Ising Transition in Frustrated Heisenberg Models

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We derive scaling equations for a 2D square Heisenberg model where frustration spontaneously breaks the Z_4 lattice symmetry. At short distances, the model behaves as two interpenetrating Néel sublattices. Short-wavelength fluctuations couple these sublattices, driving a crossover to single-lattice behavior at long distances and generating an Ising order parameter. When the spin-correlation and crossover lengths become comparable, there exists a finite-temperature Ising phase transition *independent* of the subsequent development of a sublattice magnetization.

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The possible connection between antiferromagnetism and copper-oxide superconductivity has led to considerable interest in the properties of two-dimensional (2D) Heisenberg models. It was originally proposed that these systems have a strong-coupling phase where quantum fluctuations destabilize the long-range Néel order.[1] Though the relevant 2D $S=\frac{1}{2}$ square Heisenberg antiferromagnet appears to have a finite sublattice magnetization,[2-4] the possibility of strong coupling "disordered phases" in certain generalizations of this model remains a subject of great interest.

One method of enhancing fluctuations in the 2D Heisenberg antiferromagnet is to add diagonal bond frustration. The model considered is

$$H=\sum_{(i,j)} J(\mathbf{R}_i-\mathbf{R}_j)\mathbf{S}_i\cdot\mathbf{S}_j\,, \tag{1}$$

with

$$J(\mathbf{R})=\sum_{\mathbf{q}}[2J_1(c_x+c_y)+4J_2(c_xc_y)]\cos(\mathbf{q}\cdot\mathbf{R})\,, \tag{2}$$

where $c_l=\cos(q_la)$, and J_2 and $J_1=2\eta J_2$ are the second- and first-nearest-neighbor couplings (Fig. 1). In the region $\eta\sim 1$, quantum fluctuations become large enough to destroy the sublattice magnetization.[5-7]

Previous theoretical work has focused on the limit of weak frustration $\eta\gtrsim 1$, where the relevant long-wavelength action is the O(3) nonlinear sigma model.[8,9] In this regime, it has been suggested that when the microscopic spins are not multiples of two, the strong-coupling limit is characterized by a dimer ground state. However, for strong frustration $\eta\lesssim 1$, the relevant long-wavelength action is no longer a conventional O(3) sigma model. In this regime, the magnetic wave vector $\mathbf{Q}$ of the classical ground states no longer lies along a diagonal in reciprocal space, breaking the Z_4 lattice symmetry and giving rise to a superlattice structure. Classically, these magnetic structures exhibit an internal O(3) degeneracy analogous to the phason mode of charge-density waves, whereby one sublattice may be continuously rotated about the other. According to Villain's principle of "order from disorder,"[10,11] short-wavelength fluctuations lift these degeneracies, generating new correlations at long wavelengths.

In this Letter, we explore some of the consequences in the simplest example, where $\eta<1$ and the magnet becomes collinear, with $\mathbf{Q}=(0,\pi)$ or $(\pi,0)$. Classically, the ground state consists of two interpenetrating Néel sublattices with independent staggered magnetizations $\hat{\mathbf{n}}_1$ and $\hat{\mathbf{n}}_2$. Although the exchange fields between the two sublattices cancel, the zero-point and thermal fluctuations depend on the angle θ between the two sublattices. This is most clearly understood in the analogous ferromagnetic J_1,J_2 model, $(J_1,J_2<0)$, which behaves as two interpenetrating ferromagnetic sublattices. Here, zero-point motion is completely eliminated when the two sublattices are parallel, forming a pure ferromagnet. In

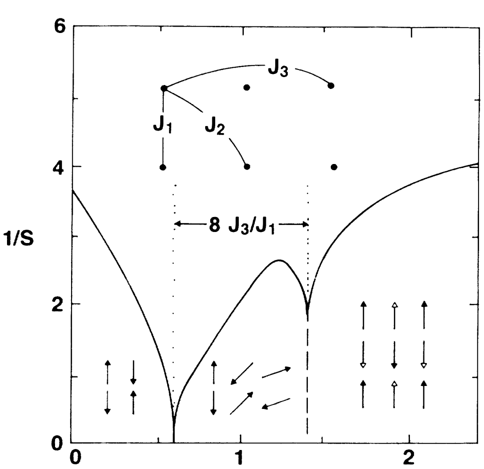

FIG. 1. Inset: Illustration of 2D square frustrated Heisenberg antiferromagnet. Main diagram: The critical value of S where the sublattice magnetization vanishes, calculated for $J_3=0.1J_1$ from spin-wave theory, showing the Néel, helicoid, and collinear phases.

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the antiferromagnetic case of interest, fluctuations can never be eliminated, but they are minimized in the configuration that is *maximally ferromagnetic.* This occurs when $\hat{\mathbf{n}}_1\cdot\hat{\mathbf{n}}_2=\pm 1$, and the spins along the x or y axes are ferromagnetically aligned. Short-wavelength fluctuations thereby select the collinear configurations, breaking the Z_4 lattice symmetry. The appearance of the soft Ising order parameter $\sigma=\hat{\mathbf{n}}_1\cdot\hat{\mathbf{n}}_2$ in these phases is an example of Villain's "order from disorder." In the 2D Heisenberg model this phenomenon is particularly marked, for Ising order survives the loss of sublattice magnetization at finite temperature, leading to a finite-temperature second-order phase transition.

A gradient expansion of the classical energy $E=\sum J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j$ in the 2D square collinear magnet yields the classical action

$$A=\frac{1}{2g}\int d^2x\left[\sum_{i=1,2}(\partial\hat{\mathbf{n}}_i)^2+2\eta(\partial_x\hat{\mathbf{n}}_1\cdot\partial_x\hat{\mathbf{n}}_2-\partial_y\hat{\mathbf{n}}_1\cdot\partial_y\hat{\mathbf{n}}_2)\right], \quad (3)$$

where $g=T/2S^2J_2$. At first sight, the second term in A is not invariant under lattice rotations. However, under a 90° lattice rotation about a site on sublattice one, up and down sites of sublattice two are *interchanged,* and the sublattice magnetization $\hat{\mathbf{n}}_2$ changes sign. Under the lattice rotation operation $(x,y)\to(-y,x)$, $\hat{\mathbf{n}}_2\to-\hat{\mathbf{n}}_2$, the action is then invariant. This action is appropriate for short wavelengths and high temperature, where the fluctuation coupling between the Néel sublattices can be neglected. The scaling behavior of A determines the spin correlations in this "two-sublattice" regime. We set $\hat{\mathbf{n}}_i(x)=[1-(\phi_i)^2]^{1/2}\hat{\mathbf{n}}_0(x)+\phi_i^a\hat{\mathbf{e}}_a$, where $\hat{\mathbf{n}}_0(\mathbf{r})$ is the slowly varying component of the magnetization,[12] and the ϕ_a^i are the short-wavelength fluctuations in directions $\hat{\mathbf{e}}_a^i$ orthogonal to $\hat{\mathbf{n}}_0^i$. In this coordinate system

$$\partial_a\hat{\mathbf{n}}_0=B_a^a\hat{\mathbf{e}}_a,\quad \partial_a\hat{\mathbf{e}}_a=A_a^{ab}\hat{\mathbf{e}}_b-B_a^a\hat{\mathbf{n}}_0^i. \quad (4)$$

Expanding the action to Gaussian terms in the symmetric and antisymmetric fluctuations $\phi_s=(\phi^1+s\phi^2)/\sqrt{2}$ $(s=\pm)$, we find

$$A=\frac{1}{2g}\int d^2x\{[(1+s\epsilon_a\eta)(\mathcal{D}_a\phi_s^a)^2+2(1+\epsilon_a\eta)(B_a^a)^2]+B_a^aB_a^b[(1+s\epsilon_a\eta)\phi_s^a\phi_s^b-\delta_{ab}(1+\eta\epsilon_a)\phi_s^2]\}, \quad (5)$$

where $(\epsilon_x,\epsilon_y)=(1,-1)$ and $\mathcal{D}_a\phi_s^a=\partial_a\phi_s^a-A_a^{ab}\phi_s^b$. Integrating out the fast fluctuations renormalizes the coupling constants through the last term in (5), according to the scaling equations

$$\partial g/\partial\ln(\Lambda)=-(1-\eta^2)^{-1/2}g^2/2\pi,$$
$$\partial\eta/\partial\ln(\Lambda)=(1-\eta^2)^{-1/2}\eta g/2\pi, \quad (6)$$

where Λ^{-1} is the short-wavelength cutoff. The last equation implies that $\eta g=\eta_0g_0$ is constant, so the anisotropy η scales to zero in the two-sublattice regime. Using this to integrate the first scaling equation, we find that g becomes of order unity at the correlation length $\xi\sim a\times\exp[2\pi/z_0g_0]$, where

$$z_0=2\eta_0/[\sin^{-1}\eta_0+\eta_0(1-\eta_0^2)^{1/2}] \quad (7)$$

is a renormalization due to the anisotropy and a is the lattice constant.

At longer length scales and lower temperatures, the fluctuation coupling between sublattices becomes important. To calculate the contribution to the free energy from the short-wavelength fluctuations, we use the spin-wave dispersion

$$\omega_\eta(\mathbf{q})^2=(4SJ_2)^2\{[1+\eta(\alpha c_x+\beta c_y)]^2-[c_xc_y+\eta(\alpha c_y+\beta c_x)]^2\}, \quad (8)$$

with $c_l=\cos q_l$ $(l=x,y)$, $(\alpha,\beta)=(\cos^2\theta/2,\sin^2\theta/2)$. This spectrum has zero modes at the four points $\mathbf{Q}_1=0$, $\mathbf{Q}_2=(\pi,0)$, $\mathbf{Q}_3=(0,\pi)$, and $\mathbf{Q}_4=(\pi,\pi)$. The free-energy contribution from the short-wavelength modes is then

$$F_{\text{fl}}(\eta)=\int_{|\mathbf{q}-\mathbf{Q}_i|>\Lambda}\frac{d^2q}{(2\pi)^2}T\ln[\sinh(\tfrac{1}{2}\beta\omega_{\mathbf{q}})]. \quad (9)$$

The angle-dependent component $\delta F_{\text{fl}}(\eta,\theta)=F_{\text{fl}}(\eta)-F_{\text{fl}}(0)$ contains no infrared divergences, permitting us to replace the cutoff by zero in these terms. To leading order in η^2

$$\delta F_{\text{fl}}(\eta,\theta)=-E(T)[1+\cos^2\theta], \quad (10)$$

where

$$E(T)=\left[\frac{J_1^2S^2}{2J_2}\right]\left[\gamma_Q\left(\frac{1}{S}\right)+\gamma_T\left(\frac{T}{J_2S^2}\right)\right]. \quad (11)$$

Here, the coefficients of the thermal and quantum fluctuations γ_T and γ_Q are

$$\gamma_{Q,T}=\int\frac{d^2q}{(2\pi)^2}\frac{1}{2[1-(c_xc_y)^2]^{\alpha_{Q,T}}}\times\{(c_x^2+c_y^2)[1+\tfrac{1}{2}(c_xc_y)^2]-2(c_xc_y)^2\}, \quad (12)$$

where $\alpha_Q=\frac{3}{2}$, $\alpha_T=2$, yielding $\gamma_Q=0.260$, $\gamma_T=0.318$. Thus a quadrupole coupling term

$$A_c=-[E(T)/Ta^2]\int d^2x(\hat{\mathbf{n}}_1\cdot\hat{\mathbf{n}}_2)^2 \quad (13)$$

must be added to the classical action.

At high temperatures, each sublattice behaves as an ordered Néel state up to a length scale $\xi(T)$. Within a region of this size, the quadrupole coupling then selects configurations where $\sigma=\hat{\mathbf{n}}_1\cdot\hat{\mathbf{n}}_2=\pm 1$, so σ behaves as a soft Ising order parameter. In terms of the microscopic spins around a plaquet $\sigma=(2S)^{-2}(\mathbf{S}_1-\mathbf{S}_3)\cdot(\mathbf{S}_2-\mathbf{S}_4)$. The energy barrier required to move from an x-collinear $(\sigma=1)$ to a y-collinear $(\sigma=1)$ configuration is then $W(T)\sim E(T)[\xi(T)/a]^2$. When $W(T)\sim T$, there will be an Ising phase transition into the collinear state. The phase transition temperature is then approximately

$$T_i=8\pi J_2S^2/z_0\ln[T_i/E(T_i)]. \quad (14)$$

For large S, where $S\gtrsim\ln(1/\eta)$, the dominant contribution to $E(T)$ is from thermal fluctuations, and

$$T_I = 4\pi J_2 S^2 / z_0 \ln[1/\eta(2\gamma_T)^{1/2}]\,. \tag{15}$$

The quadrupole term can be written as

$$A_c = (2g)^{-1} \int d^2x (\phi^{a}_{-})^2 / [l(g)]^2\,, \tag{16}$$

where

$$l(g) = a[T/4E(T)g]^{1/2}\,. \tag{17}$$

At high temperatures $l(g)$ is greater than the correlation length. However, at the Ising phase transition $T = T_I$, $g \sim 1$, so $l(q) \sim a[T_i/E(T_i)]^{1/2} \sim \xi(T_I)$. For $T < T_i$, the out-of-phase fluctuations in the sublattice magnetizations are exponentially damped with correlation length $l_0 = l(g(1/l_0))$. For small η,

$$l_0 = a \exp\left[-\frac{8\pi E}{T}\left(\frac{l_0}{a}\right)^2\right] \exp\left[\frac{2\pi}{z_0 g_0}\right]. \tag{18}$$

Below T_i, the two sublattice magnetizations become rigidly coupled into a collinear magnet for length scales $l > l_0(T)$. l_0 is also the typical size of a wall that would separate regions of $\sigma = 1$ and $\sigma = -1$. To explore the low-temperature regime, we modify the antisymmetric fluctuations with the mass term, which then leads to the modified scaling equations

$$\frac{\partial g}{\partial \ln(\Lambda)} = -\frac{g^2}{4\pi}\left[\frac{1}{(1-\eta^2)^{1/2}} + \frac{1}{(\{1+[l(g)\Lambda]^{-2}\}^2 - \eta^2)^{1/2}}\right], \quad \frac{\partial \eta}{\partial \ln(\Lambda)} = \frac{\eta g}{2\pi}\frac{1}{(\{1+[l(g)\Lambda]^{-2}\}^2 - \eta^2)^{1/2}}. \tag{19}$$

For $\Lambda \gg l_0^{-1}$, the scaling equations revert to Eq. (6). When $\Lambda \sim (l_0)^{-1}$, there is a crossover into the one-sublattice regime, where to logarithmic accuracy $\eta(\Lambda) = \eta^* = \eta_0 g_0 / g(1/l_0)$ is constant. The coupling constant for the symmetric fluctuations of the long-wavelength one-sublattice structure is now $\tilde{g} = \frac{1}{2} g[1-(\eta^*)^2]^{-1/2}$, (the factor of $\frac{1}{2}$ accounts for the doubling of the stiffness once the sublattices become locked), which obeys the conventional scaling equation $\partial \tilde{g}/\partial \ln(\Lambda) = -\tilde{g}^2/2\pi$. Thus the correlation length for in-phase spin fluctuations is now

$$\xi(T) = l_0 \exp\left(\frac{4\pi[1-(\eta^*)^2]^{1/2}}{g(1/l_0)}\right) = l_0 \exp\left(\frac{16\pi[1-(\eta^*)^2]^{1/2}E}{T}\left(\frac{l_0}{a}\right)^2\right), \tag{20}$$

which grows to be exponentially larger than the out-of-phase fluctuations at low temperatures. In summary then, the magnetic spatial correlations at low temperatures are given by

$$\langle \mathbf{n}_+(\mathbf{R}) \cdot \mathbf{n}_+(0) \rangle \sim e^{-R/\xi(T)},$$
$$\langle \mathbf{n}_-(\mathbf{R}) \cdot \mathbf{n}_-(0) \rangle \sim e^{-R/l_0}, \tag{21}$$
$$\langle \sigma(\mathbf{R})\sigma(0) \rangle \xrightarrow{R\to\infty} \langle \sigma \rangle^2,$$

where $\mathbf{n}_\pm = \hat{\mathbf{n}}_1 \pm \hat{\mathbf{n}}_2$ are the symmetric and antisymmetric fluctuations. As $T \to 0$, $\xi \to \infty$, and $T/g(1/l_0) \to 2J_2S^2$, so the value of l_0 is determined by the zero-point fluctuations,

$$l_0(0)/a = (2\eta_0)^{-1}(S/\gamma_Q)^{1/2}\,. \tag{22}$$

The out-of-phase fluctuations then have a "quantum exchange gap" $\Delta = c/l_{T=0}$, as first considered by Shendar for 3D Heisenberg models.[13] This has interesting consequences for finite-size studies of this model. In cases where the size of the lattice is small in comparison with l_0, there will be a small size-dependent splitting of the twofold-degenerate ground state ΔE produced by tunneling. As η decreases, the tunneling barrier becomes smaller, and ΔE rises. [A crude analysis suggests $\ln(1/\Delta E) \sim L^2(\eta S)^{1/2}$, where L is the size of the lattice.] Qualitative agreement with this behavior has been observed in recent finite-size studies.[7,14]

The previous discussion is strictly only valid for small values of η. For larger η, higher multipole terms appear in $\delta F_{fl}(\theta)$. Within spin-wave theory, the quadrupolar term continues to dominate the fluctuation coupling even when $\eta = 1$, so our expressions for the scaling and the Ising temperature are qualitatively correct. Figure 2 plots the behavior predicted by Eq. (14). As η increases, the fluctuation coupling between the sublattices rises giving rise to a growth in T_i, and a reduction in both ξ and l_0.

The case $\eta \to 1$ deserves special attention, for in this limit both ξ and l_0 are comparable with the lattice spacing. Here, $T_i \sim J_2 S^2$, and the two sublattices are locally locked, even though the spin directions remain disordered. For classical spins, entropy arguments establish the presence of collinearity at this special point. Doucot[15] has shown that for $\eta = 1$, the frustrated Heisenberg model assumes the form $H = (J_2/2)\sum(S_1 + S_2 + S_3 + S_4)^2$. Classical ground states of this model

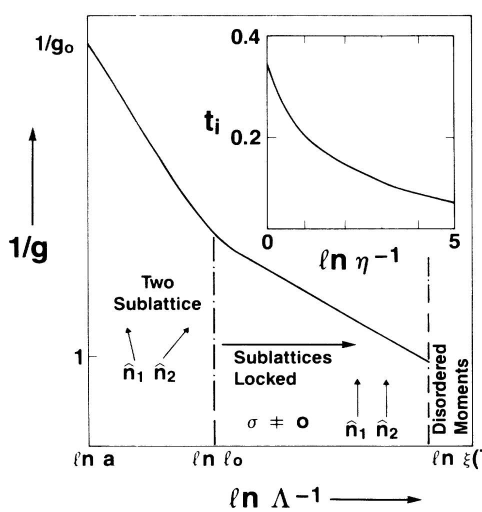

FIG. 2. The scaling behavior of $1/g$ as a function of length scale. Inset: The Ising phase transition as a function of frustration, where $t_i = z_0 T_i / 8\pi J_2 S^2$.

can be constructed by setting the spin configurations along the x axis, and then growing the spin configurations in the y direction using the condition that the energy of each plaquet is zero. The resulting states are all collinear ($\sigma > 0$), with the isolated exception of the Néel state. Growing away from the y axis produces states with $\sigma < 0$, and the two types of states cannot be joined without forming a wall with energy $J_2 S^2$ per unit area. Thus at finite temperatures $T \lesssim J_2 S^2$, the fully frustrated classical Heisenberg model will exhibit a collinearity. At finite S, the additional zero-point fluctuations reinforce the Ising order already present in the classical limit. We are left with the amusing conclusion that the Ising phase transition reaches its maximum value as we approach the frustrated point $\eta = 1$ from the collinear regime.

The nature of the finite-temperature phase transition between collinear and noncollinear phases in the large-S limit appears to be quite complex, and is dependent on the sign and magnitude of the next-nearest-neighbor coupling J_3. When J_3 is finite, $\eta_0 = J_1/(2J_2 - 4J_3)$. If J_3 is negative (ferromagnetic) and large in comparison with J_2, then there is a first-order phase transition between finite-temperature Néel and collinear phases, with a vertical phase boundary at $J_1 = 2J_2$ rising to meet the second-order Ising boundary. Actually, small positive J_3 terms are generated by thermal and quantum fluctuations.[5] In this case, there is the interesting possibility of a second-order phase transition from a noncollinear phase into a phase with short-range helicoidal order along the x or y axis. As η is reduced, there will then be a crossover where first the helicoidal spin-correlation length shrinks to a, followed by a rise in the spin-correlation length for the simple collinear phase.

Finally, we would like to comment on the implications of this work for regions of the phase diagram where the ground state has no sublattice magnetization at zero temperature. Figure 1 shows the critical value of S deduced in spin-wave theory, for the case of a small positive J_3. At large S, for all values of $J_2 > (J_1 - 4J_3)/2$, $\langle\sigma\rangle \neq 0$, stabilized by short-wavelength quantum fluctuations. Above the line $S = S_c$ in this region, the spin-correlation length is large but finite, so a finite-temperature Ising phase transition is still expected.[16] In contrast with the conclusions for the O(3) sigma model,[8,9] this collinearity is driven by frustration and our conclusions are stable against the effects of tunneling between different hedgedog configurations of the order parameter. Since the size of a point defect l_d is much larger than the size of an Ising wall ($\sim l_0$), the Berry-phase calculation must be carried out with the Néel sublattices locked. The effective spin that appears in the Berry-phase calculation will therefore be $S^* = 2S$, which is always an integer. When S^* is even, there are no collective topological effects. When S^* is odd, the collective tunneling will act only to reinforce the twofold degeneracy driven by fluctuations. Since S^* is never half integer, we are led to the interesting conclusion that "order from disorder" suppresses the topologically generated fourfold-degenerate spin Peierls states. It would be interesting to extend our analysis to the case of helicoidal magnets, where a richer classical degeneracy is present.[17] In this case the (2+1)-dimensional short-range quantum fluctuations appear to stablize not only scalar σ, but also the *vector* order associated with the twist $\mathbf{S}_i \times \mathbf{S}_j$ of the selected helicoidal state.[18] This will be a subject of future work.

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