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Abstract

The ground-state energy of a spin-density wave of wave vector Q in a Heisenberg ferromagnet with competing interactions is calculated for small Q as $E_G(Q) = E_G(0) + A_1 Q^2 + A_2 Q^4 + \dots$. The coefficients A_1 and A_2 are calculated *exactly* at zero temperature in the limit as the ferromagnet to helix transition is approached. For some ranges of parameters we find that quantum zero point motion causes A_2 to become negative thus leading to a first-order transition not present in the classical system.

Disciplines

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First-order phase transition induced by quantum fluctuations in Heisenberg helimagnets

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The ground-state energy of a spin-density wave of wave vector $\mathbf{Q}$ in a Heisenberg ferromagnet with competing interactions is calculated for small $\mathbf{Q}$ as $E_G(\mathbf{Q}) = E_G(0) + A_1 Q^2 + A_2 Q^4 + \dots$. The coefficients A_1 and A_2 are calculated *exactly* at zero temperature in the limit as the ferromagnet to helix transition is approached. For some ranges of parameters we find that quantum zero point motion causes A_2 to become negative thus leading to a first-order transition not present in the classical system.

It is well known that Heisenberg systems with competing exchange interactions can produce a very rich phase diagram, including not only ferromagnetic (F) and antiferromagnetic (AF) phases, but also helical (H) phases.^{1,2} In particular we consider a Heisenberg system of quantum spins of magnitude S at temperature $T = 0$ on a hexagonal Bravais lattice governed by the Hamiltonian

$$H = -2 \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where $\langle ij \rangle$ indicates a sum over pairs of sites i, j and the J_{ij} are as follows. Between nearest neighbors in adjacent basal planes $J_{ij} = J'$ is ferromagnetic. In a basal plane the interactions between nearest neighbors J_1 are ferromagnetic, between second and third neighbors J_2 and J_3 can have either sign. In this paper we shall be concerned with H phases described by a wave vector $\mathbf{Q}$ such that $\mathbf{S}_i(\mathbf{r}_i)$ is in the direction

$$\mathbf{S}_i(\mathbf{r}_i) = S [\cos(\mathbf{Q} \cdot \mathbf{r}_i) \hat{\mathbf{y}}_c - \sin(\mathbf{Q} \cdot \mathbf{r}_i) \hat{\mathbf{x}}_c], \quad (2)$$

where $(\hat{\mathbf{x}}_c, \hat{\mathbf{y}}_c, \hat{\mathbf{z}}_c)$ is a coordinate axis fixed with respect to the crystal axes: $\hat{\mathbf{z}}_c$ lies along the crystal c axis, and $\hat{\mathbf{x}}_c$ lies in the basal plane along a nearest-neighbor direction. Since the model we consider has no anisotropy, we assume arbitrarily that the spins always lie in a basal plane. Also, since J' is ferromagnetic, $\mathbf{Q}$ will also always lie in a basal plane. (The hexagonal lattice we treat is simple, not close packed, so all spins on a given line parallel to the crystal c axis are parallel to one another.) In the classical approximation (i.e., for $S \rightarrow \infty$) the phase diagram² in the parameter space $j_2 = J_2/J_1$ and $j_3 = J_3/J_1$ is divided into five regions corresponding to F, AF, H, and 120° phases, as shown in Fig. 1. The phases H_2 and H_1 differ in that for the former $\mathbf{Q}$ lies along an in-plane nearest-neighbor direction, δ_1 , whereas for the latter $\mathbf{Q}$ lies along an in-plane second neighbor direction, i.e., $\mathbf{Q} \perp \delta_1$. In the classical approximation the F-H and AF-H₁ transitions are continuous. (For the F-H transition to be continuous, $\mathbf{Q}$ in the H phase must tend to zero as the phase boundary is approached.)

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It is of interest to know how quantum corrections^{3,4} (for finite S) affect the above conclusions. Clearly the ground-state energy per spin, E_G , of the F phase has no quantum corrections, whereas other phases have a lower energy due to zero point motion. However, to treat the effect of zero-point motion on the transitions in a clear way is not easy. The most serious problem concerns the value of $\mathbf{Q}$. Near a phase boundary the correct value of $\mathbf{Q}$ can be one for which the classical spin-wave Hamiltonian has unstable modes, and is therefore an inconvenient starting point for a conventional perturbation theory. To avoid such problems we determine the F-H phase boundary by a Landau-type construction in which the ground-state energy of a helical state of wave vector $\mathbf{Q}$ in the basal plane is calculated in powers of Q for small Q :

$$E_G(\mathbf{Q}) = E_G^{(0)} + A_1 Q^2 + A_2 Q^4 + \dots + K_\theta^6 Q^6 \cos(6\theta_Q) \dots, \quad (3)$$

where θ_Q is the angle between $\mathbf{Q}$ and δ_1 . Note that the in-plane anisotropy first enters at order Q^6 and that $K_\theta^6 > 0$ leads to $\mathbf{Q} \perp \delta_1$, and $K_\theta^6 < 0$ to $\mathbf{Q} \parallel \delta_1$. Within the F phase $A_1 > 0$. As the F-H transition is approached $A_1 \rightarrow 0$. If the F-H transition is continuous, then at the phase transition $A_2 > 0$, whereas if $A_2 < 0$, the transition is discontinuous. In the classical approximation²

$$A_1^{\text{cl}} = \frac{3}{2} J_1 S^2 (1 + 3j_2 + 4j_3), \quad (4a)$$

$$A_2^{\text{cl}} = -\frac{3}{32} J_1 S^2 (1 + 9j_2 + 16j_3), \quad (4b)$$

where the superscript cl indicates the classical ($S = \infty$) value. Thus, classically, $A_2 > 0$ along the entire F-H phase boundary ABC in Fig. 1. In this paper we study quantum corrections to A_1 and A_2 over the entire range of the F-H transition. In previous work⁵ we have found that quantum fluctuations gave a negative contribution to A_2 , but did not change the sign of A_2 for the case considered unless uniaxial anisotropy was invoked. The new result of the present paper is that this quantum effect becomes large enough in the vicinity of the multicritical points labeled A and C in Fig. 1 to cause A_2 to become negative. As we shall discuss, this phenomenon is due to the extreme softness of spin waves in these vicinities.

FIG. 1. Phase diagram² at $T=0$ of the classical Heisenberg helimagnet with reduced exchange interactions j_2 and j_3 as discussed in the text with ferromagnetic in-plane interactions. On the H-F phase boundary, $1 + 3j_2 + 4j_3 = 0$, and on the H₁-H₂ phase boundary $j_2 = 2j_3$.

We now describe briefly the calculation of A_1 and A_2 at $T=0$. Full details are given elsewhere.⁶ To calculate quantum corrections we use the Dyson-Maleev transformation^{7,8}

$$S_i^+ \equiv S_i^x + iS_i^y = \sqrt{2S}(1 - a_i^+ a_i/2S)a_i, \quad (5a)$$

$$S_i^- \equiv S_i^x - iS_i^y = \sqrt{2S}a_i^+, \quad (5b)$$

$$S_i^z = S - a_i^+ a_i, \quad (5c)$$

where $\hat{x}$, $\hat{y}$, and $\hat{z}$ are local axes for spin i such that $\hat{z}$ is a unit vector in the direction of S_i , as given by Eq. (2). For the F phase where $\hat{z}$ is independent of i , one has $(Q=0)$ and the Hamiltonian is

$$H(Q=0) = E_G(Q=0) + \sum_k \epsilon_k(Q=0) a_k^+ a_k + \frac{1}{2NS_{1,2,3,4}} \Phi_{1234}(Q=0) \times \delta(1+2-3-4) a_1^+ a_2^+ a_3 a_4 \quad (6)$$

$$\equiv E_G(0) + H_0 + V_{DM}, \quad (7)$$

where $\epsilon_k(Q=0)$ is the energy of a ferromagnetic spin wave of wave vector k ,

$$a_k^+ = N^{-1/2} \sum_i a_i^+ \exp(ik \cdot r_i),$$

in the second term 1 denotes k_1 , 2 denotes k_2 , etc., and Φ_{1234} is the famous Dyson-Maleev interaction potential.^{7,8} Both ϵ_k and Φ depend on all the J 's. For small wave vectors in the basal plane one has

$$\epsilon_k(Q=0) = 3J_1 S a^2 k_\perp^2 (1 + 3j_2 + 4j_3) - \frac{3}{16} J_1 S a^4 k_\perp^4 (1 + 9j_2 + 16j_3), \quad (8)$$

where $k_\perp^2 = k_x^2 + k_y^2$, and a is the nearest-neighbor separation. This dispersion relation indicates that an instability in basal plane spin waves occurs at the F-H phase boundary, as one would expect.

When Q is no longer zero, ϵ_k and Φ_{1234} are modified, but also many additional terms arise. Of these we write here only those which affect the calculation of A_1 and A_2 . Thus, we write for small Q :

$$H(Q) = \sum_k \epsilon_k(Q) a_k^+ a_k + \frac{1}{2NS_{1,2,3,4}} \Phi_{1234}(Q) \times \delta(1+2-3-4) a_1^+ a_2^+ a_3 a_4 + \frac{1}{2} \sum_k B_k(Q) (a_k a_{-k} + a_k^+ a_{-k}^+) + E_G^{\text{cl}}(Q), \quad (9)$$

where

$$B_k(Q) = -\frac{1}{2} \sum_{\delta} J_{\delta} S (Q \cdot \delta)^2 \cos k \cdot \delta. \quad (10)$$

The only terms in the complete $H(Q)$ which have nonzero matrix elements with the ferromagnetic ground state are the pair creation and pair annihilation terms written in the third line of Eq. (9). Note that $B_k(Q) \sim Q^2$. This fact implies that corrections to the classical value of E_G are of order Q^4 at least: A_1 has no quantum corrections. To evaluate A_2 we study

$$E_G(Q) = E_G^{\text{cl}}(Q) + \left\langle 0 \left| V \sum_{n=0}^{\infty} (GV)^n \right| 0 \right\rangle_c, \quad (11)$$

where V is the perturbation, $\langle \rangle_c$ indicates that only connected diagrams are used, and $G \equiv (E_0 - H_0)^{-1}$. For this calculation we take

$$H_0 = \sum_k \epsilon_k(0) a_k^+ a_k$$

and V therefore includes all other terms in $H(Q)$. Since $\langle 0|V|0\rangle$ and $V|0\rangle$ are each of order Q^2 , we see that all other V 's appearing in Eq. (11) can be evaluated at $Q=0$, i.e., we may set $V = V_{DM}$ for such "internal" V 's. Thus, if

$$V_2^+ = \sum_k B_k(Q) a_k^+ a_{-k}^+ = \text{h.c.}(V_2^-), \quad (12)$$

where h.c. indicates hermitian conjugate, we may then write

$$E_G(Q) = E_G^{\text{cl}}(Q) + \langle 0|V_2^- G V_2^+|0\rangle + \langle 0|V_2^- G t_{DM} G V_2^+|0\rangle, \quad (13)$$

where t_{DM} is the t matrix for repeated scatterings by V_{DM} :

$$t_{DM} = V_{DM} + V_{DM} G t_{DM}. \quad (14)$$

Thus, our formal result is

$$A_1 = A_1^{\text{cl}}, \quad A_2 = A_2^{\text{cl}} + \delta A_2, \quad (15)$$

where

$$\delta A_2 = (\langle 0|V_2^- G V_2^+|0\rangle + \langle 0|V_2^- G t_{DM} G V_2^+|0\rangle)/Q^4. \quad (16)$$

Here we have used the fact that the only form of order Q^4 consistent with hexagonal symmetry is Q^4 . (In order Q^6 we would get contributions to both A_3 and K_6^* .)

The detailed construction of t_{DM} and evaluation of δA_2 are given in a full paper.⁶ Here we make a few comments on the results. A crucial result is that A_2 becomes negative on the F-H phase boundary at $T=0$ near the multicritical points A and C of Fig. 1. For $J'/J=0.1$ and $S=\frac{1}{2}$, we find $A_2 < 0$ for $j_3 < -0.913$ and $j_3 > 0.168$, so the largest effect is near A . The region over which A_2 is negative decreases as either S or J' is increased. As S increases quantum fluctu-

ations are reduced. As J' increases, the spin waves become stiffer and reduce the fluctuations. However, even for $J' = J_1$ and $S = \frac{1}{2}$, A_2 is negative, leading to a first-order transition, for a significant range ($0.36 < j_3 < 0.5$) of the F-H transition. That the first order region is large near A is attributed to the extreme softness of basal plane spin waves. All along the F-H transition $\epsilon_k \sim c_1 k_1^4 + c_2 k_z^2$, but $c_1 \rightarrow 0$ at A , so at A $\epsilon_k \sim k_1^6$ for basal plane spin waves, leading to large fluctuation effects. The points on the line ABC where A_2 becomes negative may be denoted A' and C' . From a separate total energy calculation one can determine to order $1/S$ the locations A'' and C'' of the multicritical points where three phases coexist. Since the point C' is very close to C , we believe that it lies in the interval $C-C''$, in which case the F- H_2 transition would always be continuous. In contrast, quantum fluctuations cause A' to be rather far from A , so that A' falls outside the interval $A-A''$. Thus, we expect that there is actually a regime in which the F- H_1 transition is discontinuous.

This work also leaves several issues unresolved. In the regime where the F-H transition is discontinuous it would be of interest to estimate the size of the discontinuity in Q as a function of the exchange parameters. Finally, a major question which we have not addressed is whether this phenomenon occurs for nonzero temperature.

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