Phase transitions of the bilayered spin-S Heisenberg model

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We study the ground state and the phase transitions of the bilayered spin-S antiferromagnetic Heisenberg model using the Schwinger boson mean-field theory. The interplane coupling initially stabilizes but eventually destroys the long-range antiferromagnetic order. The transition to the disordered state is continuous for small $S$, and first order for large $S$. The latter is consistent with an argument based on spin-wave theory. [S0163-1829(96)01818-8]

I. INTRODUCTION

Recently there has been considerable interest in quantum spin liquids, which are magnetic systems without long-range order (LRO) at low temperature. While in general, the ground state of quantum spin systems lack true LRO in one-dimensional (1D), the ground state of the 2D Heisenberg antiferromagnet (AF) exhibits Néel ordering even for $S=1/2$, albeit with a sublattice magnetization that is considerably decreased from its classical value. Since the spin is quantized, the spin value cannot be decreased beyond 1/2, hence the model does not have a spin-liquid ground state. On the other hand, when two planes of antiferromagnetic spins are coupled together,3–11 and if the interplane coupling is strong enough, the ground state is easily seen to be one of valence bond solid of interplane singlets (IVBS). Thus, there should be a transition from the LRO Néel state to a spin-liquid state as the interplane coupling is increased. It has been suggested that the unusual magnetic properties of Y-Ba-Cu-O, with its basic unit of a pair of coupled CuO planes, may be due to its lying close to this quantum transition.3

It is of interest to study the nature of this quantum transition. Within a nonlinear sigma-model (NLSM) description, Haldane12 has pointed out that for a single plane of spins, topological Berry phase terms exist which differ between half-integer, odd integer, and even integer spins. One way to understand this is to consider the degeneracy of the valence bond solid states which maximize the number of resonating plaquettes in each case (fourfold, twofold, and nondegenerate, respectively). On the other hand, the mapping of the two-plane system to the NLSM does not yield a topological term, which is consistent with the valence bond solid state for two planes with large interplane vs intraplane coupling being zero-dimensional-like and nondegenerate. Since the 2+1 D NLSM has only one phase transition which is second order, this suggests the same for the 2D quantum Heisenberg AF at $T=0$. However, the NLSM mapping assumes slow variation on the scale of lattice spacing, and so additional disordered phases and/or first-order transition cannot be ruled out conclusively.

In this paper we investigate the ground state of the 2D bilayered Heisenberg AF for general $S$ using the Schwinger boson mean-field theory1,2 with no additional approximation. Our calculation complements previous calculations for $S=1/2$ only and/or using additional approximations, as well as a calculation using the related Takahasi bosons approach.4–6 Our results show that the transition from the AF ordered state to disordered state is second order for small $S$, and first order for large $S$. A simple argument using spin-wave theory helps to explain why a first-order transition occurs for large $S$. In the latter case, the magnetization decreases slowly as the interplane coupling $J_\perp$ increases, and it remains finite when the IVBS becomes lower in energy. Quantitatively the critical $S$ separating first from second-order transition $S_c$, is found to be 0.35 within the mean-field theory (MFT). While we should not expect the MFT to give correct critical $S$ and the critical $J_\perp$, we believe the qualitative features described by the MFT are correct because the topological effect mentioned above is not important in the present geometry. The actual value of $S_c$ should be larger than 1/2, as more accurate calculations6,8 showed the transition for the $S=1/2$ systems to be second order.

II. SCHWINGER BOSON MEAN-FIELD THEORY FOR BILAYERED AF HEISENBERG MODEL

We begin with a quick review of Schwinger boson mean-field theory2 as applied to the translationally invariant nearest-neighbor Heisenberg antiferromagnet on a bipartite lattice. The Hamiltonian is

$$H = \sum_{\langle ij \rangle} J_{ij} S_i^\tau S_j^\tau; \quad J_{ij} > 0, \quad \langle ij \rangle = \text{NN}.$$
In the Schwinger boson representation, spin operators in each lattice site are replaced by spin 1/2 bosons as follows:

\[ S_i^+ = b_i^\dagger b_i, \quad S_i^- = b_i^\dagger b_i, \quad S_i^z = \frac{1}{2}(b_i^\dagger b_i - b_i^\dagger b_i). \]

The number of bosons at each lattice site is subject to the constraint

\[ \sum_\sigma b_i^\dagger b_i = 2S, \]

which can be implemented by introducing a Lagrange multiplier on each site. The Hamiltonian can now be written as

\[ H = -2\sum_{\langle ij \rangle} J_{ij} \vec{A}_{ij}^\dagger \vec{A}_{ij} + \frac{1}{2} \sum_{\langle ij \rangle} \sum_{\sigma} \lambda_{ij}(\vec{b}_{ij}^\dagger \vec{b}_{ij} - 2S), \]

where \( \vec{A}_{ij}^\dagger = \frac{1}{2} \sum_\sigma \vec{b}_{ij}^\dagger \vec{b}_{ij} \) and \( \vec{b}_{ij} = b_i^\dagger b_j \), \( \vec{b}_{ij} = -b_i^\dagger b_j \) for sites on one sublattice and \( b_i = b_i^\dagger \) for sites on the other sublattice. Physically, the product \( \vec{A}_{ij}^\dagger \vec{A}_{ij} \) acts as the valence bond (singlet) number operator for sites \( \langle ij \rangle \). In the mean-field approximation, this product is decoupled by the Hartree-Fock decomposition. In addition, the exact local constraint is relaxed to one for the average

\[ \left( \sum_\sigma b_i^\dagger b_i \right) = 2S, \]

leading to the mean-field Hamiltonian

\[ H_{MF} = E_0 + \sum_{\langle ij \rangle} \sum_\sigma J_{ij} A_{ij} (\vec{A}_{ij}^\dagger + \vec{A}_{ij}), \]

where we have taken \( A_{ij} = \langle \vec{A}_{ij} \rangle \) to be real.

First consider the case that all the bonds are identical by symmetry, and assuming no spontaneous dimerization, then all \( A_{ij} \) must be the same \( A_{ij} = A \). In this case \( E_0 = \frac{1}{2} N z J S^2 - 2 \lambda N S + J A S^2 z \), where \( z \) is the coordination number. \( H_{MF} \) can be diagonalized by going to momentum space and perfoming the Bogoliubov transformation:

\[ H_{MF} = E_0 - \lambda N + \sum_k \omega_k (a_k^\dagger a_k + b_k^\dagger b_k + 1), \]

where \( \omega_k = [\lambda^2 - (J A z \gamma_k)^2]^{1/2}, \gamma_k = (1/2) \sum_i \delta \cos k_i / d. \) At \( T = 0 \), the energy should be minimized with respect to \( \lambda \) and \( A \), yielding the set of self-consistent equations:

\[ S + \frac{1}{2} = \frac{1}{2 N} \sum_k \frac{\mu}{(\mu^2 - \gamma_k^2)^{1/2}}, \]

\[ \vec{A} = \frac{1}{2 N} \sum_k \frac{\gamma_k^2}{(\mu^2 - \gamma_k^2)^{1/2}}, \]

where we define \( \mu = \lambda/(J A z) \). An essential point of the theory is that a nonzero mean-field amplitude \( A \), which gives rise to boson hopping, indicates short-range antiferromagnetic order. Long-range order is achieved if the hopping amplitude is sufficiently large to give Bose condensation. This occurs when these equations cannot be satisfied by having \( \mu > 1 \), in which case \( \mu = 1 \), and the \( k = 0 \) term gives a finite contribution when converting the momentum sums into integrals:

\[ S + \frac{1}{2} = m_s + \frac{1}{2} \int_0^\pi \frac{d^d k}{(2 \pi)^d} \frac{1}{(1 - \gamma_k^2)^2}, \]

\[ A = m_s + \frac{1}{2} \int_0^\pi \frac{d^d k}{(2 \pi)^d} \frac{\gamma_k^2}{(1 - \gamma_k^2)^2}. \]

It has been shown that the condensate density \( m_s \) is also the sublattice magnetization. For the Heisenberg antiferromagnet on a square lattice, it was found that Bose condensation occurs for all \( S > S_c \), where \( S_c = 0.2 \), with a gapless linear excitation spectrum characteristic of spin waves. For \( S < S_c \), \( \mu > 1 \), and there is an energy gap for excitations. Thus, for all physical values of \( S \), there is AFLRO.

On the other hand, if two such planes are coupled together antiferromagnetically, and the interplane coupling is very large compared to intraplane coupling, the ground state is obviously a valence bond solid of interplane singlets, and the intraplane correlation length is zero. Thus, there must be at least one phase transition as the interplane coupling is increased. We now analyze this for general \( S \) using Schwinger boson MFT.

The Hamiltonian in this case is

\[ H = J \sum_{\langle ij \rangle} S_i S_j + J_\perp \sum_{\langle ij \rangle} S_i S_j, \]

where \( \Sigma_{\langle ij \rangle} \) sums over nearest neighbor (NN) on the same plane and \( \Sigma_{\langle ij \rangle} \) sums over NN on different planes. Since there is still translational invariance, the mean-field Lagrange multiplier will be the same on all sites. However, the lack of symmetry between intraplane and interplane bonds means two mean-field amplitudes must be introduced for the bond decoupling. Letting these be \( A \) and \( B \), respectively, and taking them to be both real, the mean-field Hamiltonian is now

\[ H_{MF} = E_0 + \lambda \sum_{\langle ij \rangle} \sum_\sigma (\vec{b}_{ij}^\dagger \vec{b}_{ij}) - 2 J A \sum_{\langle ij \rangle} (\vec{A}_{ij}^\dagger + \vec{A}_{ij}) \]

\[ -2 J_\perp B \sum_{\langle ij \rangle} (\vec{A}_{ij}^\dagger + \vec{A}_{ij}), \]

where \( E_0 = 2 N J S^2 - 2 \lambda N S + 4 J A^2 N + J_\perp S^2/2 + J_\perp B^2 N \). As before, we diagonalize \( H_{MF} \) through the Bogoliubov transformation, giving

\[ H_{MF} = E_0 - \lambda N + \sum_{\kappa \sigma} \omega_{\kappa \sigma} (a_{\kappa \sigma}^\dagger a_{\kappa \sigma} + b_{\kappa \sigma}^\dagger b_{\kappa \sigma} + 1). \]

The excitation energies are given by

\[ \omega_{\kappa \sigma} = \left[ \lambda^2 - \left( 2 J A \sum_{i=1}^d \cos k_i + J_\perp B \sigma \right)^2 \right]^{1/2}, \]

where \( \sigma = \pm 1 \). Minimizing \( H_{MF} \) with respect to \( \lambda, A, \) and \( B \) gives the self-consistent equations.
$S + \frac{1}{2} = \frac{1}{2N} \sum \frac{\mu}{(\mu^2 - \Gamma_{k,a}^2)^{1/2}},$

$A = \frac{1}{2N} \sum \frac{\Gamma_{k,a}}{(\mu^2 - \Gamma_{k,a}^2)^{1/2}} \left( \frac{\sum_{d=1}^{d} \cos k_d}{d} \right),$

$B = \frac{1}{2N} \sum \frac{\Gamma_{k,a} \alpha}{(\mu^2 - \Gamma_{k,a}^2)^{1/2}}$ \hspace{1cm} (2)

where $\Gamma_{k,a} = (\sum_{d=1}^{d} \cos k_d + Q \alpha) / d$ and $Q = J_1 B / (2JA)$. Note that $\mu$, the excitation gap, must be greater than or equal to $1/Q/d$. In particular, in the case of Bose condensation, the value of $\mu$ is fixed to $1/Q/d$ and hence the summations in Eq. (2) turn out to be a function of the parameter $Q$ only. The magnetization $m_s$ is calculated by solving the self-consistent equations with the summations converted into integrals:

$S + \frac{1}{2} = m_s + \frac{1}{4} \int \frac{d^d k}{(2\pi)^d} \sum \frac{\mu_0}{(\mu_0^2 - \Gamma_{k,a}^2)^{1/2}},$

$\bar{A} = m_s + \frac{1}{4} \int \frac{d^d k}{(2\pi)^d} \sum \frac{\Gamma_{k,a}}{(\mu_0^2 - \Gamma_{k,a}^2)^{1/2}} \left( \frac{\sum_{d=1}^{d} \cos k_d}{d} \right),$

$\bar{B} = m_s + \frac{1}{4} \int \frac{d^d k}{(2\pi)^d} \sum \frac{\Gamma_{k,a} \alpha}{(\mu_0^2 - \Gamma_{k,a}^2)^{1/2}}$ \hspace{1cm} (3)

where $\mu_0 = 1 + Q/d$. These equations hold so long as they give $m_s > 0$, i.e., Bose condensation, otherwise Eqs. (3) should be used with $\mu$ also as an unknown parameter. In principle, we can solve for $Q$ and $m_s$ or $\mu$. In practice, the form of these equations allow us to avoid this by plugging in an arbitrary values of $Q$ into the equations to find out $m_s$ or $\mu$, and then $A$ and $B$. The self-consistency is then reduced to using the values of $A$, $B$, and $Q$ to determine the value of $\beta = J_1 / J$.

III. MEAN-FIELD SOLUTIONS

In this section, we present the solutions of the Schwinger boson mean-field theory. The solutions represent various phases and their transitions. The critical values of $S$ separating these phases are often smaller than 1/2 within the MFT. But these phases may be realized in physical systems, which
we will discuss in the next section.

We start to discuss the behavior of $Q$ as a function of $\beta$, as shown in in Fig. 1 for $S=1/2$, which is a representative of all $S$. Discounting the trivial solutions $Q=0$ and $Q=\infty$, corresponding to independent planes and IVBS, respectively, there are $Q\neq0$ solutions indicating both intraplane and interplane correlations. For small $\beta$, there is only one solution, with $Q$ increasing from 0 with $\beta$. For $\beta>4(S+1/2)^2$, a second branch of solution, beginning at infinity appears. The two solutions merge at some larger value of $\beta$, and beyond that, only the trivial solutions remain. The significance of these solutions can be understood if we consider the energy $E(Q)$ obtained by minimizing the energy with respect to all other parameters except $Q$. Then, the nontrivial solutions are extrema of $E(Q)$. Thus, for $\beta<\beta_0=4(S+1/2)^2$, the solution of $Q$ corresponds to a global minimum in $E(Q)$, and describes the ground state. For $\beta>\beta_0$, the upper branch corresponds to a local maximum while the lower branch remains a local minimum. The local maximum begins at $Q=\infty$ at $\beta_0$, and moves towards the local minimum with increasing $\beta$. Eventually, the two extrema merge into a saddle point at $\beta_2$. Beyond that, $E(Q)$ is strictly decreasing with $Q$. By continuity, this means somewhere between $\beta_0$ and $\beta_2$, $E(\infty)$ must cross from being greater than $E(Q_1)$ to less than it, where $Q_1$ is the lower branch solution. Thus, at this value $\beta_1$, the ground state jumps from the 2D correlated state described by $Q_1$ to the interplane VBS state. The analysis leading to this "first-order transition" in $Q$ is somewhat similar to the argument for first-order transition within Landau theory for a Landau free-energy functional with a cubic term. A very important difference is that $Q$ represents only short-range correlations and is not an order parameter. Thus, the jump in $Q$ can but does not necessarily lead to a first-order transition in the AFLRO.

We can solve for the value of $m_j$ at the nontrivial solutions. Initially, $m_j$ increases with increasing $Q$, but eventually will decrease, vanishing at some $Q_c$. For sufficiently large $S$, $Q_c$ will belong to the upper branch (maximum energy) solution. More importantly, in the case where $Q_c$ lies in the lower branch, its $\beta$ value changes from less than to greater than $\beta_1$ with increasing $S$. Thus, the transition from the LRO state to disordered state is second order for small $S$, but becomes first order for larger $S$. In the former case, there is a subsequent transition from a disordered state with finite $Q$, hence with both interplane and intraplane short-range correlations, to the $Q=\infty$ state with only interplane correlations. Along with the jump in $Q$ is a discontinuous jump in the gap. It is tempting to associate this jump as a transition from some disordered state associate with a single plane to the nondegenerate IVBS. More likely this transition is probably an artifact of the Schwinger boson MFT, and indicates a relative sharp drop in the intraplane correlation length and a sharp rise in the gap. This is similar to the finite temperature MFT solution for a single plane, where for a given $\beta$, hence short-range correlation, drops to zero above some finite temperatures. In the latter case of first-order transition in sublattice magnetization, the ground state jumps from one with LRO to the IVBS state. Since this latter state should be the correct ground state only in the $\beta$ goes to infinity limit, we interpret this as the MFT way of showing a transition into a disordered state with a very short intraplane correlation length. The behavior of $m_j$ and the gap $\Delta$ as a function of $\beta$ is shown in Fig. 2 for representative values of $S$. Figure 2(c) shows an example of reentrance, where LRO first develops with increasing $\beta$, but is subsequently destroyed when $\beta$ gets too large. This occurs for $S$ smaller than $S_{C2}\approx0.2$, below which the ground state for $\beta=0$ has no LRO, but greater than $S_{C3}\approx0.13$, the minimum value of $S$ below which there is no LRO at any $\beta$.

The phase diagram of $S$ vs $\beta$ is shown in Fig. 3. For $S<S_{C1}$, the ground state is always disordered. For $S_{C3}<S<S_{C2}$, the system undergoes first a disorder-order and then a order-disorder continuous transition with increasing $\beta$. For $S>S_{C2}$, there is LRO for $\beta=0$, and only the order-disorder transition remains. This transition is continuous until it terminates at a tricritical point at $S_{C}$, beyond which the continuous transition is preempted by a first-order transition. Within the MFT, $S_{C}=0.35$, $\beta=2.92$. Thus, for $S>S_{C}$, there are values of $\beta$ where the LRO state is not the ground state, but is nevertheless metastable. The continuous transition phase boundary remains metastable until $S$ reaches a larger value, $\approx0.4$ in the MFT, beyond which the $m_j=0$ state moves into the upper branch and becomes unstable. In all cases of $S$ where a disordered ground state with finite $Q$ exists, a subsequent "first-order transition" occurs, with a discontinuous jump in $Q$ and the gap $\Delta$. As mentioned above, we interpret the jump as unphysical, and represents in reality a relatively sharp drop in the 2D correlation length.

IV. DISCUSSIONS

The main result of our mean-field theory is that there is a first-order transition from ordered to disordered spin states for large $S$. The prediction of the existence of first-order transition in the theory is based only on the structure of the mean-field solutions of $Q$ (two branches merging and terminating at $\beta_2$) rather than numerical details of the energies.
This result does not seem to be accidental. We can understand why large $S$ favors a first-order transition quite simply in terms of spin-wave theory.\cite{4,5} The Néel state energy is $E_N = S^2(2J_zJ_z)$ while the energy of the IVBS state is $E_V = J_z S(S + 1)$. Equating the two implies an estimate for the first-order transition at $\beta_1$ of the order of $S$ for large $S$. Within spin-wave theory, the sublattice magnetization is given by $m_s$, in Eq. (3) with $B/A = 1$. For large $\beta$, the integral on the LHS scales as $\sqrt{\beta}$. If we set $m_s = 0$ as an estimate for the critical value $\beta_c$ for continuous transition, then $\beta_c$ is of order $S^2$. Thus, for large $S$, $\beta_1$ is much less than $\beta_c$.

Within MFT, the tricritical point and even the metastable continuous transition boundary occurs below the minimum physical value of $\beta = 1/2$. Thus, a first-order transition is predicted for all physical systems described by the model. In fact, the sublattice magnetization jump at transition for $\beta = 1/2$ is about 30% of that at $\beta = 0$, clearly contradicting the results of numerical work\textsuperscript{6–8} on the model for $\beta = 1/2$, which supports a continuous transition in the same universality class as the finite temperature transition of the 3D classical Heisenberg model. On the other hand, there is no reason to expect the Schwinger boson MFT to give the exact answer, so the true position of the tricritical point might very well be above $\beta = 1/2$. This is particularly so since by relaxing the local constraint to a global one, unphysical states are included in the mean-field solution, and the MF energy is not even variational. Thus, using these MF energies to find the position of the first-order transition is necessarily suspect. Nevertheless, we believe the prediction of larger $S$ favoring a first-order transition to be correct, and the nature of phase transition in the bilayer system is nonuniversal. For example, the transition for $\beta = 1/2$ may become first order if there is a sufficiently large next-nearest-neighbor ferromagnetic interaction. The seeming contradiction to the fact that the $2 + 1$ D NLSM has only continuous transition is resolved by noting that the mapping of the Heisenberg model into the NLSM is legitimate only if the correlation length is long, which does not have to be the case of the disordered state close to a first-order transition.

The reentrance behavior for small $S$ found in our MFT may have relevance in some physical systems. Since $\beta = 1/2$ at least, all the physical Heisenberg antiferromagnets in a square lattice with nearest-neighbor coupling are LROed, and the reentrance behavior will not occurred. However, with sufficient frustration, the single-layered system can be disordered for $\beta = 1/2$ or other physical values. Introducing the interplane coupling may first develop the LRO and the reentrance behavior of Fig. 2(c) discussed for small $S$ in the bilayered system may be physically observed in the frustrated physical systems.

Within our MFT and according to general arguments, a first-order transition implies the existence of metastable states with finite sublattice magnetization. This may lead to observable dynamics characteristic of macroscopic quantum tunneling. It would also be of significance with respect to Monte-Carlo-type numerical calculations\textsuperscript{6–9} due to problems of being "stuck" in the metastable minimum. For example, the first-order transition may be missed if the metastability persists till the would-be continuous transition.

Finally we discuss the critical phenomena of the continuous transition of this model. Analyzing Eqs. (2) and (3) close to the transition, we find the staggered magnetization vanishes linearly, while the gap vanishes as $(\beta - \beta_c)^s$ with $s = 1/(d - 1)$ for $d < 3$, and $s = 1/2$ for $d = 3$ (there are logarithm corrections at $d = 3$). These MF exponents are the same as those for the finite temperature transition of a single hypercube with the substitution $d \rightarrow d + 1$, reflecting the quantum nature of the present transition.

In conclusion we have used the Schwinger boson mean-field theory to study the bilayer antiferromagnetic Heisenberg model for general spins $S$. Our main results are that the phase transition from the ordered to disordered states induced by the interplane coupling is second order for small $S$, and first order for large $S$. Although the obtained critical lines in the phase diagram need to be modified using more accurate methods, the qualitative features predicted in the mean-field theory should be correct.

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\textsuperscript{10}D. Yoshioka \textit{et al.} (unpublished).