Bi-layer Heisenberg model studied by the Schwinger-boson
Gutzwiller-projection method

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Abstract

A two-dimensional bi-layer, square lattice Heisenberg model with different intraplane($J_\parallel$) and interplane($J_\perp$) couplings is investigated. The model is first solved in the Schwinger boson mean-field approximation. Then the solution is Gutzwiller projected to satisfy the local constraint that there should be only one boson at each site. For these wave functions, we perform variational Monte Carlo simulation up to $24 \times 24 \times 2$ sites. It is shown that the Néel order is destroyed as the interplane coupling is increased. The obtained critical value, $J_\perp/J_\parallel = 3.51$, is smaller than that by the mean-field theory. Excitation spectrum is calculated by a single mode approximation. It is shown that energy gap develops once the Néel order is destroyed.

75.10.-b, 75.10.Jm, 75.50.Ee
I. INTRODUCTION

Spin pseudogap observed in underdoped YBa$_2$Cu$_3$O$_{7-x}$ is one of the fascinating characters of the high-$T_c$ cuprates. NMR experiments showed that even above the transition temperature of superconductivity, $T_c$, static uniform susceptibility and the NMR relaxation rate, $T_1$, decrease with decreasing temperature. Neutron scattering experiments showed the decrease of low energy magnetic excitation with decreasing temperature and found precursor of a finite spin gap. It has been pointed out that these astonishing experimental results can be explained provided that there is a spin pseudogap in the normal state of high $T_c$ materials. These phenomena indicating the spin pseudogap, however, have not been observed in the La$_{2-x}$Sr$_x$CuO$_4$ systems. Therefore it is speculated that the number of the CuO$_2$ layers between the insulating layers is essential for the formation of this gap, although a successful theory has not been presented.

It is conceivable that the finite concentration of holes affect the spin configuration and the excitation considerably. However, as a first step toward understanding of the spin pseudogap behavior, it is meaningful to study the properties of the bi-layer CuO$_2$ system at zero doping. Namely we investigate a bi-layer square-lattice Heisenberg model of spin 1/2.

\[ H = J_\parallel \sum_i \sum_w \sum_{a=1,2} S_{i,a} \cdot S_{i+w,a} + J_\perp \sum_i S_{i,1} \cdot S_{i,2}, \]

where $w = x, y$, $i + w$ represents a site next to the site $i$ in the $w$ direction, and $S_{i,a}$ is a spin 1/2 operator at site $i$ in plane $a$. The nearest neighbor spins interact antiferromagnetically with intraplane coupling constant $J_\parallel$ and interplane coupling constant $J_\perp$. What we want to know is how the properties of the system changes as $J_\perp/J_\parallel \equiv \alpha$ increases: at what value of $\alpha$ the Néel order is destroyed, and how the excitation spectrum varies.

As for the zero-temperature critical value of $\alpha_c$ for the destruction of the Néel order, there have been several investigations by various methods: spin wave approximation given by Matsuda and Hida and the Schwinger boson mean-field theory resulted in quite large critical value, $\alpha_c = 4.24$ for the former and 4.48 for the latter. On the other hand, more
sophisticated methods have resulted in much lower critical value. Quantum Monte Carlo
calculation gives it as $2.51 \pm 0.01$ and the dimer expansions, which is an approach from
the $\alpha \to \infty$ limit, gives $2.56$. One of the aim of the present paper is to obtain this critical
value by another method, the Schwinger-boson Gutzwiller-projection method.

In Schwinger-boson Gutzwiller-projection method we first solve the Hamiltonian by
Schwinger-boson mean-field theory. The obtained ground-state wave function is Gutzwiller
projected to fix the spin at each site to be $1/2$. The wave function thus obtained is a kind
of RVB wave function where long-range bonds are allowed with amplitude depending on
the distance between the sites. This method was first used by Chen and Xiu for the square
lattice antiferromagnetic Heisenberg model. It was shown that the wave function obtained
this way is quite close to the true ground-state. This method has also been applied to the
anisotropic Heisenberg model. There it was shown that even in the one-dimensional limit
the ground-state energy, $-0.4377J$ per site, is quite close to the exact value, $-0.4431J$ per
site. Therefore we expect that this method gives wave functions quite close to the actual
ground-state in the present system, too. A merit of the present method is that the wave
function is given as an RVB wave function. Thus vertically coupled dimer state in the limit
of $\alpha \to \infty$, disordered state in the intermediate value of $\alpha$, and the Néel state at small $\alpha$
can be described in a unified way by wave functions with the same structure.

In this paper, using this method we show that the Néel order at small $\alpha$ is destroyed at
$\alpha_c = 3.51$. It is expected that gap appears in the excitation spectrum at $\alpha > \alpha_c$. This is
confirmed by our calculation of the spectrum by a single mode approximation. To obtain
these results we solve the present Hamiltonian by the Schwinger-boson mean-field theory
in Sec.II. The obtained ground-state wave function is Gutzwiller-projected in Sec.III. The
single mode approximation for the RVB wave function is discussed in Sec.IV. In Sec.V,
we perform variational Monte Carlo simulation for these wave functions and calculate its
energy, spin-spin correlation, staggered magnetization and low-lying excitation spectrum.
In Sec.VI critical point and the excitation spectrum are discussed.
II. MEAN-FIELD SOLUTION

We introduce four kinds of bose operators, \( s_{i,a,\uparrow}, s_{i,a,\downarrow} \) \((a = 1, 2)\) to express the spin operators

\[
S_{i,a}^{\pm} = s_{i,a,\uparrow}^\dagger s_{i,a,\downarrow}, \quad S_{i,a}^z = \frac{1}{2}(s_{i,a,\uparrow}^\dagger s_{i,a,\uparrow} - s_{i,a,\downarrow}^\dagger s_{i,a,\downarrow}).
\]  

(2)

The commutation relations of the spin operators \( S_i \) are satisfied in this replacement. We impose a constraint,

\[
s_{i,a,\uparrow}^\dagger s_{i,a,\uparrow} + s_{i,a,\downarrow}^\dagger s_{i,a,\downarrow} = 1,
\]

(3)
in order to guarantee \( S = 1/2 \). Then Hamiltonian is rewritten as follows;

\[
H = \frac{1}{2}J_\parallel \sum_i \sum_{w,a=1,2} \sum_{\sigma}(s_{i,a,\sigma}^\dagger s_{i+w,a,-\sigma} s_{i,a,-\sigma} - s_{i,a,\sigma}^\dagger s_{i+w,a,-\sigma} s_{i,a,-\sigma}) \\
+ \frac{1}{2}J_\perp \sum_i \sum_{\sigma}(s_{i,1,\sigma}^\dagger s_{i,2,-\sigma} s_{i,2,\sigma} - s_{i,1,\sigma}^\dagger s_{i,2,-\sigma} s_{i,1,\sigma}) \\
+ \mu \sum_i \sum_{a=1,2} \sum_{\sigma} s_{i,a,\sigma}^\dagger s_{i,a,\sigma}.
\]

(4)

Here \( \mu \) is a chemical potential introduced to enforce the constraint Eq.(3) on the average.

To solve the Hamiltonian in the mean-field approximation, we introduce the following mean-field order parameters \( \Delta_{w,a}, \Delta_z, \) and \( n_{a,\sigma} \), which give the amplitudes of the intralayer singlet correlations, interlayer singlet correlations, and an averaged occupation number, respectively,

\[
\Delta_w \equiv \Delta_{w,2} = -\Delta_{w,1} = \frac{1}{2}\langle s_{i,2,\dagger} s_{i+w,2,\uparrow} - s_{i,2,\uparrow} s_{i+w,2,\dagger} \rangle, 
\]

(5)

\[
\Delta_z = \frac{1}{2}\langle s_{i,1,\dagger} s_{i,2,\uparrow} - s_{i,1,\uparrow} s_{i,2,\dagger} \rangle, 
\]

(6)

\[
n_{a,\sigma} = \langle s_{i,a,\sigma}^\dagger s_{i,a,\sigma} \rangle = \frac{1}{2}. 
\]

(7)

After decoupling the Hamiltonian, we rewrite the operator using its Fourier transformation:

\[
s_{i,a,\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{i\mathbf{k} \cdot \mathbf{r}_i} s_{k,a,\sigma},
\]

(8)

where \( N \) is the total number of lattice sites for each layer, and \( k \) summation is taken over the Brillouin zone \(-\pi \leq k_x \leq \pi, -\pi \leq k_y \leq \pi\). The mean-field Hamiltonian \( H_{MF} \) is written as follows
The ground-states are defined as the vacuum of the Bose operator \( \alpha_{k\uparrow}, \alpha_{-k\downarrow}, \beta_{k\uparrow}, \) and \( \beta_{-k\downarrow} \), such that \( \alpha_{k\uparrow}|G\rangle = \alpha_{-k\downarrow}|G\rangle = \beta_{k\uparrow}|G\rangle = \beta_{-k\downarrow}|G\rangle = 0 \).
For a finite-size system, the self consistent equations for \( \lambda, \Delta_x, \Delta_y, \Delta_z \) are given by Eqs. (5-7), which lead to

\[
1 = \frac{1}{4N} \sum_k \left( \frac{\lambda}{E_{k+}} + \frac{\lambda}{E_{k-}} \right),
\]

\[
\Delta_w = \frac{1}{4N} \sum_k \sin k_w \left( \frac{\gamma_k + \delta}{E_{k+}} + \frac{\gamma_k - \delta}{E_{k-}} \right),
\]

\[
\Delta_z = \frac{i}{4N} \sum_k \left( \frac{\gamma_k + \delta}{E_{k+}} - \frac{\gamma_k - \delta}{E_{k-}} \right).
\]

We find that the free energy takes the same minimal value for \( \Delta_x = \Delta_y \) (s-wave) and \( \Delta_x = -\Delta_y \) (d-wave). Since either state gives the same result, we consider only the s-wave state from now on. We denote \( \Delta_x = \Delta_y \equiv \Delta_\parallel \) and \(-i\Delta_z \equiv \Delta_\perp \). The solution depends on the size of the system \( N \). When \( N \) is finite, \( E_{k\pm} \) never becomes zero. However, in the limit of \( N \to \infty \) it is possible that \( E_{k\pm} \) vanishes at \( k = K_\pm = \pm(\pi/2, \pi/2) \). In such a case it is known that we need to introduce the Bose condensate \( n_B \), and Eqs. (20-22) are rewritten as

\[
1 = \frac{1}{4N} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \left( \frac{\lambda}{E_{k+}} + \frac{\lambda}{E_{k-}} \right) dk_x dk_y + n_B,
\]

\[
\Delta_\parallel = \frac{1}{4N} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \sin k_w \left( \frac{\gamma_k + \delta}{E_{k+}} + \frac{\gamma_k - \delta}{E_{k-}} \right) dk_x dk_y + n_B,
\]

\[
\Delta_\perp = \frac{1}{4N} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \left( \frac{\gamma_k + \delta}{E_{k+}} - \frac{\gamma_k - \delta}{E_{k-}} \right) dk_x dk_y + n_B.
\]

When the Bose condensate \( n_B \) becomes finite, we have \( \lambda = 4J_\parallel \Delta_\parallel + J_\perp \Delta_\perp \). The self-consistent equations are numerically solved. Figure 1 shows the \( \alpha \) dependence of order-parameters \( \Delta_\parallel, \Delta_\perp \), Bose condensate \( n_B \), and energy gap \( E_g \). Bose condensate vanishes at \( \alpha = 4.48 \), and the gap opens for \( \alpha > 4.48 \). The intralayer RVB order parameter, \( \Delta_\parallel \), vanishes at \( \alpha = 4.62 \). For \( \alpha > 4.62 \), only the interlayer nearest neighbor spin-spin correlation exists.

The intra(inter) layer spin-spin correlation \( \langle S_{i,a} \cdot S_{j,a} \rangle (\langle S_{i,1} \cdot S_{j,2} \rangle) \) in the grand-state are given as

\[
\langle S_{i,a} \cdot S_{j,a} \rangle = \frac{3}{2} \left[ \frac{1}{4N} \sum_k \left( \frac{\lambda}{E_{k+}} + \frac{\lambda}{E_{k-}} \right) \cos k \cdot r_{i,j} + n_B \cos K_+ \cdot r_{i,j} \right]^2
\]

\[
-\frac{3}{2} \left[ \frac{1}{4N} \sum_k \left( \frac{\gamma_k + \delta}{E_{k+}} + \frac{\gamma_k - \delta}{E_{k-}} \right) \sin k \cdot r_{i,j} + n_B \sin K_+ \cdot r_{i,j} \right]^2,
\]

\( n_B \) is the Bose condensate.
From Eq. (32) it is clear that the ground-state wave function obtained in the mean-field theory is expressed as

\[
\langle S_{i,1} \cdot S_{j,2} \rangle = \frac{3}{2} \frac{1}{4N} \sum_k \left( \frac{\lambda}{E_{k+}} - \frac{\lambda}{E_{k-}} \right) \sin k \cdot r_{i,j} + n_B \sin K_+ \cdot r_{i,j} \right)^2 - \frac{3}{2} \frac{1}{4N} \sum_k \left( \frac{\gamma_k + \delta}{E_{k+}} - \frac{\gamma_k - \delta}{E_{k-}} \right) \cos k \cdot r_{i,j} + n_B \cos K_+ \cdot r_{i,j} \right)^2, \tag{27}
\]

where \( r_{i,j} = r_i - r_j \). The summations over \( k \) in Eqs. (26, 27) vanish in the limit \( |r_{i,j}| \to \infty \). Therefore, the correlation extends to infinity only if \( n_B > 0 \), which means the existence of antiferromagnetic long-range order. Thus, in the mean-field approximation, the critical point of order-disorder transition is 4.48.

### III. RVB Wave Function

The ground-state wave function obtained in the mean-field theory is expressed as

\[
|G\rangle = \prod_k \exp \left[ \frac{i}{2} \frac{\tanh \theta_k^\uparrow + \tanh \theta_k^\downarrow}{2} \left( s_{k,1,\uparrow}^\dagger s_{k,2,\downarrow}^\dagger - s_{k,1,\uparrow}^\dagger s_{k,1,\downarrow}^\dagger \right) - \frac{i}{2} \frac{\tanh \theta_k^\uparrow + \tanh \theta_k^\downarrow}{2} \left( s_{-k,1,\downarrow}^\dagger s_{k,2,\uparrow}^\dagger - s_{k,1,\uparrow}^\dagger s_{-k,1,\downarrow}^\dagger \right) \right] |0\rangle, \tag{28}
\]

where \( |0\rangle \) is the vacuum of the Schwinger bosons. By the Fourier transformation for \( s_{k,1,\uparrow}^\dagger, s_{-k,1,\downarrow}^\dagger, s_{k,2,\uparrow}^\dagger, s_{-k,2,\downarrow}^\dagger \), we can get a real-space representation for this ground-state,

\[
|G\rangle = \exp \left[ \sum_{i,j} a_{i,j} \left( s_{i,1,\uparrow}^\dagger s_{j,2,\downarrow}^\dagger - s_{i,1,\downarrow}^\dagger s_{j,2,\uparrow}^\dagger \right) + b_{i,j} \left( s_{j,1,\downarrow}^\dagger s_{i,2,\uparrow}^\dagger - s_{i,1,\uparrow}^\dagger s_{j,2,\downarrow}^\dagger \right) \right] |0\rangle, \tag{29}
\]

\[
a_{i,j} = \frac{i}{2N} \sum_k \left[ \tanh \theta_k^\uparrow + \tanh \theta_k^\downarrow \right] \exp(i k \cdot r_{i,j}), \tag{30}
\]

\[
b_{i,j} = -\frac{i}{2N} \sum_k \left[ \tanh \theta_k^\uparrow - \tanh \theta_k^\downarrow \right] \exp(i k \cdot r_{i,j}). \tag{31}
\]

It is evident that the local constraint, Eq. (3) is not satisfied in this wave function. We remove this difficulty by projecting the wave function to a space where each site is singly occupied. Namely, we perform the Gutzwiller projection, using Gutzwiller projection operator \( P \),

\[
|G\rangle = P \left[ \sum_{i \neq j} a_{i,j} \left( s_{i,1,\uparrow}^\dagger s_{j,2,\downarrow}^\dagger - s_{i,1,\downarrow}^\dagger s_{j,2,\uparrow}^\dagger \right) + b_{i,j} \left( s_{j,1,\downarrow}^\dagger s_{i,2,\uparrow}^\dagger - s_{i,1,\uparrow}^\dagger s_{j,2,\downarrow}^\dagger \right) \right] |0\rangle. \tag{32}
\]

From Eq. (32) it is clear that the ground-state \( |G\rangle \) is an RVB state. The weights of the bond, \( a_{i,j} \) and \( b_{i,j} \), decay proportional to \( r_{i,j}^{-3} \) except for \( b_{i,j} \) at small \( J_{\perp} \). Although it would be
possible to regard every \(a_{i,j}\) and \(b_{i,j}\) as variational parameters, we here restrict them to be those given in Eqs. (30, 31). In the case of \(\alpha = 0\), this restriction is justified by the result itself: Chen and Xiu\(^2\) have shown that this choice of \(a_{i,j}\) gives excellent results for the ground-state energy and the staggered magnetization. The weights \(a_{i,j}\) and \(b_{i,j}\) depend on \(\alpha = J_\perp/J_\parallel\) through the order parameters. We consider this \(\alpha\) in \(a_{i,j}\) and \(b_{i,j}\) as a variational parameter. In order to avoid confusion, we use a symbol \(\alpha_p\) to mean the value of \(\alpha\) used to obtain the ground-state.

**IV. EXCITATION SPECTRUM**

Once the approximate ground-state is obtained, excitation spectrum can be calculated by a method given by Feynman for liquid \(^4\)He, namely the single mode approximation\(^21\),\(^22\). The essential point of this method is to consider a low-lying excited state intuitively and calculate excitation spectrum from a known ground-state. In our case, low-lying state of this Hamiltonian should be the spin wave excitation. Thus we consider the following excited states.

\[
|E_\pm\rangle = (S_{k,1}^- \pm S_{k,2}^-)|G\rangle , \tag{33}
\]

\[
S_{k,a}^- \equiv \frac{1}{\sqrt{N}} \sum_i S_{i,a}^- e^{ik\cdot r_i} , \tag{34}
\]

where \(|E_\pm\rangle\) is variational excited states. Excitation spectrum, \(\omega_\pm(k)\), is calculated as

\[
\omega_\pm(k) = \frac{f_\pm(k)}{S_\pm(k)} , \tag{35}
\]

\[
S_\pm(k) = \frac{1}{N} \sum_{i,j} \langle G| (S_{i,1}^\pm \pm S_{i,2}^\pm)(S_{j,1}^- \pm S_{j,2}^-)|G\rangle e^{ik\cdot r_{i,j}} , \tag{36}
\]

\[
f_\pm(k) = \frac{1}{N} \sum_{i,j} \langle G| (S_{i,1}^\pm \pm S_{i,2}^\pm)(H, (S_{j,1}^- \pm S_{j,2}^-))|G\rangle e^{ik\cdot r_{i,j}} \]

\[= \frac{J_\parallel}{N} \sum_{i,l,\omega'} \langle G| (S_{i,1}^\pm \pm S_{i,2}^\pm)(-S_{i,1}^- S_{i+\omega',1}^- + S_{i,2}^- S_{i+\omega',2}^- + S_{i,1}^z S_{i+\omega',1}^- S_{i,2}^- S_{i+\omega',2}^-)|G\rangle e^{ik\cdot r_{i,l}} \]

\[+ (1 \mp 1) \frac{J_\perp}{N} \sum_{i,j} \langle G| (S_{i,1}^\pm \pm S_{i,2}^\pm)(S_{i,1}^z S_{i,2}^- - S_{i,1}^- S_{i,2}^-)|G\rangle e^{ik\cdot r_{i,l}} . \tag{37}\]
Here, $\omega' = \pm x, \pm y, i + \omega'$ represents a site next to the site $i$ in the $\omega'$ direction, $S_{\pm}(k)$ is the static structure factor and $f_{\pm}(k)$ is a 3-point correlation function of spin operators. The two modes represent in-phase, $\omega_{+}(k)$, and out-of-phase, $\omega_{-}(k)$, spin excitations of the two layers.

Since $|G\rangle$ is an RVB state, we must consider a loop covering associated with two valence bond configurations, $|c_{1}\rangle, |c_{2}\rangle$, to calculate Eqs.(36,37). For Eq.(36) we use known results,

$$\langle c_{1}|S_{i,a}^{+}S_{j,b}^{-}|c_{2}\rangle = \begin{cases} 
\frac{1}{2} & (i, a), (j, b) \text{ belong to the same loop and the same sub-lattice.} \\
-\frac{1}{2} & (i, a), (j, b) \text{ belong to the same loop and different sub-lattice.} \\
0 & (i, a), (j, b) \text{ belong to the different loop.}
\end{cases}$$

(38)

For Eq.(37) the following rule is found,

$$\langle c_{1}|S_{i,a}^{+}S_{i+b,a}^{-}S_{i+\delta,c}^{z}|c_{2}\rangle = \begin{cases} 
\frac{1}{4} & (i, b), (i + \delta, c) \text{ belong to the same loop and } (l, a) = (i + \delta, c). \\
-\frac{1}{4} & (i, b), (i + \delta, c) \text{ belong to the same loop and } (l, a) = (i, b). \\
0 & \text{otherwise.}
\end{cases}$$

(39)

Here, $i + \delta$ means the nearest neighbor of $i$-th site. $S_{\pm}(k)$ can be calculated directly from the first rule. Using the second rule, $f_{\pm}(k)$ becomes

$$f_{\pm}(k) = \frac{J_{\parallel}}{N}(2 - \cos k_{x} - \cos k_{y}) \sum_{i} \sum_{a=1,2} \sum_{w} \langle G|S_{i+w,a}^{+}S_{i,w,a}^{-}S_{i+\delta,c}^{z}|G\rangle$$

$$+ \frac{4(1 \mp 1)J_{\perp}}{N} \sum_{i} \langle G|S_{i,2}^{+}S_{i,1}^{-}S_{i,2}^{z}|G\rangle.$$ 

(40)

Thus we have only to count the number of the nearest neighbors in the same loop for each loop covering. This simplifies the numerical calculation.

V. NUMERICAL RESULTS

In this section, we show numerical results of the ground-state energy, spin-spin correlation, staggered magnetization, and the excitation spectrum as a function of $\alpha$. We perform...
Monte Carlo simulations in which RVB states are sampled to satisfy detailed balance for lattices with $L \times L \times 2$ sites, where $L \leq 24$. All the numerical calculations are performed with periodic boundary conditions. For each system size we solve the self-consistent equations \((20,22)\), and calculate $a_{i,j}, b_{i,j}$ to be used to construct the wave function at that system size.

A. Ground-state energy

The energy per site of the bi-layer Heisenberg model, $E$, is given by the nearest-neighbor spin-spin correlations $\epsilon_{\parallel}(L, \alpha_p)$ and $\epsilon_{\perp}(L, \alpha_p)$ for a given wave function specified by the parameter $\alpha_p$:

$$E(L, \alpha_p) = 2J_{\parallel}\epsilon_{\parallel}(L, \alpha_p) + \frac{1}{2}J_{\perp}\epsilon_{\perp}(L, \alpha_p) \quad ,$$

(41)

where

$$\epsilon_{\parallel}(L, \alpha_p) = \frac{1}{4L^2} \sum_i \sum_w \sum_{a=1,2} \langle G | S_{i,a} \cdot S_{i+w,a} | G \rangle \quad ,$$

(42)

$$\epsilon_{\perp}(L, \alpha_p) = \frac{1}{L^2} \sum_i \langle G | S_{i,1} \cdot S_{i,2} | G \rangle \quad .$$

(43)

To estimate the energy in the thermodynamic limit, the size dependence is examined and we find the following size scaling for any fixed $\alpha_p$,

$$\epsilon_{\parallel}(L, \alpha_p) = \epsilon_{\parallel}(\alpha_p) + \lambda L^{-3} + \cdots \quad ,$$

(44)

$$\epsilon_{\perp}(L, \alpha_p) = \epsilon_{\perp}(\alpha_p) + \lambda L^{-3} + \cdots \quad ,$$

(45)

where $\lambda$ is a constant. This size-scaling coincides with the spin wave theory for a square lattice. In Fig. 2, $\epsilon_{\parallel}(\alpha_p)$ and $\epsilon_{\perp}(\alpha_p)$ are shown. Open circles and solid circles indicate $\epsilon_{\parallel}(\alpha_p)$ and $\epsilon_{\perp}(\alpha_p)$. Error bars show the standard deviation of the Monte Carlo simulation. The interplane nearest-neighbor spin-spin correlation $\epsilon_{\parallel}$ has a value of $-0.3333 \pm 0.0006$ at $\alpha_p = 0$, which is quite close to the best estimated value of $-0.3348$. The magnitude of $\epsilon_{\parallel}$ decreases as $\alpha_p$ increases and finally vanishes at $\alpha_p = 4.62$. On the other hand,
the magnitude of $\epsilon_\perp(\alpha_p)$ increases and saturates to 0.75 at $\alpha_p = 4.62$. At $\alpha_p \geq 4.62$ the intraplane spin correlation vanishes and dimerized state is realized.

The ground-state energy per site at a given $\alpha$ is calculated as a minimum of $E(\alpha_p) = 2J_\parallel \epsilon_\parallel(\alpha_p) + \frac{1}{2}J_\perp \epsilon_\perp(\alpha_p)$ with respect to $\alpha_p$. Thus, we can get an optimal variational parameter and energy for a given $\alpha$. The relation between the variational parameter($\alpha_p$) and a real coupling($\alpha$) is shown in Fig. 3, and the ground-state energy per site is shown in Fig. 4. In Fig. 4 we also show the energy of dimerized state per site, $-\frac{3}{8}\alpha J_\parallel$(straight line) for reference. The difference between the optimal energy and the dimerized energy becomes smaller with increasing interlayer coupling.

**B. Staggered magnetization**

We calculated the spin-spin correlation, $\langle \mathbf{S}_{i,a} \cdot \mathbf{S}_{j,b} \rangle$, between arbitrary two sites $(i, a)$ and $(j, b)$. The results for $24 \times 24 \times 2$ lattice system are shown in Fig. 5, where absolute value of the intralayer spin-spin correlation is plotted as a function of the distance between the two sites. Open circles are for $\alpha = 0.4$ and solid circles are for $\alpha = 4.6$. It is obvious that there is a long-range order at $\alpha = 0.4$ and no long-range order at $\alpha = 4.6$. In the latter case, the correlation decreases exponentially and the typical correlation length for the disordered state is of the order of a lattice constant.

The long-range order is of the antiferromagnetic one. In the ordered phase staggered magnetization of the infinite size system is obtained from size dependence of the staggered spin-spin correlation between the mostly separated pairs. For a given lattice size $L$, we calculated both the intralayer correlation $M_0(L)^2$, and interlayer correlation $M_1(L)^2$:

$$M_0(L)^2 \equiv \frac{1}{2N} \sum_{i,j}^\prime \sum_{a=1,2} \langle |S_{i,a} \cdot S_{j,a}| \rangle,$$  \hspace{1cm} (46)

$$M_1(L)^2 \equiv \frac{1}{N} \sum_{i,j}^\prime \langle |S_{i,1} \cdot S_{j,2}| \rangle,$$  \hspace{1cm} (47)

where the summation is taken for all the pair of $i$ and $j$ such that $r_i - r_j = (\pm L/2, \pm L/2)$. 

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Except at $\alpha = 0$, $M_0(L)$ and $M_1(L)$ coincide within the Monte Carlo statistical error. As shown in Fig. 6, they are well fitted by the size scaling,

$$M_0(L) = M_1(L) = M(\infty) + \mu L^{-1} + \cdots,$$

where $\mu$ is a constant. This scaling agrees with the prediction of the spin wave theory and arguments given by Huse. The staggered magnetization $M_0 = M(\infty)$ as a function of $\alpha$ is given in Fig. 7. In this figure, the results of the mean-field theory (MFT) are also shown. In the case of small $\alpha$, the interlayer coupling enhances the antiferromagnetic long-range order. This is because the system acquires a weak three-dimensionality and quantum fluctuation is suppressed. On the other hand, for larger $\alpha$, the magnetizations are suppressed. This behavior is consistent with the result of Matsuda and Hida in the spin-wave theory. The staggered magnetization vanishes at $\alpha_c = 3.51 \pm 0.05$.

C. Excitation spectrum

We calculate the structure factor, $S_{\pm}(k)$, and excitation spectrum, $\omega_{\pm}(k)$ as a function of coupling $\alpha$. The calculations are done for $24 \times 24 \times 2$ lattice. The behavior of $S_{\pm}(k)$ and $\omega_{\pm}(k)$ strongly depends on whether the system has long-range order or not. The result of $S_{\pm}(k)$ is shown in Fig. 8 and $\omega_{\pm}(k)$ is shown in Fig. 9. Here, three typical couplings are taken; $\alpha = 0.4$ (open circles), $\alpha = 2.4$ (closed circles), $\alpha = 3.6$ (open squares). The third coupling is for the system in the disordered phase. For each figure, (a) is for the plus mode and (b) is for the minus mode, and $\Gamma = (0,0)$, $X = (0,\pi)$, $M = (\pi,\pi)$ in momentum space.

It is obvious from Fig. 8 that $S_+(k)$ of the ordered state ($\alpha = 0.4, 2.4$) is proportional to $k$ near $\Gamma$ point and $S_-(k)$ has an antiferromagnetic peak at $M$ point. On the other hand, $S_+(k)$ at $\alpha = 3.6$ increases quadratically with $k$ near $\Gamma$ point. (See inset of Fig. 8(a)). In the Néel state, the excitation is gapless at two points. One is $\omega_+(k)$ at $\Gamma$ point. Around this point, since the function $f_+(k)$ in Eq. (33) behaves like $f_+(k) \propto k^2$ and the structure factor does $S_+(k) \propto k$, the excitation is proportional to $k$. The other is $\omega_-(k)$ at $M$ point where
$S_- (k)$ diverges due to the antiferromagnetic long-range order. Thus, the gap opens when the structure factor becomes proportional to the square of $k$ for the former point and when the structure factor does not diverge, that is, the system becomes the disordered state for the latter point. In the former case, we should determine the critical coupling, $\alpha_{c2}$, where the gap opens. We take five $k_x$ points and do the following fitting along the $\Gamma - X$ line; $S_+(k_x) = a_1 k_x + a_2 k_x^2 + a_3 k_x^3$, where $a_1, a_2$, and $a_3$ are fitting parameters. The result of $a_1$ versus $\alpha$ is shown in Fig. 7 (open squares). Comparing the result of staggered magnetization with this coefficient, we find that the critical point $\alpha_{c2}$ is equal to the $\alpha_c$ within the statistical and fitting errors, which gives $\alpha_c = 3.51 \pm 0.05$. The $\alpha$ dependence of the gap is shown in Fig. 10. All values are scaled by $J_\parallel$. Open circles are for $\omega_+(0,0)$ and closed circles are for $\omega_-(\pi,\pi)$. In the disordered phase, excitation energy $\omega_-(\pi,\pi)$ always takes smaller value. Spin wave velocity along the $\Gamma - X$ line is calculated for the ordered state and the result is shown in the inset of Fig. 10. Here, $Z_c$ is the renormalization factor. Namely spin wave velocity is given by $\sqrt{2Z_cJ_\parallel}$. As the coupling increases, the velocity first slightly decreases and then suddenly increases near the critical point.

VI. DISCUSSIONS

In this paper we first solved the Hamiltonian by the Schwinger-boson mean-field theory. Then the solution is Gutzwiller projected to obtain variational ground state wave functions, which are examined by the Monte Carlo simulation for finite sizes.

We first see the advantage of our variational Monte Carlo simulation. In the mean-field calculation, the system becomes dimerized for $\alpha > 4.62$. For this region, interlayer order parameter, $\Delta_\parallel$, is zero and only dimer coupling between the layers is permitted. In addition, excitation spectrum becomes flat in momentum space; $E_g(k) = \sqrt{\lambda^2 - \delta^2}$. As a matter of fact, theoretically, this state must be only realized at $\alpha \to \infty$. This disadvantage is removed in Monte Carlo simulation. It is estimated from Fig. 4 that the virtual critical point where the system stabilizes with the dimerized state is 11.0. This means that the Gutzwiller projection
improves the wave functions. The improved wave function can describe the disordered state without dimerization at least up to $\alpha = 11.0$.

There have been many investigations for the order-disorder critical point. Our mean-field result is essentially same as the previous report and the modified spin wave theory. These give the critical value of $\alpha$ around 4.5. This value is much larger than the results by the other methods: 2.56 by the dimer expansion, and $2.51 \pm 0.01$ by the quantum Monte Carlo method. However, these latter values are still formidable larger than the value of $\alpha$ realized in the bi-layer cuprates. Our motivation for this work was to see if our method gives the critical value closer to the experimental value or not. Our result, $\alpha_c = 3.51 \pm 0.05$, is not for this expectation, and confirms the previous theories that without doping bi-layer Heisenberg model will not give an explanation for the spin gap behavior of the experiments.

We also calculated the excitation spectrum, especially for the disordered phase. It is not obvious whether the system has always a finite gap in disordered state. For instance, there is no long-range order for the one-dimensional $s = 1/2$ antiferromagnetic Heisenberg model, though the excitation spectrum is gapless. In our bi-layer two-dimensional Heisenberg model, we find that there is always a finite gap for the disordered state. Within the statistical and fitting errors, it occurs at $\alpha_c = 3.51 \pm 0.05$. In disordered region, the spin-spin correlation decays as the distance exponentially. The structure factor, $S_\perp(k)$, near the critical coupling, however, has a large maximal value at $M$ point, which makes the excitation spectrum be minimized at that point. This shows that even in the disordered state the antiferromagnetic spin fluctuation is strong. It should be remarked that even though the spectrum $\omega_\perp(k)$ at $\alpha = 3.6$ looks singular at $Q = (\pi, \pi)$, this is not the case. Around $Q$ it should be quadratic in $(k - Q)$. Such a behavior is not apparent in Fig. 9(b) due to the lack of data close enough to $Q$.

At $\alpha = 0$ where the model becomes the single layer Heisenberg model, our result can be compared with other methods: spin wave theory, series expansions and single mode approximation. Our result of the spectrum is roughly proportional to those of other methods over the entire Brillouin zone. The maximal value is around $2.65J_\parallel$ at $X$ or $L =$
$$(\pi/2, \pi/2)$$ point. Series expansions predicted the maximum is about $2.35J_\parallel$ at $L$ point$^{28}$ and single mode approximation based on the expansions around the Ising limit estimated the maximum about $2.5J_\parallel$ at $L$ point.$^{29}$ Both results are close to our result. The most remarkable difference from the other methods is the spin wave velocity. The renormalization factor, $Z_c$, is $1.99 \pm 0.03$ at $\alpha = 0$ which is 1.69 times larger than the best estimated value around $1.18\pm0.02$. This difference indicates that multi-magnon contribution to $S_+(k)$ is not negligible. However, since this method gives qualitatively correct behavior, we believe it gives qualitatively correct spectrum at $\alpha > 0$ also. Finally we remark that the non-monotonous behavior of spin wave velocity with increasing interlayer coupling can be understood from that of the coefficient($a_1$) of the structure factor shown in Fig. 7, since the spin wave velocity is inversely proportional to $a_1$.

In conclusion, we have investigated the bi-layer Heisenberg model using the Schwinger-boson Gutzwiller-projection method. We find that there is an order-disorder transition with increasing interlayer coupling. The critical point is $\alpha_c = 3.51 \pm 0.05$. Excitation spectrum can be calculated for wide range of coupling and we find that the spin excitation has always a finite gap for disordered phase and the minimum of the spectrum is located at $M$ point. Our model corresponds to the half-filled case for high-$T_c$ cuprates. Although $\alpha_c$ in this case is quite large, it is possible that hole doping reduces the value extremely. Then it will be possible that our disordered state continuously changes into the spin gap state. The similar treatment for a hole doped model, $t - t' - J$ model, is our next problem.

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REFERENCES

1 M. Takigawa, A. P. Reyes, P. C. Hammel, J. D. Thompson, R. H. Heffner, Z. Fisk, and K. C. Ott, Phys. Rev. B 42, 243 (1991).

2 J. M. Tranquada, P. M. Gehring, G. Shirane, S. Shamoto, and M. Sato, Phys. Rev. B 46, 5561 (1992).

3 K. Yamada, Y. Endoh, C. H. Lee, S. Wakimoto, M. Arai, K. Ubukata, M. Fujita, S. Hosoya, and S. M. Bennington, J. Phys. Soc. Jpn. (to be published).

4 B. L. Altshuler and L. B. Ioffe, Solid State Communications 82, 253 (1992).

5 B. L. Altshuler, L. B. Ioffe, A. I. Larkin, and A. J. Millis, JETP Lett. 59, 65 (1994).

6 M. Ubbens and P. A. Lee, Phys. Rev. B 50, 438 (1994).

7 A. J. Millis and H. Monien, Phys. Rev. Lett. 70, 2810 (1993).

8 A. Sokol and D. Pines, Phys. Rev. Lett. 71, 2813 (1993).

9 T. Matsuda and K. Hida, J. Phys. Soc. Jpn. 59, 2223 (1990).

10 K. Hida, J. Phys. Soc. Jpn. 59, 2230 (1990).

11 A. W. Sandvik and D. J. Scalapino, Phys. Rev. Lett. 72, 2777 (1994).

12 K. Hida, J. Phys. Soc. Jpn. 61, 1013 (1992).

13 P. W. Anderson, Mater. Res. Bull 8, 153 (1973).

14 P. W. Anderson, Science 235, 1196 (1987).

15 S. Liang, B. Douçot, and P. W. Anderson, Phys. Rev. Lett. 61, 365 (1988).

16 Y. C. Chen, K. Xiu, Phys. Lett. A 181, 373 (1993).

17 T. Miyazaki, D. Yoshioka, and M. Ogata, Phys. Rev. B 51, 2966 (1995).

18 H. A. Bethe, Z. Phys. 71, 205 (1931).
Schwinger boson mean-field theory and the modified spin wave theory are essentially the same. In the present system, the latter has given the smaller critical value because the possibility of the first order phase transition is considered.

In term of $\alpha_p$ this transition occurs at $\alpha_p = 2.57 \pm 0.02$.

R. R. P. Singh and A. Watabe, Phys. Rev. B 43, 13456 (1991); 44, 5057 (1991).

R. R. P. Singh and M. P. Gelfand, preprint.

R. R. P. Singh, Phys. Rev. B 47, 12337 (1993).

E. Manousakis, Rev. Mod. Phys. 63, 1 (1991).
FIGURE CAPTIONS

FIG. 1. Mean-field values of order parameters $\Delta_\parallel, \Delta_\perp$, Bose-condensate $n_B$ and energy gap $E_g$ as a function of $\alpha$.

FIG. 2. The nearest neighbor spin correlation for each direction is shown. Open circles are for $\epsilon_\parallel$, and solid circles are for $\epsilon_\perp$. Error bars result from Monte Carlo statistical errors.

FIG. 3. The variational parameter $\alpha_p$ which minimizes the ground state energy for a given parameter $\alpha$.

FIG. 4. Total energy per site as a function of $\alpha$. Open circles are for variational Monte Carlo results and straight line is for dimerized state, $-0.375\alpha$.

FIG. 5. Spin-spin correlation for $\alpha = 0.4$(open circles) and $\alpha = 4.6$(solid circles). Each calculation is done for $24 \times 24 \times 2$ lattice. Here, $r_{i,j}$ means the distance between two sites. It is obvious that there is a long-range order for $\alpha = 0.4$ but no long-range order for $\alpha = 3.6$.

FIG. 6. $M_0(L)$ versus $1/L$ for $\alpha = 0.0, 0.8, 1.7, 3.1, \text{and} 4.6$.

FIG. 7. Staggered magnetization as a function of $\alpha$. Open circles are for the mean-field theory, and solid circles are for variational Monte Carlo results. The magnitude of the $k$-linear term in the expansion of $S_+(k)$ around the $\Gamma$ point, $a_1$, is also shown by open squares.

FIG. 8. The structure factors (a)$S_+(k)$ and (b)$S_-(k)$. Open circles, closed circles, and open squares are for $\alpha = 0.4, 2.4, \text{and} 3.6$, respectively. Inset shows the detailed structure
of $\alpha = 3.6$ along the $\Gamma - X$ line. Note that the value at $M$ point of $S_-(\mathbf{k})$ is too large to be shown in the figure.

FIG. 9. Excitation spectrum (a)$\omega_+(\mathbf{k})$ and (b)$\omega_-(\mathbf{k})$. The same values for $\alpha$ are chosen and indicated by the same symbols as in Fig. 8. At $\alpha = 3.6$, gap opens at $\Gamma$ point for $\omega_+(\mathbf{k})$ and at $M$ point for $\omega_-(\mathbf{k})$.

FIG. 10. The $\alpha$ dependence of the gap for $\omega_+(0, 0)$ and $\omega_-(\pi, \pi)$. In the inset, the renormalization factor of the linear spin wave velocity, $Z_c$, is also shown.