Bond-Operator Mean Field Theory for the Bilayer Heisenberg Model

Yasuhiro Matsushita*, Martin P. Gelfand1 and Chikara Ishii

Department of Physics, Faculty of Science, Science University of Tokyo,
Shinjuku-ku, Tokyo 162
1Department of Physics, Colorado State University,
Fort Collins, Colorado 80523, USA

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Bond-operator mean field equations for the square-lattice, $S = 1/2$ bilayer Heisenberg model are developed and solved numerically. In the vicinity of both the zero-field critical point and the field-induced transitions, comparisons are made with $T = 0$ and finite-temperature strong coupling expansions. The mean-field theory suggests that the quantum critical region for the field-induced transitions is restricted to significantly lower temperatures than one might have concluded based on strong-coupling expansions or other numerical studies.

KEYWORDS: bilayer Heisenberg model, field-induced transition, quantum critical phenomena, bond-operator mean-field theory, strong-coupling expansion

§1. Introduction

The appearances of unconventional superconductivity and non-Fermi-liquid behavior near the quantum critical point of antiferromagnetic instability in strongly correlated electronic systems, such as copper oxides or heavy fermion systems, has attracted great interest in recent years. These observations have led to the investigation of the interplay between magnetic long-range order and novel quantum disordered states. Particular attention has been paid to low-dimensional quantum spin systems in which the classical ground states are destabilized by strong quantum fluctuations, which are experimentally realizable in several compounds.

The bilayer Heisenberg model

$$H = J \left( \sum_{\langle i,j \rangle} S_{1,i} \cdot S_{1,j} + \sum_{\langle i,j \rangle} S_{2,i} \cdot S_{2,j} \right) + \sum_i S_{1,i} \cdot S_{2,i},$$

(taking the interlayer exchange as the unit of energy, and with $\langle i, j \rangle$ running over nearest neighbor pairs on the square lattice) has attracted considerable interest² as a testing ground

* E-mail: matusita@grad.ap.kagu.sut.ac.jp
for notions of quantum criticality. On increasing $J$ from zero, at $T = 0$ the model passes from a spin-disordered ground state through a critical point to a Néel-ordered state — the same phase diagram as the nonlinear $\sigma$ model, with $1/J$ playing the role of the coupling parameter $g$.

For $S = 1/2$, this model is directly relevant to the magnetic properties of several cuprate high-$T_c$ parent, antiferromagnetic compounds (and possibly the high-$T_c$ materials themselves), and also to the spin-gap system BaCuSi$_2$O$_6$.

If an external field

$$H_{\text{Zeeman}} = -h \sum_i (S_{1,i}^z + S_{2,i}^z)$$

is applied to the bilayer Heisenberg model, new $T = 0$ phases and phase transitions are introduced. In particular, if at $h = 0$ the system is in the disordered, gapped phase then there is a critical field $h_c$, trivially related to the zero-field triplet gap $\Delta$, since there is a simple Zeeman splitting of the triplet elementary excitations. For $h > h_c$ the gap is closed and the system exhibits algebraic order in the spin components transverse to the applied field.

A great deal is known about this $T = 0$ field-induced transition. In particular, $d = 2$ is the upper critical dimension, so critical exponents take on their classical values (modulo log corrections) in the bilayer Heisenberg model. In all dimensions above the lower critical dimension $d = 1$, the dynamic exponent $z = 2$ and the correlation length exponent $\nu = 1/2$. A variety of detailed model studies for one-dimensional spin-gap systems have been carried out. Work on two-dimensional systems exhibiting this transition is sparser and what is particularly not well known is how high in temperature the associated quantum critical region extends. This is a matter of some significance, if one is to ascribe the temperature dependence of properties of an experimental system to quantum critical behavior.

In this paper, we study the field-induced transition in the bilayer Heisenberg model by means of bond-operator mean-field theory and strong-coupling expansions. Our principal conclusion is that the quantum critical regime is rather narrow, and that “quantum-critical-like” temperature dependences of quantities such as the magnetization are not sufficient to demonstrate that the system is in the true quantum critical regime.

Bond operator mean-field theory has been applied to the spin-ladder (1D) and weakly coupled spin-ladder (3D) models and shown to yield quantitatively correct results. Mean-field theory is a particularly appropriate tool for the problem at hand because the model is at its upper critical dimension, and so the asymptotic critical behavior will be correctly described up to logarithms. The strong-coupling expansions provide a good check of the accuracy of the mean-field theory, in the regimes where the former are reliable.

In §2, we describe the bond-operator mean-field theory, where the bilayer Heisenberg model is described in terms of three types of interacting bosons with a local constraint. In §3, ground state phase diagram in the $h-J$ plane and the critical properties of phase transitions are discussed. In
§4, thermodynamic properties of quantum disordered and quantum critical phases in a magnetic field are presented. The last section (§5) offers a summary and discussions.

§2. Bond-Operator Mean-Field Theory

Let us consider the quantum disordered phase of (1.1) in the limit $J \ll 1$ which is the analytic continuation of the interlayer dimer Hamiltonian ($J = 0$). Then we describe the phase by introducing bosonic degrees of freedom corresponding to local dimer states (singlet and triplet states) following the bond-operator representation of Sachdev and Bhatt:

| $s$ > = $s^\dagger|0>$ = \frac{1}{\sqrt{2}}(|\uparrow\downarrow> - |\downarrow\uparrow>)

| $t_x$ > = $t_{x}^\dagger|0>$ = \frac{-1}{\sqrt{2}}(|\uparrow\uparrow> - |\downarrow\downarrow>)

| $t_y$ > = $t_{y}^\dagger|0>$ = \frac{i}{\sqrt{2}}(|\uparrow\uparrow> + |\downarrow\downarrow>)

| $t_z$ > = $t_{z}^\dagger|0>$ = \frac{1}{\sqrt{2}}(|\uparrow\downarrow> + |\downarrow\uparrow>)

Here the four types of bosons satisfy bosonic commutation relations, and the left and right arrows in the kets represent the spin states on the first and second layers respectively. However there is a significant difference from usual bosonic systems because in the physical subspace only a single boson is allowed on each dimers. Thus the Hilbert space is restricted by a local constraint on the number operators of these bosons in each dimer

$s^\dagger s_i + t_{\alpha,i}^\dagger t_{\alpha,i} = 1$

where the summation convention is used for Greek indices.

In terms of these bosons, the spin operators in each layer can be expressed as

$S_{1,i}^\alpha = \frac{1}{2}(s_{i}^\dagger t_{\alpha,i} + t_{\alpha,i}^\dagger s_i - i\epsilon_{\alpha\beta\gamma}t_{\beta,i}^\dagger t_{\gamma,i})$

$S_{2,i}^\alpha = \frac{1}{2}(-s_{i}^\dagger t_{\alpha,i} - t_{\alpha,i}^\dagger s_i - i\epsilon_{\alpha\beta\gamma}t_{\beta,i}^\dagger t_{\gamma,i})$.

Then the bond-operator expression of Hamiltonian (1.1) is obtained in the form

$H = \sum_i \left( -\frac{3}{4}s_i^\dagger s_i - \frac{1}{4}t_{\alpha,i}^\dagger t_{\alpha,i} \right) - \sum_i \mu_i(s_i^\dagger s_i + t_{\alpha,i}^\dagger t_{\alpha,i} - 1)

+ \frac{J}{2} \sum_{\langle i,j \rangle} \left( s_i^\dagger s_j^\dagger t_{\alpha,i} t_{\alpha,j} + s_i s_j t_{\alpha,i} t_{\alpha,j} + \text{h.c.} \right)

- \frac{J}{2} \sum_{\langle i,j \rangle} \left( 1 - \delta_{\alpha\beta})(t_{\alpha,i}^\dagger t_{\beta,j} t_{\alpha,j}^\dagger t_{\beta,i} - t_{\alpha,i}^\dagger t_{\beta,j} t_{\alpha,j}^\dagger t_{\beta,i} ) \right)$.

Here we have introduced local chemical potentials $\mu_i$ to account for the local constraint (2.5). Mean-field theory of the disordered phase is constructed by the following procedures. (1) An
average chemical potential $\mu \equiv \mu_i$ is introduced to approximate the local constraints by a global constraint. (2) Bose-Einstein condensation of singlet states is assumed: $\langle s_i^\dagger \rangle = \langle s_i \rangle = s$, where $\langle \cdot \cdot \cdot \rangle$ denotes the thermodynamic average. (3) Terms containing four triplet operators are dropped. Here we would like to comment on the last numerically simplified assumption. The quadratic terms in $t_\alpha$-operators will in tern lead to a nonzero expectation value of $\langle t_\alpha t_\alpha \rangle$. By taking quadratic decouplings of fourth-order terms in $t_\alpha$, we found that the inclusion of these terms changes the numerical results only slightly, even near the critical coupling (for example, this lowers $J_c$ discussed in the next section about 5%).

The resulting mean-field Hamiltonian is easily diagonalized using the Bogoliubov transformation:

$$\xi_{k\alpha} = \cosh \theta_k t_{k\alpha} + \sinh \theta_k t_{k\alpha}^\dagger$$  \hspace{1cm} (2.9)$$

$$\cosh^2 \theta_k = \frac{1}{2}(\Lambda_k / \omega_k + 1)$$  \hspace{1cm} (2.10)$$

$$H_{MFT}(\mu, s) = N(-\frac{3}{4}s^2 - \mu s^2 + \frac{5}{2} \mu - \frac{3}{8}) + \sum_k \omega_k (\xi_{k\alpha}^\dagger \xi_{k\alpha} + \frac{3}{2})$$  \hspace{1cm} (2.11)$$

$$\omega_k = \sqrt{\Lambda_k^2 - 4\Delta_k^2}$$  \hspace{1cm} (2.12)$$

$$\Lambda_k = \frac{1}{4} - \mu + 2Js^2 \gamma_k, \Delta_k = Js^2 \gamma_k$$  \hspace{1cm} (2.13)$$

$$\gamma_k = \frac{1}{2}(\cos k_x + \cos k_y).$$  \hspace{1cm} (2.14)$$

The only effect of including an external field is to Zeeman-split the excitations, so that instead of all three lying at $\omega_k$ they have energies $\omega_k$ and $\omega_k \pm h$.

The above mean-field description of the disordered phase will be valid if the temperature is much less than the minimum energy gap. However, at intermediate and higher temperatures the density of triplet bosons becomes sufficiently large that their interactions cannot be neglected. Troyer, Tsunetsugu and Würtz have presented a simple prescription to modify the mean-field theory so that it correctly treats both the low and high-temperature limits. They noticed that the main problem of the bosonic description is its overcounting of entropy due to the global constraint on the number of elementary excitations. They reweighted the $M$-boson part in the partition function so that each multiplet contributes the correct entropy. In their formulation, the free energy of the triplet bosons in a uniform magnetic field is expressed (per dimer) as

$$f = -\frac{1}{\beta} \ln \left\{ 1 + [1 + 2 \cosh(\beta h)]z(\beta) \right\}$$  \hspace{1cm} (2.15)$$

where

$$z(\beta) = \frac{1}{N} \sum_k e^{-\beta \omega_k}.$$  \hspace{1cm} (2.16)$$

Using these formulae, one obtains self-consistent equations for the mean-field parameter $s$ and chemical potential $\mu$ by minimizing the total free energy ($F(s, \mu) = f(s, \mu) + \text{constant}(s, \mu)$) with
respect to those parameters:

\[-\frac{3}{2} - 2\mu + \frac{1}{N} \sum_k J \frac{2\gamma_k}{\sqrt{1 + 2r\gamma_k}} \left[ 3 + \frac{2(1 + 2\cosh(\beta h))e^{-\beta\omega_k}}{1 + [1 + 2\cosh(\beta h)]z(\beta)} \right] = 0 \]  

(2.17)

\[-s^2 + \frac{5}{2} - \frac{1}{2N} \sum_k \frac{1 + \gamma_k}{\sqrt{1 + 2r\gamma_k}} \left[ 3 + \frac{2(1 + 2\cosh(\beta h))e^{-\beta\omega_k}}{1 + [1 + 2\cosh(\beta h)]z(\beta)} \right] = 0 \]  

(2.18)

where

\[ r = \frac{2Js^2}{\left(\frac{1}{4} - \mu\right)} . \]  

(2.19)

It is straightforward to verify that this approach leads to the correct free energy and magnetization for isolated dimers \((J = 0)\) for all temperatures and external fields. The numerical analysis of the above equations when \(J \neq 0\) is discussed below.

§3. Ground State Phase Diagram

In the classical (large-\(S\)) limit, the Heisenberg bilayer with \(h > 0\) has three types of ground states. One is the fully polarized ferromagnet, realized in the high-field region. The others are canted phases in which the \(z\) component of the magnetization is parallel to the external field to gain Zeeman energy, while \(x\) and \(y\) components of the spins are ordered to gain exchange energy. For quantum spins a disordered (dimer) phase appears around \(J = 0\) for sufficiently small \(h\). As mentioned in Introduction, the phase diagram of (1.1) in zero magnetic field has been extensively studied. The order-disorder transition lies in the universality class of classical \(d = 3\) Heisenberg model, and is associated with a dynamical exponent \(z = 1\). However, the field-induced transitions have dynamical exponent \(z = 2\) and so should lie in the universality class of a \(d = 4\) classical model. The reduction of symmetry from \(O(3)\) to \(U(1)\) due to the magnetic field leads one to anticipate that the universality of the transition is \(d = 4\) \(XY\) type.

To estimate the phase boundary between dimer and canted phases, we performed \(T = 0\) strong-coupling expansions of the longitudinal susceptibilities transverse to the applied field up to the 8th order at the ordering vectors from interlayer dimer Hamiltonian (i.e. series expansions in powers of the intralayer couplings \(J\) about the interlayer dimer singlet state) using connected cluster method. By applying the differential approximant method assuming power-law divergence of the susceptibilities at critical points for fixed values of the applied field \(h\), \(\chi \sim (J_c(h) - J)^{-\gamma}\), we obtained estimates for the critical lines \(J_c(h)\) (and found associated critical exponents \(\gamma\) close to the expected value of 1). We could also estimate phase boundaries using the triplet excitation gaps at zero field which had been studied by strong-coupling expansions previously. These different estimates of the critical lines are consistent with each other, as shown in Fig. 1. The boundaries between the fully polarized phase and canted phases shown in that figure can be obtained from the lowest one magnon excitation gap in linear spin-wave theory.
Next we compare the results of the bond-operator mean-field theory at $T = 0$ and $h = 0$ with the results from the series expansions. At $T = 0$, the self-consistent equations (2.17), (2.18) for the two parameters $s$ and $\mu$ can be reduced to a single equation for the parameter $r$ introduced in (2.19), namely,

$$r = J(5 - 3K(r))$$  \hspace{1cm} (3.1)

with

$$K(r) = \frac{1}{N} \sum_k \frac{1}{\sqrt{1 + 2r \gamma_k}}.$$  \hspace{1cm} (3.2)

Once the parameter $r$ is determined from the above set of equations, the mean-field parameter $s$ and chemical potential $\mu$ are obtained from

$$s^2 = \frac{5}{2} - \frac{3}{4}(E(r) + K(r))$$  \hspace{1cm} (3.3)

and

$$\mu = -\frac{3}{4} + \frac{3}{2r}(E(r) - K(r))$$  \hspace{1cm} (3.4)

where

$$E(r) = \frac{1}{N} \sum_k \sqrt{1 + 2r \gamma_k}.$$  \hspace{1cm} (3.5)

As $J$ grows from 0, the triplet gap at the wave vector $k = (\pi, \pi)$ decreases, and the gap vanishes at $J = J_c$, signaling the instability of dimer phase. The critical value $J_c$ can be obtained by setting $r = 1/2$ and $J = J_c$ in (3.1), giving the value $J_c = 0.437$ which is somewhat larger than the series expansion estimate 0.393. In addition we obtain a critical spin-wave velocity 0.715 which is somewhat smaller than the series expansion estimate 0.744. The triplet gap for various values of $J$ in the dimer phase, and excitation spectra for $J = 0.2$ and 0.35, were obtained from numerical solutions of the mean-field equations, with the results shown in Figs. 2 and 3. For negative $J$, the mean-field theory gives the same critical parameters, changing only the sign of $J_c$. For comparison, the series expansion estimate for the negative critical coupling is $-0.433$, so mean field theory is remarkably accurate in that case.

In the following section, we restrict our discussion of several thermodynamic properties only for positive $J$ but the qualitative results of thermodynamic behavior are the same for negative $J$.

§4. Finite Temperature Properties

Our principal purpose in this section is to discuss the finite temperature quantum critical properties of the bilayer system, where a magnetic field is the tuning parameter and the system has a quantum disordered ground state at zero field. We analyzed these properties on the basis of the bond-operator mean-field theory as well as finite-temperature strong-coupling expansions up to 5th order (i.e. series expansions of the free energy in powers of the intralayer coupling $J$) using connected cluster method.\textsuperscript{28} Calculations of the latter variety for some parameter cases have already
been carried out to 8th order by Elstner and Singh for bilayers both with \( J = 0.2 \) and without \( J = 0.2 \) an external field. It turns out that the results from directly summing 5th order series are not very different from those of 8th order series, at least in the regimes where we expect these calculations to be most reliable.

Let us first discuss the thermodynamic properties of the system when \( h = 0 \). In Fig. 4, we show the energy gap \( \Delta \) of triplet excitations as a function of temperature as obtained from the mean-field theory. For values of \( J \) less than \( J_c \), \( \Delta \) is finite at \( T = 0 \) and shows a sharp rise with increasing temperature and eventually tends to saturate, reflecting a rapid extinction of long-range correlations. However, at \( J = J_c \), \( \Delta \) rises from zero linearly with temperature, consistent with the prediction of the non-linear \( \sigma \) model, \( \Delta \approx 1.04T \). We have calculated the specific heat \( C_V \) and uniform susceptibility \( \chi \) for \( J = 0.2 \) as functions of temperature, using both mean-field theory and series expansions, with the results shown in Fig. 5. Since the system has a quantum disordered ground state, the thermodynamic quantities show thermally activated behavior. For the specific heat, both methods yield nearly identical results. For the susceptibility, mean-field theory deviates by about 10% at intermediate temperatures from the results of series expansions.

Let us now discuss the temperature dependence of properties of the system at a field-induced transition. In Figs. 6 and 7, we show the magnetization and specific heat as functions of \( T \) at the critical field \( h = h_c = \Delta \) for \( J = 0.2 \). In general, we expect power-law dependences of thermodynamic quantities at low temperatures if the parameters of a system are set to a quantum critical point. Mean-field theory gives a linear \( T \) dependence for both quantities in a very narrow low temperature region, \( T \leq 0.1 \ll \Delta \). The agreement between two approaches is fairly good except for some artificial features seen in the summed series expansions at low temperatures.

The series expansions at finite temperature should reduce to the strong-coupling expansion from the dimer singlet state in the limit \( T = 0 \). Thus the thermodynamic quantities obtained by direct summation of finite series necessarily decrease exponentially at sufficiently low temperature. However we might have the possibility of seeing quantum critical behavior at intermediate \( T \) temperatures if the tuning parameter is set equal or close to the quantum critical point of the infinite system. Thereby we must be careful to judge whether or not the system is really exhibiting quantum critical behavior in the relevant temperature regime. In Fig. 6, it is found that the magnetization starts to show apparently linear behavior towards \( T = 0 \) at \( T \sim 0.3 \), but mean-field theory indicates that the system has not yet entered the quantum critical region, since at \( T = 0 \) the magnetization has a different slope than in the intermediate-\( T \) "linear" regime. The specific heat behaves similarly, as seen in Fig. 7. (The series expansion result exhibits a pair of peaks and a dip but this should be regarded as an artifact due to low order of the expansion and the crudeness of the extrapolation technique.)

The case we have presented above, for \( J = 0.2 \), is actually the one in which there is the best
chance of observing the true quantum critical regime for the field induced transition. As $J \to 0$ the quantum critical regime vanishes since there is no way that the critical properties will be exhibited for $T > J$. As $J \to J_c$, $h_c \to 0$ and it is natural to expect that for $T > h_c$ (but not too large) the system will exhibit the quantum critical behavior associate with the zero-field transition. Thus the field-induced transition’s quantum critical regime is squeezed at both ends. We have made rough estimates of the extent of that regime as a function of $J$, based on the behavior of $M(T)$, with the results shown in Fig. 8. It therefore appears that observing the quantum critical regime for the field-induced transition will, in general, be very difficult to achieve either in numerical simulations or experiments.

§5. Summary and Discussion

We have investigated the ground state phase diagram and thermodynamic properties of bilayer Heisenberg model on the square-lattice in a uniform magnetic field. The ground state phase diagram of the model has been investigated by means of strong-coupling expansion around the dimer limit (considering both the gap and longitudinal susceptibility) and linear spin-wave theory. We found that the longitudinal susceptibility exponent for the field-induced transition appears to be very close to $z \nu = 1$, as expected. However, we cannot exclude the possibility of logarithmic corrections to scaling expected at upper critical dimensions, and further field-theoretical investigations are needed to clarify this point. It might also be interesting to calculate the transverse susceptibility, for which one expects an exponent of $(z + d) \nu = 2$.

Thermodynamic properties of the model were investigated also by means of bond-operator mean-field theory, and its results were compared to those of the finite temperature strong-coupling expansions. We found the theory provides a simple but reasonably good description of thermodynamic quantities at all temperatures. It appears that the quantum critical region for field-induced transitions in this system is restricted to extremely low temperatures, even though the magnetization exhibits what might appear to be the expected quantum critical power law behavior at higher temperatures.

Finally, we mention that a transition entirely analogous to the field induced transition in Heisenberg bilayers can take place in bilayer quantum Hall systems. Recently, Troyer and Sachdev presented quantum Montecarlo simulation on Heisenberg bilayers in a magnetic field to determine the universal Kosterlitz-Thouless transition temperature $T_{KT}$ in the vicinity of a zero-field quantum critical point. The universality of $T_{KT}$ when the ground state is ordered leads us to an anticipation of the universality of a quantum critical crossover temperature when the ground state is disordered ($h < h_c = \Delta$) (which is not our estimated one but the one between field-induced quantum critical and quantum disordered regions). We leave this issue to a future study.
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FIGURE CAPTIONS

Fig. 1. Phase diagram of bilayer Heisenberg model in the magnetic field. The canted phases are specified by the ordering vectors \((\pi, \pi; \pi)\) and \((0, 0; \pi)\), where the third component \(\pi\) indicates antiferromagnetic orientation between layers. The open circles are series expansion estimates of the triplet excitation gaps.

Fig. 2. Triplet gap as a function of \(J(>0)\). The dots and solid line are series expansion estimates and mean-field theory results, respectively.

Fig. 3. Triplet excitation spectra for \(J = 0.2, 0.35\). The dots and lines are series expansion estimates and mean-field theory results, respectively.

Fig. 4. Triplet gaps for various \(J(\leq J_c)\) as a function of temperature \(T\).

Fig. 5. Uniform susceptibility and specific heat (per a dimer) as a function of temperature for \(J = 0.2\) and \(h = 0\). The dots and solid lines are the results of series expansion up to the 5-th order and mean-field theory, respectively.

Fig. 6. Magnetization at the critical field for \(J = 0.2\) as a function of temperature. The symbols are the same as in Fig. 5. The broken line is just a guide to the eye.

Fig. 7. Specific heat at the critical field for \(J = 0.2\) as a function of temperature. The symbols are the same as in Fig. 5. The broken line is just a guide to the eye.

Fig. 8. Estimates of the extent of the quantum critical regime for the field-induced transition, as a function of \(J\). The curved line is just a guide to the eye.
\& \& Q=(\& P, \& P)
\[ \mathcal{S}_Q = \mathcal{S}_Q(P, P) \]

- \( J = 0.2 \)
- \( J = 0.35 \)
- \( J = J_c \)

non-linear \& R model
