First-order transition in frustrated quantum antiferromagnets

Andrey Chubukov
Department of Physics, Science and Technology Center for Superconductivity, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801
and Institute for Physical Problems, 117334 ul. Kosygina, 2 Moscow, U.S.S.R.
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A two-dimensional frustrated quantum Heisenberg model with first-, second- (diagonal), and third-neighbor couplings (J_1-J_2-J_3 model) is studied near the phase boundary of the antiferromagnetic (π,π) phase. It is shown that quantum corrections remove accidental classical degeneracy and ensure a nonzero hysteresis width for the $J_3=0$ transition between commensurate (π,π) and $(\pi,0)$ phases, so that finite J_3 is necessary to produce a continuous transition through the intermediate disordered phase.

The discovery of high-temperature superconductivity renewed an interest in the study of quantum fluctuations in two-dimensional (2D) quantum antiferromagnets. Besides the effort undertaken in order to establish whether or not quantum fluctuations are strong enough to destroy long-range order in $S=\frac{1}{2}$ Heisenberg antiferromagnets on various lattices,[1,2] there is also a considerable interest in the study of frustrated antiferromagnets with most of the efforts focused on the so-called J_1- J_2-J_3 model with first-, second- (diagonal), and third-neighbor couplings:[3-9]

$$H=J_1\sum_{l,\Delta}\mathbf{S}_l\cdot\mathbf{S}_{l+\Delta}+J_2\sum_{l,\Delta_{\rm diag}}\mathbf{S}_l\cdot\mathbf{S}_{l+\Delta_{\rm diag}} +J_3\sum_{l,\Delta}\mathbf{S}_l\cdot\mathbf{S}_{l+2\Delta}\ . \tag{1}$$

For positive (antiferromagnetic) J_i, next-neighbor couplings compete with the nearest-neighbor one and, approaching some critical values, provide an instability of the (π,π) antiferromagnetic ground state.

For classical spins, the (π,π) configuration becomes unstable at $J_c>J_1$, $J_c=2J_2+4J_3$, against a transition or into a symmetrical (Q,Q) incommensurate state with $\cos Q=-J_1/J_c$, or into a nonsymmetrical state $(\pi,\tilde{Q})$ with

$$\cos\tilde{Q}=-\frac{1}{a}\left[\frac{J_1}{J_c}(1+a)-1\right]$$

and $a=2J_3/J_2$, depending on whether or not the ratio of next-neighbor couplings a is greater than one, correspondingly.[8] In the latter case, a subsequent increase of frustration leads to a second transition at $J_1=J_c(1-a)/(1+a)$ into a commensurate $(\pi,0)$ state. For diagonal frustration only, i.e., when $J_3=0$, the intermediate region disappears and (π,π) configuration transforms directly into $(\pi,0)$ state at $J_2=J_1/2$.

What ensures interest in this simple model is that it is believed to have a region of a disordered spin-liquid phase. The possibility for a breakdown of long-range order comes from the fact that, on a transition line $J_1=J_c$, antiferromagnetic spin-wave excitations, generally linear in k for k close to (0,0) and $\boldsymbol{\pi}=(\pi,\pi)$, undergo additional softening and along $J_1=J_c$, the spin-wave spectrum

$$\begin{gathered}\varepsilon_{\mathbf{k}}=2J_2S(\varphi_{\mathbf{k}}\varphi_{\mathbf{k}+\pi})^{1/2}\ ,\\ \varphi_{\mathbf{k}}=\{2(1-\nu_x)(1-\nu_y)+a[(1-\nu_x)^2+(1-\nu_y)^2]\}\ ,\end{gathered} \tag{2}$$

where $\nu_i=\cos k_i$, is quadratic in k both at low momentum and near $\boldsymbol{\pi}$.[8,9] As a result, in the quantum version of the problem, the corrections due to quantum fluctuations turn out to be logarithmically divergent in two dimensions and one comes to a possibility that different ordered states may be separated by an intermediate spin-liquid state.

For $S=\frac{1}{2}$, numerical simulations[2,4,8] point out that this is most likely the case. The intermediate phase with a restored continuous symmetry was identified as a dimer phase with columnar dimerization. In this paper, I will focus instead on the situation for large S.

The question of whether or not a region of a spin-liquid state really exists even for arbitrary large S is a subject of recent controversy. Ioffe and Larkin[5] used a renormalization-group (RG) technique and showed that, along a critical line, the coupling constants measuring the strength of quantum fluctuations also grow logarithmically in passing to larger scales exactly in the same way as in the O(n) σ model with $n>2$. This means that fluctuations not only destroy on-site magnetization but also generate an internal scale (correlation length, $\xi\propto\exp S$ for $S\gg1$); that is, finite shift from a critical line is necessary to produce long-range order. This approach is valid only for strong enough J_3 since, in the case of $J_3\to0$, the bare coupling constants, normally small to the extent of $1/S$, acquire a logarithmically divergent (as $\ln J_2/J_3$) factor. The case $J_3=0$ was first considered by Chandra and Doucot.[6] They calculated the first correction to sublattice magnetization and claimed that a disordered region exists in the lack of J_3 as well (see also Refs. 8 and 9).

Contrary to these results, Read and Sachdev[7] explored the $1/N$ expansion for $S_p(N)$ frustrated magnets (the physical picture is restored by setting $N=1$) and did not detect any intermediate disordered phase in the "quasiclassical" limit when, besides large N, one also assumes that the ratio n_b/N, where n_b is the number of bosons at each site ($n_b=2S$ for $N=1$), is also large.

The purpose of this Brief Report is to show that the contradiction can be partly resolved by the standard Hartree-Fock calculations for ordinary SU(2) spins. Specifically, I will show that the same Hartree-Fock corrections, which are well known to lift an accidental degeneracy in the $(\pi,0)$ phase[3,8,10,11] also produce a finite hysteresis width for the $J_3=0$ transition between the (π,π) and $(\pi,0)$ states, that is finite J_3 is necessary for a continuous transition to occur. This is very natural since, at the transition point $J_2=J_1/2$, the two states have different spin-wave spectra:

$$\varepsilon_{\mathbf{k}}=4J_2S|\sin k_x||\sin k_y| \tag{3}$$

for the (π,π) phase and

$$\varepsilon_{\mathbf{k}}=4J_2S|\sin k_x|(1+\cos k_y) \tag{3'}$$

for the $(\pi,0)$ phase, and there are absolutely no reasons to expect quantum fluctuations to be absolutely equal in both phases. This is to be contrasted with the cases when hysteresisless first-order transitions result from exact infinite *quantum* degeneracy at criticality.[12,13] Since the *lines* of soft modes in the spin-wave spectrum of Eqs. (3) and (3′) were associated with the hysteresisless transition for classical spins, the finite hysteresis width due to quantum fluctuations also removes the accidental classical degeneracy (this phenomena is often referred to as "order from disorder"[14]).

The calculations are very simple and, in essence, require only a decoupling procedure for the fourfold anharmonic terms in the bosonic version of the original spin Hamiltonian obtained with, say, a Dyson-Maleev transformation. In the absence of cubic anharmonisms this is enough to get the leading corrections in $1/S$. The realization of this procedure for the (π,π) phase produces a shift in the instability point when the excitation spectrum first becomes unstable at $\mathbf{k}=0$ and π:

$$\delta_c^{(\pi,\pi)}=1+2J_2\sum_k \frac{\nu_x^2(1-\nu_y^2)}{\varepsilon_k} , \tag{4}$$

where $\delta=2J_2/J_1$. The logarithmical divergence on the right-hand side (rhs) of (4) with ε_k as in (3), is an aftereffect of the classical "soft lines" at criticality. The evaluation of the integral with logarithmic accuracy gives

$$\delta_c^{(\pi,\pi)}=1+\frac{\ln S}{\pi^2 S} . \tag{4'}$$

The same procedure applied to the $(\pi,0)$ phase lifts an accidental degeneracy at $k=(0,\pi)$ and (π,π). However, quantum corrections do not produce any shift in the instability point since the transition is now governed by *ferromagnetic* fluctuations in the y direction, which are well known to be insensitive to a transformation from classical to quantum spins [mathematically, this is manifested in that, for ε_k as in (3′), the coefficients of the unitary transformation diagonalizing the quadratic form in bosons do not depend on ν_y]. Hence,

$$\delta_c^{(\pi,0)}=1 . \tag{5}$$

It follows from (4′) and (5) that the stability regions of the (π,π) and $(\pi,0)$ phases overlap and thus for quantum spins the first-order transition has a finite hysteresis width. The energies of the (π,π) and $(\pi,0)$ states touch each other at

$$\delta_{\rm cr}=1+\frac{1}{\pi^2 S}(\pi-2) . \tag{6}$$

Note that, by evident reasons, $\delta_{\rm cr}$ has no logarithmical factor in S.

The fact that, up to logarithmic terms, $|\delta_{\rm cr}-\delta_c|$ grows linearly with $1/S$ violates a possibility of disordered intermediate phase which was believed to result from *logarithmical* corrections to the sublattice magnetization which become relevant only exponentially close to the instability lines in both (π,π) and $(\pi,0)$ phases. This complements the Read and Sachdev results for $J_3=0$.[7] The only difference is that their expression for the instability point of the (π,π) phase does not contain a logarithmical factor in n_b/N.

For classical spins, no matter how small J_3 produces a continuous transition through the intermediate (π,Q) phase. For quantum spins, however, the finite hysteresis width for $J_3=0$ points out that finite J_3 is necessary to make a transition continuous. Moreover, since, in *both* phases, J_3 couples ferromagnetically ordered spins and

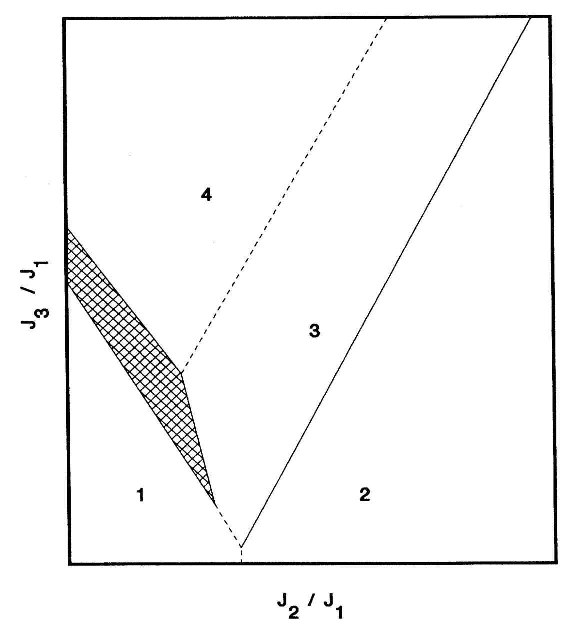

FIG. 1. A schematic $T=0$ phase diagram of the J_1-J_2-J_3 model on the J_2/J_1 and J_3/J_1 planes. Solid and dashed lines correspond to second- and first-order transitions. Due to quantum fluctuations, finite J_3 is necessary to produce a continuous transition through the intermediate disordered phase (shown hatched). The numbers denote the stability regions of different phases: 1 (π,π); 2 $(\pi,0)$; 3 (π,Q); and 4 (Q,Q).

the logarithmical in S term enters into the expression for $\delta_c^{(\pi,\pi)}$ only, then, with J_3 increasing, the type of transition will change first along the instability line of the $(\pi,0)$ phase: for $J_3 > J_3^{(1)}$, where

$$J_3^{(1)} = J_1 \frac{\pi-2}{4\pi^2 S} , \tag{7}$$

it will transform into the (π,Q) phase via continuous transition. Meanwhile, a transition from the (π,π) phase will continue to be first-order until J_3 exceeds a second critical value, $J_3^{(2)}$. One could expect that $J_3^{(2)} \simeq (1/S)\ln S$. However, the self-consistent solution of when the quadric in the $(\pi-Q)$ term in the low $(\pi-Q)$ expansion of the energy of the (π,Q) phase changes a sign along the (π,π) instability line shows, that on this scale, only the hysteresis width decreases, while the first-order transition itself survives up to much higher values of J_3. The calculations yield

$$J_3^{(2)} = \frac{J_1}{2} \left[\frac{\ln S}{2\pi^2 S} \right]^{1/2} . \tag{8}$$

In between $J_3^{(1)}$ and $J_3^{(2)}$ the (π,π) phase will undergo a first-order transition into the (π,Q) phase with some intermediate Q [although small for $J_3 \gg (1/S)\ln S$].

On the other hand, for sufficiently large J_3 ($J_3 > J_3^{(2)}$), the (π,π) phase will lose a stability via a continuous transition. In this case, Hartree-Fock corrections only shift a critical line and renormalize the bare values of the couplings but do not change a conclusion of Ref. 5 about the existence of an intermediate disordered phase for arbitrary large S. The proposed phase diagram with the tricritical point, where a continuous transition via intermediate disordered phase changes to first-order transition (dashed curve), is presented in Fig. 1. Note that quantum fluctuations do not diverge along the $(\pi,0)\rightarrow(\pi,Q)$ transition line and, thus, no disordered state separates these two phases.

A phase diagram for $n_b/N = 1$ was obtained by Read and Sachdev.[7] They found a first-order transition for small J_3 but did not detect any intermediate phase between the ordered (π,π) and (Q,Q) or (π,Q) states in the region where one expects a continuous transition to occur. The reason for the discrepancy is unknown to me.

Note added in proof. After submitting this paper I learned that the first-order transition in the large-S J_1-J_2 model was also obtained in the frameworks of a Schwinger-boson approach.[15]

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