the arrangement of antiphase boundaries in binary alloys[3]. A given compound may exhibit many different modulated structures of differing wavelength as a control parameter such as the temperature is varied. Some modulated structures can usefully be viewed as an assembly of domain walls when the energy for introducing a wall passes through zero. The stability of the different structures is then determined by the interactions between pairs, trios, etc. of walls[4]. It has been established that these interactions can result from entropic contributions to the free energy[5] and from softening of the spins[6]. Here our aim is to show that quantum fluctuations can also stabilize long-period modulated structures.

The Hamiltonian we consider is

\[ H = -J_1 \sum_{ij} S_{i,j} \cdot S_{i+1,j} + \frac{J_2}{S^2} \sum_{ij} S_{i,j} \cdot S_{i+2,j} - \frac{J_0}{S^2} \sum_{i(jj')} S_{i,j} \cdot S_{i,j'} - \frac{D}{S^2} \sum_{ij} ([S_{i,j}^z]^2 - S^2) , \tag{1} \]

where \( i \) labels the planes of a cubic lattice perpendicular to the \( z \)-direction and \( j \) the position within the plane. Also \( \langle jj' \rangle \) indicates a sum over pairs of nearest neighbors in the same plane and \( S_{i,j} \) is a quantum spin of magnitude \( S \) at site \( (i,j) \). For \( D = \infty \), only the states \( S_{iz} = \sigma_i S \), where \( \sigma_i = \pm 1 \) are relevant and \( H \) reduces to the axial next-nearest neighbor Ising (ANNNI) model, first proposed to describe helical phases of the heavy rare earths[7],

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

The ground state of the ANNNI model is ferromagnetic for \( \kappa \equiv J_2/J_1 < 1/2 \) and an antiphase structure with layers ordering in the sequence \( \{ \sigma_i \} = \{ \ldots 1, 1, -1, -1, 1, 1, -1, -1 \ldots \} \) for \( \kappa > 1/2 \). \( \kappa = 1/2 \) is a multiphase point[8], where the ground state is infinitely degenerate with all possible configurations of ferromagnetic and antiphase orderings having equal energy. For classical spins \( S = \infty \), the ground state (and therefore the multiphase point) is
maintained as $D$ is reduced from infinity as long as $D$ is larger than about 1/2. For higher order anisotropies this is not the case[6].

To describe how the degeneracy is broken at the multiphase point we use a notation similar to that of Fisher and Selke[5] so that $\langle n_1, n_2, \ldots n_m \rangle$ denotes a state in which spins form domains (of parallel spins) whose widths repeat periodically the sequence $n_1, n_2, \ldots n_m$.

Fisher and Selke[5] showed that at nonzero temperature $T$ the degeneracy at the multiphase point is broken to give a sequence of phases $\langle 2^k3 \rangle$, for $k = 1, 2, 3, \ldots$ Fisher and Szpilka[4,8] later recast their analysis in terms of domain wall interactions and we will follow their formulation.

In view of this interesting phase diagram in the $\kappa$-$T$ plane, we are led to study the phase diagram in the $\kappa$–$D^{-1}$ plane when the spins are quantum operators. That quantum fluctuations can remove ground–state degeneracies was pointed out by Shender[9] and given the apt name "ground state selection" by Henley[10]. In this paper we show how the multiphase degeneracy is resolved by quantum fluctuations.

To study quantum fluctuations we introduce the Dyson-Maleev[11] transformation

$$
\begin{align*}
S_i^z &= \sigma_i (S - a_i^+ a_i) \\
S_i^+ &= \sqrt{2S} \left( \delta_{\sigma_i,1} \left[ 1 - \frac{a_i^+ a_i}{2S} \right] a_i + \delta_{\sigma_i,-1} a_i^+ \left[ 1 - \frac{a_i^+ a_i}{2S} \right] \right) \\
S_i^- &= \sqrt{2S} \left( \delta_{\sigma_i,1} a_i^+ + \delta_{\sigma_i,-1} a_i \right),
\end{align*}
$$

(3)

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 $i$. We thereby transform the Hamiltonian of Eq. (1) into the bosonic form

$$
\mathcal{H}(\{\sigma_i\}) = E_0 + \mathcal{H}_0 + V_{||} + V_{\perp} + V^{(4)},
$$

(4)

where $E_0 \equiv \mathcal{H}_A$,

$$
\begin{align*}
\mathcal{H}_0 &= \sum_{i,j} \left[ 2\tilde{D} + J_1 \sigma_{i,j} (\sigma_{i-1,j} + \sigma_{i+1,j}) \\
&\quad - J_2 \sigma_{i,j} (\sigma_{i-2,j} + \sigma_{i+2,j}) \right] S^{-1} a_i^+ a_i \\
&\quad \left( a_i^+ a_i \right)^2.
\end{align*}
$$

(5)
with $\tilde{D} = D + 2J_0$ and $V_{\parallel} (V_{\parallel})$ is the interactions between spins which are parallel (antiparallel)

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

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

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. In Eq. (6), $V^{(4)}$ represents the four operator terms proportional to $1/S^2$.

Fluctuations out of the classical ground state (the boson vacuum) only occur at the walls due to $V_{\parallel}$. We do not consider quantum fluctuations within a plane, since the phase diagram is determined by the interplanar quantum couplings. Also, since the walls in this three-dimensional system are flat at $T = 0$, we may characterize states of the system in terms of distances between walls.

We now consider the structure of perturbation theory for all states which are degenerate at the multiphase point $\kappa = 1/2$. Perturbation theory generates corrections to the diagonal energy of the classical states in powers of $1/S$ and $J/\tilde{D}$, where $J = J_1$ or $J_2$. Off-diagonal matrix elements (for example, in which two domain walls both move through one lattice constant) first occur in 2Sth order perturbation theory and may be ignored. We will only include effects of the quadratic Hamiltonian, i.e. we will work to leading order in $1/S$.

Instead of a direct evaluation of the energy of all possible phases, we follow the methods of Fisher and Szpliaka[8] and study the sequence of wall interaction energies: $E_w$, the 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 energy of the system when there are walls at positions $m_i$ as
\[ E = E_0 + n_w E_w + \sum_i V_2(m_{i+1} - m_i) \\
+ \sum_i V_3(m_{i+2} - m_{i+1}, m_{i+1} - m_i) \\
+ \sum_i V_4(m_{i+3} - m_{i+2}, m_{i+2} - m_{i+1}, m_{i+1} - m_i) \\
+ \ldots , \]

(8)

where \( E_0 \) is the energy with no walls present and \( n_w \) is the number of walls. The scheme of Ref. [8] for calculating the general wall potentials \( V_k \) is illustrated in Fig. 1. Let all spins to the left of the first wall have \( \sigma_i = \sigma \) and those to the right of the last wall have \( \sigma_i = \eta \) for \( k \) even and \( \sigma_i = -\eta \) for \( k \) odd. The energy of such a configuration is denoted \( E_k(\sigma, \eta) \). If \( \sigma = -1 \) (\( \eta = -1 \)) the left (right) wall is absent. Then the energy ascribed to the existence of \( k \) walls is given by[12]

\[ V_k(n_1, n_2, \ldots n_{k-1}) = \sum_{\sigma, \eta = \pm 1} \sigma \eta E_k(\sigma, \eta) . \]

(9)

Contributions to \( E_k \) which are independent of \( \sigma \) or \( \eta \) do not influence \( V_k \). \( E_k(\sigma, \eta) \) is calculated by developing the energy in powers of the perturbations \( V_|| \) and \( V_\perp \). To lowest order in \( 1/\tilde{D} \), contributions to \( V_k \) can be obtained, for instance, by creating an excitation at the left wall (using \( V_\perp \)) and (for wall separations \( n_1 > 3 \)) using \( V_|| \) to hop the excitation sufficiently near the other wall that one (or more) energy denominator depends on \( \eta \). Examples of such processes are shown in Fig. 2.

For instance for the top diagram of Fig. 2, we get

\[ E_2(\sigma, \eta) = - \left( \frac{J_2^2}{4\tilde{D} + J_1 + J_2 + \eta(J_2 - J_1)} \right) \frac{\delta_{\sigma,1}}{S} , \]

(10)

which gives a contribution to \( V_2(2) \) at order \( J^3/\tilde{D}^2 S \) of

\[ \sum_{\sigma, \eta = \pm 1} \sigma \eta E_2(\sigma, \eta) = \frac{2J_2^2(J_2 - J_1)}{16\tilde{D}^2 S} . \]

(11)

Collecting all such processes we find the general result

\[ V_2(2n + 1) = \frac{16\tilde{D}}{S} \left( \frac{J_2}{4\tilde{D}} \right)^{2n+1} \]

(12)

\[ V_2(2n) = \frac{4n^2(J_1^2/J_2) - 4J_1 + 8J_2}{S} \left( \frac{J_2}{4\tilde{D}} \right)^{2n} . \]

(13)
These results may be understood in terms of a correlation length $\xi \sim [1/\ln(4\tilde{D}/J_2)]$ which governs wall–wall interactions.

More generally, power counting shows that

$$V_3(2n, 2n) \sim V_3(2n, 2n + 1) \sim J(J/\tilde{D})^{4n}$$

$$V_3(2n - 1, 2n - 1) \sim V_3(2n - 1, 2n) \sim J(J/\tilde{D})^{4n-1}$$

(14)

and $V_k(n_1, n_2, \ldots n_{k-1}) \sim J(J/\tilde{D})^x$, where $x \geq \sum_j n_j - 2$. Second order perturbation theory yields the result

$$E_w = 2J_1 - 4J_2 - \frac{J_1^2 + 2J_2^2}{4\tilde{D}S} + O(J^3/\tilde{D}^2S).$$

(15)

When $E_w > 0$, the ferromagnetic phase is stable. This happens for $J_2 < J_c = J_1/2 - (3J_1^2/8\tilde{D}S)\ldots$.

We wish to describe the sequence of phases which occur as $J_2/J_1$ is decreased starting from $\langle 2 \rangle$ when $J_2/J_1 > 1/2$ and reaching $\langle \infty \rangle$ when $J_2 < J_c$. As Fisher and Szpilka show, the phase boundary along which $\langle n \rangle$ and $\langle n + 1 \rangle$ have the same energy is given by

$$E_w = nV_2(n) - (n + 1)V_2(n + 1) + nV_3(n,n)$$

$$- (n + 1)V_3(n + 1, n + 1) + \ldots$$

(16)

This relation yields a critical value of $J_2$, denoted $J_{nc}$ which can be expressed as $J_{nc} = J_c + \Delta J_2(n)$, where

$$\Delta J_2(n) = \frac{nV_2(n) - (n + 1)V_2(n + 1)}{\partial E_w/\partial J_2} + \ldots \bigg|_{J_2 = J_1/2}.$$  

(17)

Thus, to elucidate the topology of the phase diagram, it is not necessary to know $J_c$ accurately. For $n$ not too large, Eqs. (12), (13), and (17) give $\Delta J_2(n) \sim V_2(n) \sim J(J^2/\tilde{D}^2)^{[n/2]}$, where $[x]$ is the integer part of $x$. The tentative conclusion is that one has successive regions of stability of the phase $\langle n \rangle$, where $n$ increases as $J_2$ decreases, as shown in Fig. 3. However, we must check the stability of the phase boundary to mixed phases of $\langle n \rangle$ and $\langle n + 1 \rangle$.  

6
As Fisher and Szpilka show, the condition that this phase boundary be stable is that $F_n < 0$, where

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

(18)

Here the last term is higher order in $1/\D$ than the first two and can be neglected. All perturbative terms which contribute at lowest order in $1/\D$ to $V_3(n, n + 1)$ have their analogs for $V_3(n, n)$. By an appropriate grouping of terms one can show that for $n > 2$, $F_n < 0$. Basically this happens because even order ground-state-to-ground-state terms in perturbation theory are negative. The case $n = 2$ is special in that $F_2 = 0$ at lowest order. Then it is necessary to go to the next order, where we find

$$V_3(2, 2) = \frac{8J_2^2}{(4D)^3S}[-J_1^2 + 2J_1J_2 - 2J_2^2]$$

$$+ \frac{12J_2^2}{(4D)^4S}[-4J_1^3 + 12J_1^2J_2 - 5J_1J_2^2 + 10J_2^3].$$

(19)

$$V_3(2, 3) = -\frac{8J_2^4}{(4D)^3S} + \frac{12J_2^4}{(4D)^4S}[2J_1^2J_2 + 4J_1J_2^2 + 5J_2^3].$$

(20)

$$V_3(3, 3) = O(J^6/\D^5S).$$

(21)

To leading order in $1/S$ we may set $J_2 = J_1/2$, in which case the above results indicate that $F_2 \sim A/\D^4$, where $A < 0$. Thus all the phase boundaries between phases $\langle n \rangle$ and $\langle n + 1 \rangle$ are stable against subdivision.

The above results are valid (as we shall see) for $n < \sqrt{\D/J}$. When this limit is violated, the entropy of more complicated perturbation contributions can compensate for taking more powers of $J/\D$. We overcome this limitation with respect to $V_2(n)$ as follows. We work to lowest (second) order in $V_4$ (A pair of excitations is created, one to the left of the left wall and one to the right of the left wall, as in Fig. 2, and is later destroyed.) To simplify the result we assume that the excitation created to the left of the left wall does not propagate. We work to first order in the field exerted on spins $n - 1$ and $n$ by the spins in the neighboring
domain. The result for the ground state energy is then expressed in terms of the EXACT spin-wave Green’s function, $G^{(n)}$, for an isolated domain of $n$ spins. In this way we sum over all trajectories of the spin deviation inside the domain of $n$ parallel spins. For small $n$ we reproduce the above results[13]. For large $n$ the result at leading order in $J/\tilde{D}$ is

$$V_2(n) = 4J_2^2 G^{(n)}(2, n - 1)^2/S,$$  \hspace{1cm} (22)

where

$$G^{(n)}(i, j) = \sum_{\alpha} \frac{\phi_{\alpha}(i)\phi_{\alpha}(j)}{2\tilde{D} + \epsilon_{\alpha}}. \hspace{1cm} (23)$$

Here $\phi_{\alpha}$ and $\epsilon_{\alpha}$ are the exact eigenstates and energies for the single–spin excitations of an isolated system of $n$ parallel spins. We carried out an exact evaluation of $G^{(n)}(2, n - 1)$. For large $n$, we found

$$G(2, n - 1)^2 = \frac{4\tilde{D}}{J_2^3} e^{-n/\tilde{\xi}} \sin^2(n\delta), \hspace{1cm} n \text{ even}$$

$$= \frac{4\tilde{D}}{J_2^3} e^{-n/\tilde{\xi}} \cos^2(n\delta), \hspace{1cm} n \text{ odd}, \hspace{1cm} (24)$$

where $\delta = J_1/\sqrt{16\tilde{D}J_2}$ and $\tilde{\xi} - \xi$ differs from zero due to corrections which are higher order in $J/\tilde{D}$. Eqs. (22) and (24) seem to imply that $V_2(n)$ can become arbitrarily close to zero. That is an artifact of truncating these equations at leading order in $J/\tilde{D}$. Where $V_2(n)$ would be small, one must keep the appropriate terms which are otherwise corrections. So doing we have a result which is uniformly asymptotically correct for $n \gg \sqrt{\tilde{D}/J}$[14]:

$$V_2(n) = \frac{16\tilde{D}}{S} e^{-n/\tilde{\xi}} \left( \sin^2(n\delta + \phi) + \frac{J_1J_2}{2\tilde{D}^2} \right), \hspace{1cm} n \text{ even}$$

$$= \frac{16\tilde{D}}{S} e^{-n/\tilde{\xi}} \left( \cos^2(n\delta + \phi) + \frac{J_1J_2}{2\tilde{D}^2} \right), \hspace{1cm} n \text{ odd}, \hspace{1cm} (25)$$

where $\phi$ is a phase shift of order $1/\sqrt{D}$.

An elegant graphical interpretation of the phase boundaries suggested by Fisher and Szpilka is that one should construct the extremal convex envelope of $V_2(n)$ versus $n$. The
points \([n, V_2(n)]\) which make up the envelope correspond to the phases \(\langle n \rangle\) which occur when \(V_2(n)\) is not convex, as Eq. (24) shows to be the case. As a result, we conclude that there is an infinite sequence of phase boundaries. When \(2n\delta/\pi\) is nearly an integer, the phase boundaries will be between phases \(n\) and \(n+2\) because of the nonconvexity of \(V_2(n)\). Note that in contrast to the ANNNI model, here \(V_2(n)\) does not pass through zero. 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, giving rise to the factor \(G^2\) in Eq. (22). In the ANNNI model the analogous factor involves only a one-way connection corresponding to \(G\). As a consequence, for the ANNNI model the sequence of phases terminates at a value, \(n_0\), which diverges as \(T \to 0\). There is no cut-off on \(n\) in the present model.

We were unable to carry out a precise analysis for \(V_3\) at large \(n\). Accordingly, at large \(n\) we can not guarantee the stability of these phase boundaries. It is conceivable that our result for small \(n\) breaks down and that the phase boundaries obtained from \(V_2(n)\) become unstable to mixing, which could even be hierarchical.

To summarize: 1) We have shown that quantum fluctuations do remove the infinite degeneracy of the multiphase point of the ANNNI model. 2) We have shown that quantum fluctuations at \(T = 0\) lead to a sequence of first order transitions similar to that for the ANNNI model, but involving a different sequence of phases. 3) In contrast to the ANNNI model there is no cut-off at large \(n\) on the appearance of phases because here \(V_2(n)\) never becomes negative. As we explained, this is a peculiarly quantum effect.

ACKNOWLEDGEMENTS: JMY is supported by an EPSRC Advanced Fellowship, ABH by an EPSRC Visiting Fellowship, and CM by an EPSRC Studentship and the Fondazione "A. della Riccia," Firenze.
REFERENCES


13 For small $n$ and to lowest order in $J/\tilde{D}$, Eq. (22) holds for $n$ odd. For $n$ even and small we have $V_2(n) = 4J_2^2[G^{(n)}(2, n - 1) - 2G(1, n - 1)]^2/S$.

14 We also checked numerically (for $\tilde{D}/J_2$ up to 400) that in the intermediate region (where neither the small $n$ nor the large $n$ results apply) $V_2(n)$ remains positive. In fact, Eq. (25) is a reasonable approximation for all $n$. 

10
FIGURE CAPTIONS

**FIG. 1** Configurations needed to calculate the interaction energy for two walls at separation $n$ (top) and three walls at separations $n$ and $m$ (bottom).

**FIG. 2** Examples of configurations needed to calculate $V_2(2)$ (top), $V_2(3)$ (middle), and $V_2(4)$ (bottom). Here ”+” (”−”) indicate creation (destruction) of a spin excitation and the arrow indicate a hopping using $V_||$.

**FIG. 3** Schematic phase diagram of the ”soft” ANNNI model. The phase boundary between $\langle n \rangle$ and $\langle n + 1 \rangle$ depends on a power of $1/\tilde{D}$ which increases with $n$. We did not attempt to represent this dependence on $\tilde{D}$ correctly.
FIG. 1
FIG. 2
FIG. 3