4-10-1995

Quantum Fluctuations in the Axial Next-Nearest-Neighbor Ising Model

A. Brooks Harris
University of Pennsylvania, harris@sas.upenn.edu

Cristian Micheletti

Julia M. Yeomans

Recommended Citation

Harris, A., Micheletti, C., & Yeomans, J. M. (1995). Quantum Fluctuations in the Axial Next-Nearest-Neighbor Ising Model. *Physical Review Letters, 74* (15), 3045-3048. http://dx.doi.org/10.1103/PhysRevLett.74.3045

Quantum Fluctuations in the Axial Next-Nearest-Neighbor Ising Model

Abstract

We obtain the axial next-nearest-neighbor Ising 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 a sequence of first order transitions in which p increases monotonically.

Disciplines

Physics | Quantum Physics

Quantum Fluctuations in the Axial Next-Nearest-Neighbor Ising Model

A. B. Harris,[1,2] C. Micheletti,[1] and J. M. Yeomans[1]

[1]*Theoretical Physics, Oxford University, 1 Keble Road, Oxford OX1 3NP, United Kingdom*

[2]*Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6396*

(Received 22 November 1994)

We obtain the axial next-nearest-neighbor Ising 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 a 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

$$\mathcal{H} = -\frac{J_1}{S^2}\sum_{i,j}\mathbf{S}_{i,j}\cdot\mathbf{S}_{i+1,j} + \frac{J_2}{S^2}\sum_{i,j}\mathbf{S}_{i,j}\cdot\mathbf{S}_{i+2,j} - \frac{J_0}{S^2}\sum_{i\langle jj'\rangle}\mathbf{S}_{i,j}\cdot\mathbf{S}_{i,j'} - \frac{D}{S^2}\sum_{i,j}([S^z_{i,j}]^2 - S^2), \quad (1)$$

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 $\mathbf{S}_{i,j}$ 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 $\mathcal{H}$ reduces to the axial next-nearest-neighbor Ising (ANNNI) model [7], first proposed to describe helical phases of the heavy rare earths,

$$\mathcal{H}_A = -J_0\sum_{i\langle jj'\rangle}\sigma_{i,j}\sigma_{i,j'} - J_1\sum_{i,j}\sigma_{i,j}\sigma_{i+1,j} + J_2\sum_{i,j}\sigma_{i,j}\sigma_{i+2,j}. \quad (2)$$

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 [5], 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 $\langle 2^k 3\rangle$, 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 κ-T plane, we are led to study the phase diagram in the κ-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 Letter we show how the multiphase degeneracy is resolved by quantum fluctuations.

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

$$S_i^z = \sigma_i(S - a_i^\dagger a_i),$$
$$S_i^+ = \sqrt{2S}\left(\delta_{\sigma_i,1}\left[1 - \frac{a_i^\dagger a_i}{2S}\right]a_i + \delta_{\sigma_i,-1}a_i^\dagger\left[1 - \frac{a_i^\dagger a_i}{2S}\right]\right),$$
$$S_i^- = \sqrt{2S}\,(\delta_{\sigma_i,1}a_i^\dagger + \delta_{\sigma_i,-1}a_i), \quad (3)$$

where $\delta_{a,b}$ is unity if $a = b$ and is zero otherwise and $a_i^\dagger$ (a_i) creates (destroys) a spin excitation at site i. We thereby transform the Hamiltonian of Eq. (1) into the bosonic form

$$\mathcal{H}(\{\sigma_i\}) = E_0 + \mathcal{H}_0 + V_{\parallel} + V_{\nparallel} + V^{(4)}, \quad (4)$$

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

$$\mathcal{H}_0 = \sum_{i,j}[2\tilde{D} + J_1\sigma_{i,j}(\sigma_{i-1,j} + \sigma_{i+1,j}) - J_2\sigma_{i,j}(\sigma_{i-2,j} + \sigma_{i+2,j})]S^{-1}a_{i,j}^\dagger a_{i,j}, \quad (5)$$

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

$$V_{\parallel} = \frac{1}{S} \sum_{i,j} [-J_1 X(i, i+1; j) (a_{i,j}^{\dagger} a_{i+1,j} + a_{i+1,j}^{\dagger} a_{i,j}) + J_2 X(i, i+2; j) (a_{i,j}^{\dagger} a_{i+2,j} + a_{i+2,j}^{\dagger} a_{i,j})], \tag{6}$$

$$V_{\nparallel} = \frac{1}{S} \sum_{i,j} [-J_1 Y(i, i+1; j) (a_{i,j}^{\dagger} a_{i+1,j}^{\dagger} + a_{i+1,j} a_{i,j}) + J_2 Y(i, i+2; j) (a_{i,j}^{\dagger} a_{i+2,j}^{\dagger} + a_{i+2,j} a_{i,j})], \tag{7}$$

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. (4) $V^{(4)}$ 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 $V_{\nparallel}$. 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 $2S$th 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 Szpilka [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

$$E = E_0 + n_w E_w + \sum_i V_2(m_{i+1} - m_i) + \sum_i V_3(m_{i+2} - m_{i+1}, m_{i+1} - m_i) + \sum_i V_4(m_{i+3} - m_{i+2}, m_{i+2} - m_{i+1}, m_{i+1} - m_i) + \cdots, \tag{8}$$

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

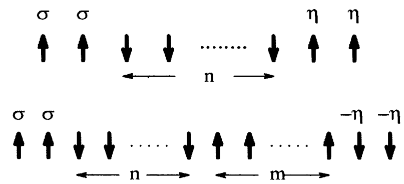

FIG. 1. Configurations needed to calculate the interaction energy for two walls at separation n (top) and three walls at separations n and m (bottom).

$\sigma_i = -\eta$ 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]

$$V_k(n_1, n_2, \ldots, n_{k-1}) = \sum_{\sigma,\eta=\pm 1} \sigma \eta E_k(\sigma, \eta). \tag{9}$$

Contributions to E_k which are independent of σ or η do not influence V_k. $E_k(\sigma, \eta)$ is calculated by developing the energy in powers of the perturbations $V_{\parallel}$ and $V_{\nparallel}$. 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 $V_{\nparallel}$) and (for wall separations $n_1 > 3$) using $V_{\parallel}$ to hop the excitation sufficiently near the other wall that one (or more) energy denominator depends on η. Examples of such processes are shown in Fig. 2.

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

$$E_2(\sigma, \eta) = -\left[\frac{J_2^2}{4\tilde{D} + J_1 + J_2 + \eta(J_2 - J_1)} \right] \frac{\delta_{\sigma,1}}{S}, \tag{10}$$

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

$$\sum_{\sigma,\eta=\pm 1} \sigma \eta E_2(\sigma, \eta) = \frac{2J_2^2(J_2 - J_1)}{16\tilde{D}^2 S}. \tag{11}$$

Collecting all such processes we find the general result

$$V_2(2n+1) = \frac{16\tilde{D}}{S} \left(\frac{J_2}{4\tilde{D}} \right)^{2n+1}, \tag{12}$$

$$V_2(2n) = \frac{4n^2(J_1^2/J_2) - 4J_1 + 8J_2}{S} \left(\frac{J_2}{4\tilde{D}} \right)^{2n}. \tag{13}$$

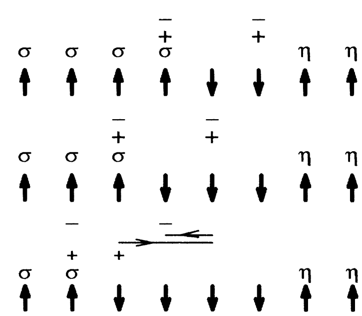

FIG. 2. Examples of configurations needed to calculate $V_2(2)$ (top), $V_2(3)$ (middle), and $V_2(4)$ (bottom). Here "+" ("−") indicates creation (destruction) of a spin excitation and the arrow indicates a hopping using $V_{\parallel}$.

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

$$V_3(2n,2n) \sim V_3(2n,2n+1) \sim J(J/\tilde{D})^{4n},$$
$$V_3(2n-1,2n-1) \sim V_3(2n-1,2n) \sim J(J/\tilde{D})^{4n-1}, \tag{14}$$

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

$$E_w = 2J_1 - 4J_2 - \frac{J_1^2 + 2J_2^2}{4\tilde{D}S} + O(J^3/\tilde{D}^2S). \tag{15}$$

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

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

$$E_w = nV_2(n) - (n+1)V_2(n+1) + nV_3(n,n) - (n+1)V_3(n+1,n+1) + \cdots. \tag{16}$$

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

$$\Delta J_2(n) = \left.\frac{nV_2(n) - (n+1)V_2(n+1)}{\partial E_w/\partial J_2} + \cdots\right|_{J_2=J_1/2}. \tag{17}$$

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 $\langle n+1\rangle$.

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

$$F_n \equiv V_3(n,n) - 2V_3(n,n+1) + V_3(n+1,n+1). \tag{18}$$

Here the last term is higher order in $1/\tilde{D}$ than the first two and can be neglected. All perturbative terms which contribute at lowest order in $1/\tilde{D}$ to $V_3(n,n+1)$ have

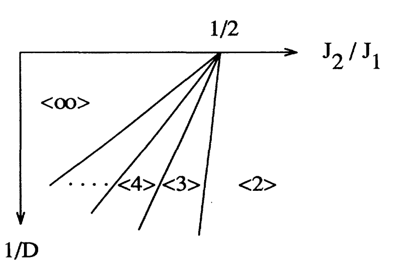

FIG. 3. Schematic phase diagram of the "soft" ANNNI model. The phase boundary between $\langle n\rangle$ and $\langle n+1\rangle$ depends on a power of $1/\tilde{D}$ which increases with n. We did not attempt to represent this dependence on $\tilde{D}$ correctly.

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

$$V_3(2,2) = \frac{8J_2^2}{(4\tilde{D})^3S}[-J_1^2 + 2J_1J_2 - 2J_2^2] + \frac{12J_2^2}{(4\tilde{D})^4S}[-4J_1^3 + 12J_1^2J_2 - 5J_1J_2^2 + 10J_2^3], \tag{19}$$

$$V_3(2,3) = -\frac{8J_2^4}{(4\tilde{D})^3S} + \frac{12J_2^2}{(4\tilde{D})^4S}[2J_1^2J_2 + 4J_1J_2^2 + 5J_2^3], \tag{20}$$

$$V_3(3,3) = O(J^6/\tilde{D}^5S). \tag{21}$$

To leading order in $1/S$ we may set $J_2 = J_1/2$, in which case the above results indicate that $F_2 \sim A/\tilde{D}^4$, 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 $n \ll \sqrt{\tilde{D}/J}$. When this limit is violated, the entropy of more complicated perturbation contributions can compensate for taking more powers of $J/\tilde{D}$. We overcome this limitation with respect to $V_2(n)$ as follows. We work to lowest (second) order in $V_\parallel$. (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. The result at leading order in $J/\tilde{D}$ is

$$V_2(n) = 4J_2^3(\Delta G)^2/S, \tag{22}$$

where $\Delta G = G^{(n)}(2,n-1) - 2G^{(n)}(1,n-1)$ with

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

Here ϕ_α and ϵ_α 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 ΔG. To leading order in $\tilde{D}/J_2$ we found

$$V_2(n) = \begin{cases} \frac{16\tilde{D}}{S}e^{-n/\tilde{\xi}}\sin^2(n\delta + \phi), & n \text{ even}, \\ \frac{16\tilde{D}}{S}e^{-n/\tilde{\xi}}\cos^2(n\delta + \phi), & n \text{ odd}, \end{cases} \tag{24}$$

where $\delta = J_1/\sqrt{16\tilde{D}J_2}$, $\tilde{\xi}$ includes corrections to ξ which are higher order in $J/\tilde{D}$, and ϕ is a phase shift of order δ^3. We have verified that Eq. (24) reduces to Eqs. (12) and (13) when n is small.

This result differs from that for the ANNNI model for which $V_2(n)$ has a similar form but with the trigonometric functions not squared. 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 we now discuss, this difference can have an important effect on the nature of the phase diagram. An elegant graphical interpretation of the phase boundaries suggested by Fisher and Szpilka [8] is that one should construct the lower convex envelope of $V_2(n)$ vs 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 in Eq. (24). It is therefore important to know whether or not $V_2(n)$ is always positive for finite n. If so, there will be an infinite sequence of phase boundaries. If not, then the sequence of phases is finite, ending with phase n_0. Thus the nature of the correction terms to Eq. (24) determines the nature of the phase diagram. These corrections come from various sources, including (a) finite size effects in $G^{(n)}$; (b) corrections to Eq. (22) involving $G^{(n)}(1, n-1)$ and/or $G^{(n)}(1, n)$; (c) propagation of the excitation to the left of the wall; (d) propagation of the excitations along nonstraight paths for a three-dimensional system. Inclusion of effects (a), (b), and (c) shows that for a one-dimensional model the small correction term in Eq. (24) does make $V_2(n)$ negative with an n_0 which we estimate to be of order D/J. For the three-dimensional system a definitive analysis becomes quite difficult. Our tentative conclusion is that in this case there is a range of the parameters J_0/D and J/D for which $V_2(n)$ is always positive, so that the devil's staircase never terminates, in contrast to the behavior of the ANNNI model, where the sequence of phase terminates at a value n_0, which diverges as $T \to 0$.

We were unable to carry out a precise analysis for V_3 at large n. Accordingly, at large n we cannot 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, we have shown that quantum fluctuations do remove the infinite degeneracy of the multiphase point of the ANNNI model. We have also 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. For some values of the parameters there may be no cutoff on the appearance of phases at large n. As explained above this possibility is a peculiarly quantum effect.

J. M. Y. is supported by an EPSRC Advanced Fellowship, A. B. H. by an EPSRC Visiting Fellowship, and C. M. by an EPSRC Studentship and the Fondazione "A. della Riccia," Firenze.

[1] *Rare Earth Magnetism Structures and Excitations,* edited by J. Jensen and A. R. Mackintosh (Oxford University Press, Oxford, 1991).
[2] J. M. Yeomans, in *Solid State Physics* (Academic Press, Orlando, 1988), Vol. 41.
[3] A. Loiseau, G. Van Tendeloo, R. Portier, and F. Ducastelle, J. Phys. (Paris) **46**, 595 (1985).
[4] A. M. Szpilka and M. E. Fisher, Phys. Rev. Lett. **57**, 1044 (1986).
[5] M. E. Fisher and W. Selke, Phys. Rev. Lett. **44**, 1502 (1980).
[6] F. Seno and J. M. Yeomans, Phys. Rev. B **50**, 10 385 (1994).
[7] R. J. Elliott, Phys. Rev. **124**, 346 (1961); J. Villain and M. B. Gordon, J. Phys. C **13**, 3117 (1980); P. Bak and J. von Boehm, Phys. Rev. B **21**, 5297 (1980); W. Selke, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1992), Vol. 15.
[8] M. E. Fisher and A. M. Szpilka, Phys. Rev. B **36**, 644 (1987).
[9] E. F. Shender, Sov. Phys. JETP **56**, 178 (1982).
[10] C. Henley, Phys. Rev. Lett. **62**, 2056 (1989).
[11] F. J. Dyson, Phys. Rev. **102**, 1217 (1956); S. V. Maleev, Sov. Phys. JETP **6**, 776 (1958).
[12] K. E. Bassler, K. Sasaki, and R. B. Griffiths, J. Stat. Phys. **62**, 45 (1991).