Phase Transitions in Bilayer Heisenberg Model with General Couplings

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The ground state properties and phase diagram of the bilayer square-lattice Heisenberg model are studied in a broad parameter space of intralayer exchange couplings, assuming an antiferromagnetic coupling between constituent layers. In the classical limit, the model exhibits three phases: two of these are ordered phases specified by the ordering wave vectors \((\pi, \pi, \pi)\) and \((0, 0, \pi)\), where the third component of each indicates antiferromagnetic orientation between layers, while another is a canted phase, stabilized by competing interactions. The effects of quantum fluctuations in the model with \(S = 1/2\) have been explored by means of dimer mean-field theory, exact diagonalization of \(2\sqrt{2} \times 2\sqrt{2} \times 2\) clusters, and high-order perturbation expansions about the interlayer dimer limit.

KEYWORDS: bilayer Heisenberg model, dimer mean-field theory, exact diagonalization, series expansion, phase diagram

§1. Introduction

Quantum magnets in two dimensions have been a fascinating topic of numerous studies over the past decade. The interest has primarily focused on the competition between long-range magnetic order and novel disordered phases at \(T = 0\) as a result of enhanced quantum fluctuations. In this paper, we consider a bilayer square-lattice Heisenberg model with general nearest-neighbor exchange couplings in each layer and antiferromagnetic coupling between corresponding sites of each layer, described by the Hamiltonian

\[
H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_{1,i} \cdot \mathbf{S}_{1,j} + J_2 \sum_{\langle i,j \rangle} \mathbf{S}_{2,i} \cdot \mathbf{S}_{2,j} + \sum_i \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i},
\]  

(1.1)

where the interlayer coupling is taken as the unit of energy.

A particular limit of the model in which \(J_1 = J_2 = J > 0\) has attracted special attention for several reasons. Several cuprate superconductors contain \(\text{CuO}_2\) bilayers, so that model may be relevant to their magnetic properties — and it is certainly an appropriate model for the

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magnetic properties of their parent compounds. Its phase diagram has been studied numerically by quantum Monte Carlo and perturbation expansions about $J = 0$, and analytically using linear spin-wave theory, Schwinger boson mean-field theory, and an alternative bosonic mean-field calculation. This one-parameter subspace of the Hamiltonian (1.1) has two well known limits. For $J \gg 1$, the model describes a pair of two-dimensional Heisenberg antiferromagnets, weakly interacting with each other. In the isolation limit, each would be in the ordered state at $T = 0$ and would possess Goldstone modes related to spontaneous breakdown of spin-rotational symmetry. Upon weak coupling, their sublattice magnetizations are phase-locked and half of the Goldstone modes acquire gaps. For $J \ll 1$, the ground state is very close to the “dimer” state, the product of spin singlets composed of adjacent interlayer pairs of spins. This state has a gap of order unity. Thus the system has a singlet ground state both for $J \gg 1$ and $J \ll 1$, and one can anticipate that there should be a critical value $J_c$ of the intralayer coupling at which a continuous transition between the two phases is expected; furthermore, we can anticipate that this transition belongs to the universality class of the classical $d = 3$ Heisenberg model.

We were led to consider the more general Hamiltonian (1.1) on the following grounds. First of all, for $J_2 = 0$ the model is related to the “Kondo necklace” model introduced by Doniach as a simple model to describe the competition between the intra-atomic Kondo coupling (favoring local singlet states) and the inter-atomic RKKY interaction (favoring magnetic order and local high-spin states) in heavy fermion systems. The model for $J_2 = 0$ may also be viewed as the symmetric Hubbard-Kondo lattice model in the limit of strong on-site repulsion $U$ between conduction electrons. In the conventional symmetric Kondo lattice model ($U = 0$) on the square lattice with Kondo coupling $J_K$, it is known that a transition from spin-liquid to antiferromagnetic phase takes place when the transfer energy $t$ is increased beyond $t_c \approx 0.7J_K$. Our calculation in §3.2 (the case $\theta = 0$) indicates that there is such a transition at $t_c \approx 0.42\sqrt{UJ_K}$ (for $U \gg J_K$): The antiferromagnetic order is suppressed by the strong on-site repulsion. This result is consistent with a finding by Shibata et al. for the one-dimensional symmetric Hubbard-Kondo lattice model, that the spin gap and inverse spin-spin correlation length are increasing functions of $U$. For $J_2 \neq 0$, our results describe the effects of direct interactions between localized spins on the stability of the Kondo-singlet phase, which is neglected in the most analyses. As would be naively expected, the antiferromagnetic direct interactions are shown to favor the long-range ordered phase over Kondo singlets, while the opposite is true for (weak) ferromagnetic direct interactions.

When $J_1$ and $J_2$ have opposite signs, the model is uniformly frustrated: The product of couplings around any four-spin plaquette that encompasses both layers is negative. Uniform frustration has been shown to lead to exotic magnetic behavior in many cases, both for theoretical models and real materials. Therefore it would be of great interest to see what are expected in the present...
relatively simple model. We find no evidence for any exotic magnetic singlet phases, such as a spontaneously dimerized or plaquettized phase.

We have carried out several types of analyses in order to identify the phases and phase transitions exhibited by the Hamiltonian (1.1). The classical ground state phase diagram is first considered (in §2). Then quantum effects for $S = 1/2$ spins are included, and it is clearly shown that a spin-disordered phase (the aforementioned dimer phase) appears in the vicinity of $J_1 = J_2 = 0$. We examine the instabilities of this phase by means of mean-field theory, small-system exact diagonalization (in §3.1), and higher-order perturbation expansions for susceptibilities and excitation spectra (in §3.2). The last technique also allows us to determine the spin-wave velocity in the magnetically ordered states in the vicinity of the phase boundary. The last section (§4) is devoted to summary and discussion. In particular, Sachdev and Senthil recently considered a quantum rotor model which is closely related to the model (1.1), and in §4 we will compare their results with ours.

§2. The classical limit

For our purpose in the following, it is instructive to consider the ground state phase diagram in the classical limit, where the operators $S$ in the Hamiltonian (1.1) are replaced by classical vectors. By noting that the interchange $J_1 \leftrightarrow J_2$ simply corresponds to relabeling the layers, we only need to consider the half space $J_1 \geq J_2$ of the $J_1$-$J_2$ plane.

One can easily determine the ground states in the part of parameter space where the two intralayer couplings have the same sign. When $J_1$ and $J_2$ are both positive the ground state is composed of a pair of Néel ordered layers with an ordering wave vector $(\pi, \pi; \pi)$, where the third component indicates the antiferromagnetic orientation between layers. When $J_1$ and $J_2$ are both negative the ground state is composed of two ferromagnetically (but oppositely) ordered layers with an ordering wave vector $(0, 0; \pi)$. In each case, both intra- and interlayer energies of the system can be minimized simultaneously.

The $(\pi, \pi; \pi)$ phase and $(0, 0; \pi)$ phase both extend into the quadrant $J_1 > 0 > J_2$, bordered on a phase which will be referred to as the weakly ferromagnetic phase (WF). This phase is composed of a canted Néel-ordered and a canted ferromagnetic layers, as is shown in Fig. 1. The direction of the staggered moment in the antiferromagnetically coupled layer is perpendicular to the uniform moment on the ferromagnetic layer. The canting angles $\psi$ and $\phi$ in the layers satisfy

$$\sin \psi = \xi_2 \sqrt{(1 - \xi_1^2)/(1 - (\xi_1 \xi_2)^2)}$$  \hspace{1cm} (2.1)

and

$$\sin \phi = \xi_1 \sqrt{(1 - \xi_2^2)/(1 - (\xi_1 \xi_2)^2)}$$  \hspace{1cm} (2.2)

with $\xi_i$ defined by

$$\xi_i = 4J_i \left(-1 + \sqrt{1 + 1/(16J_1J_2)}\right).$$  \hspace{1cm} (2.3)
When $J_1$ and $J_2$ are large, the canting angles behave like $\psi \approx 1/(8J_1)$ and $\phi \approx 1/(8J_2)$.

The boundary between the $(0, 0; \pi)$ phase and the WF phase is the line $1/J_1 + 1/J_2 = 8$, while the boundary between the $(\pi, \pi; \pi)$ phase and the WF phase is the line $1/J_1 + 1/J_2 = -8$. In both cases the phase transition is continuous. The classical phase diagram is plotted in Fig. 2.

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**Fig. 1.** Canting angles $\psi$, $\phi$ in the antiferromagnetic (AF) and ferromagnetic (F) layers respectively.

**Fig. 2.** Phase diagram in the classical spin limit ($S \to \infty$).
§3. Phase diagram for the quantum model

3.1 Simple considerations

There is at least one region in parameter space where the classical phase diagram, Fig. 2, should be modified for the quantum spin model with $S = 1/2$. When $J_1$ and $J_2$ are both small, the ground state is approximately a product of interlayer-dimer singlets and does not exhibit long-range order in its spin-spin correlation function. Since there is an energy gap of 1 (the interlayer coupling) for $J_1 = J_2 = 0$, we can expect that the “dimer” phase is stable in a region enclosing the origin with diameter of order unity. Let us try to make this statement more precise, by means of relatively simple calculations.

An estimate of the boundaries between the dimer phase and long-range ordered phases $[(\pi, \pi; \pi), (0, 0; \pi), \text{WF}]$ can be obtained from dimer mean-field theory. One considers the following two-site Hamiltonian

$$S_1 \cdot S_2 - h_1 S_1^z - h_2 S_2^z - g_1 S_1^x - g_2 S_2^x$$

and imposes the self-consistency conditions

$$h_1 = 4J_1 \langle S_1^z \rangle \quad h_2 = 4J_2 \langle S_2^z \rangle \quad g_1 = g_2 = 0$$

for the $(\pi, \pi; \pi)$ phase, or

$$h_1 = -4J_1 \langle S_1^z \rangle \quad h_2 = -4J_2 \langle S_2^z \rangle \quad g_1 = g_2 = 0$$

for the $(0, 0; \pi)$ phase, or

$$h_1 = 4J_1 \langle S_1^z \rangle \quad h_2 = 4J_2 \langle S_2^z \rangle \quad g_1 = -4J_1 \langle S_1^x \rangle \quad g_2 = -4J_2 \langle S_2^x \rangle$$

for the WF phase. In the above self-consistency conditions, the angular brackets denote ground-state averages.

As usual in mean-field theory, one finds that $h_1 = h_2 = g_1 = g_2 = 0$ is the only solution, and hence the dimer phase is stable, for a small interdimer couplings. It is straightforwardly shown that the dimer phase is unstable against the $(\pi, \pi; \pi)$ phase for $J_1 + J_2 > 1/2$, and the $(0, 0; \pi)$ phase for $J_1 + J_2 < -1/2$; in both cases the transitions are continuous. Much more effort is needed to determine the boundary of the WF phase, and we have not been able to derive any analytical results. Instead, we have carried out numerical calculation, solving the mean-field equations iteratively (starting with a set of prescribed magnetizations to calculate the fields and solving the two-site Hamiltonian for the magnetizations, repeating these process until convergent results are obtained). The resulting phase boundaries are shown in Fig. 3. An unphysical feature of our results is that the ground-state energy exhibits a discontinuous decrease on entering the WF phase. This might be due to the WF solutions which are not stable under iteration, so that we have underestimated the domain of stability of the WF phase.
We have also considered another type of mean-field calculation, which was applied to the special case $J_1 = J_2$ by Chubukov and Morr\(^8\). Their calculation can be readily generalized. Let us omit all details, which are clearly described in their paper, and just describe the results. By rewriting the Hamiltonian in terms of three types of bosonic operators, corresponding to the three triplet excited states of an $S = 1/2$ dimer, and keeping only the quadratic terms, one ends up with a three-fold degenerate excitation spectrum of the form

$$\epsilon(q) = \sqrt{1 + (J_1 + J_2)(\cos q_x + \cos q_y)}.$$  \hspace{1cm} (3.5)

(The in-plane lattice spacing is taken as the unit of length.) At small intralayer couplings the spectrum has a gap, characteristic of the dimer phase. When $|J_1 + J_2|$ is increased beyond 1/2, some of the excitation energies pass through zero onto the imaginary axis, signaling an instability of the dimer phase. This analysis agrees completely with the dimer mean-field calculations for the transitions to the $(0,0;\pi)$ and $(\pi,\pi;\pi)$ phases, as described above. It also yields the result that the spin-wave velocity on both of those phase boundaries is given simply by $c = 1/2$. However, this analysis does not appear capable of describing the transition to the WF phase.

\[Fig. 3.\] Phase diagram for $S = 1/2$ spins from dimer mean-field theory.

Finally, we have carried out finite-size exact diagonalization studies on $2 \times 2 \times 2$ and $2\sqrt{2} \times 2\sqrt{2} \times 2$ systems with periodic boundary conditions.\(^9\) In Fig. 4 the low-lying energy levels are plotted as functions of $J \equiv |J_1| = |J_2|$ for the three distinct choices of the signs of couplings. One finds that when the intralayer couplings have the same sign the ground state is always a singlet and when the couplings have opposite signs there are level crossings to high-spin states as the magnitude of the couplings increases. The latter is associated with the transition from the dimer phase to the WF
phase; in the WF phase the ground state has a net moment and therefore must have nonzero spin. We will have more to say about the finite size calculations in the following subsection.

3.2 Series expansions and extrapolations

In order to obtain more quantitative estimates of the domain of stability of dimer phase and the spin-wave velocity in the magnetically ordered phases adjacent to those phase boundaries, we have carried out perturbation expansions in powers of the intralayer couplings about the pure interlayer dimer Hamiltonian.

For convenience, the intralayer couplings are parametrized by

\[ J_1 = \lambda \cos \theta \quad J_2 = \lambda \sin \theta. \] (3.6)
Expansions in $\lambda$ can then be carried out at fixed $\theta$, rather than carrying out a double expansion in powers of $J_1$ and $J_2$ simultaneously. Note that only expansion for $\theta$ in the range $-\pi/4$ to $\pi/4$ is needed, since negative values of $\lambda$ correspond to $\theta$ in the range $3\pi/4$ to $5\pi/4$, which then maps to $-\pi/4$ to $-3\pi/4$ under the interchange $J_1 \leftrightarrow J_2$. In this way full $2\pi$ coverage is obtained by carrying out calculations only for a quarter of the circle, which were done at intervals of $\pi/16$.

Series expansions for several susceptibilities $\chi(q)$ at $T = 0$ and the Fourier transform of the triplet elementary excitation spectrum $\epsilon(q)$ were performed up to the order $\lambda^8$ using connected cluster methods.\textsuperscript{19, 4}

The values of $\lambda$ corresponding to continuous transitions out of the dimer phase can be accurately estimated by constructing differential approximants\textsuperscript{20} to the susceptibility and the gap series associated with the ordering wave vector. The leading critical behavior of these quantities is described by $\chi \sim (\lambda_c - \lambda)^{-\gamma}$ and $\epsilon \sim (\lambda_c - \lambda)^{\nu}$. The dimer-$\pi, \pi; \pi$ and dimer-$0, 0; \pi$ transitions should lie in the universality class of the $d = 3$ classical Heisenberg model, and we can expect $\gamma \approx 1.4$ and $\nu \approx 0.71$. Along those critical lines, if the dimer-WF transition is continuous, the naive hypothesis is that it would lie in the $d = 3$ classical $SO(3)$ class, as has shown to be the case for canted magnets by Kawamura\textsuperscript{22} for which $\gamma \approx 1.1$ and $\nu \approx 0.53$. On the other hand, if the dimer-WF transition is of the first-order, one would expect the linearly vanishing gap, since the transition would be a result of a level crossing to a state of different symmetry. The value of $\lambda$ at which the gap vanishes would be regarded as an upper bound on the actual phase boundary, since the excitations might have attractive interactions (and as we will see below, this is the case in the relevant parameter regime).

In order to organize the following discussion, it is useful to divide the parameter space into three regions: region I, with $0 \leq \theta \leq \pi/4$; region II, with $-3\pi/4 \leq \theta \leq -\pi/2$, and region III, with $-\pi/2 < \theta < 0$.

In region I, the dimer phase is adjacent to the $(\pi, \pi; \pi)$ phase, and a continuous transition between these phases is expected as in the conventional bilayer Heisenberg antiferromagnet ($\theta = \pi/4$). Shown in Fig. 5 is the phase diagram based on biased differential approximants to the expansion series $\chi(\pi, \pi; \pi)$ and $\epsilon(\pi, \pi)$.

Note that without biasing, the critical exponents derived from approximants show good agreement with the anticipated values, but the biasing allows for more precise estimates of critical couplings than would be possible otherwise. The uncertainties in the critical value for $\lambda$ estimates are approximately 0.002.

In region II, there is a continuous transition from the dimer phase to the $(0, 0; \pi)$ phase, and again the critical exponents $\gamma$ and $\nu$ agree well with the anticipated values. Critical points derived from biased differential approximants are shown in Fig. 5.

It is to be noted that the inequality $|J_1 + J_2| > 1/2$ along these two lines of continuous transitions
is held, indicating that the mean-field theory underestimates the domain of stability of the dimer phase. This is entirely plausible, since mean-field theory neglects the effects of quantum fluctuations, which stabilize the dimer phase. Furthermore we note that these two lines are not mirror images of one another. The dimer-(π,π;π) line is slightly but noticeably curved. The curvature suggests that quantum fluctuations suppress Néel order more strongly when the coupling between dimers is evenly distributed between the layers than when the coupling is concentrated in one layer. On the other hand, the critical dimer-(0,0;π) line is almost as straight as is the case in dimer mean-field theory. We have not an clear explanation for it, but it is worth noting another point which shows that the (π,π;π) and (0,0;π) phases are affected differently by the quantum fluctuations: Within linear spin-wave theory, the spin-wave velocity is given by \(\frac{(J_1 + J_2)}{4} + 2J_1J_2\) in the former and \(-\frac{(J_1 + J_2)}{2}\) in the latter.

In region III, the situation is more complicated than in the preceding two. Based on the classical phase diagram and dimer mean-field theory, one expects that the dimer-(π,π;π) and dimer-(0,0;π) critical lines would extend somewhat into this region, and this is in fact observed. On increasing

Fig. 5. Phase diagram for \(S = 1/2\) spins based primarily on series expansions. Solid lines represent precise estimates of continuous transitions; the dashed lines are more uncertain estimates of transitions, whose characters are discussed in the text. The dot-dashed lines are based on finite-size calculations.
λ, a dimer-(π, π; π) transition takes place at \( \theta = -\pi/16 \), and likewise a dimer-(0, 0; π) transition occurs for \( \theta = -7\pi/16 \): the relevant gaps vanish and susceptibilities diverge at the same value of \( \lambda \) with the expected exponents.

However, for most values of \( \theta \) one would anticipate encountering dimer-WF phase transitions. In fact there is an evidence for such transitions from unbiased approximants to the series, but the detailed features are rather complicated, in that neither the first-order nor continuous phase transition scenario receives complete support. Along the dashed line in Fig. 5, one finds that \( \epsilon(\pi, \pi) \) vanishes with exponents close to 1/2. The staggered susceptibility diverges with exponents in the range 0.8–1.0. So far, this is consistent with the continuous transition scenario. However, the critical values of \( \lambda \) for the susceptibility are typically 20% larger than those for the gap, and the “error bars” (deduced from the consistency of the unbiased approximants) of two sets of critical points do not overlap with each other. Since the exponents of susceptibility are generally smaller than theoretically anticipated, one might hope that a biased analysis of the susceptibility would bring the two sets of estimated critical points into agreement. Unfortunately, this is not the case and biasing actually drives them farther apart. Consequently, we cannot rule out the possibility that the dimer-WF transition involves a vanishing gap but finite susceptibility, that is, a first-order transition.

![Fig. 6. A map of the total spin of ground state of 2√2×2√2×2 clusters in the J1-J2 plane.](image)

As for the phase boundaries between the WF and magnetically ordered phases, the series expansions provide no information. The mean-field and classical calculations suggest that they lie nearly parallel to the \( J_1 \) and \( J_2 \) axes. In order to obtain a crude estimates of those phase boundaries, we
have constructed a map of the total spin of ground state of $2\sqrt{2} \times 2\sqrt{2} \times 2$ clusters in the $J_1$-$J_2$ plane, determined by exact diagonalization, see Fig. 6. The region where the ground state has nonzero spin is presumed to lie in the WF phase. The dimer-WF boundary estimated in this way is consistent with that derived from the series analysis. Therefore we expect that the boundaries between the WF and magnetically ordered phases (shown by the dot-dashed lines in Fig. 5) are reasonably accurate.

At this point let us consider the properties of the excited states of the $2\sqrt{2} \times 2\sqrt{2} \times 2$ clusters in more detail. We find that in the vicinity of the singlet-singlet (dimer-to-antiferromagnetically ordered) phase transitions the lowest excitation energy in the $S = 2$ sector is twice greater than that in the $S = 1$ sector, while in the vicinity of the dimer-WF phase boundary the reverse is true: see Fig. 7.

Fig. 7. Excitation gaps ($\Delta = E_{\text{min}}(S) - E_{\text{min}}(S = 0)$) scaled by $S$ or $S(S + 1)$ in $2\sqrt{2} \times 2\sqrt{2} \times 2$ clusters as functions of $\lambda$: (a) $\theta = \pi/4$, (b) $\theta = -\pi/4$.

Thus the triplet excitations are repulsive in the former cases and attractive in the latter, as anticipated. We have also examined how the lowest excitation energies in each spin sector vary with $S$ in each of the singlet ground states. In the spin-disordered dimer phase those energies are roughly proportional to $S$, while in the ordered phases they are nearly proportional to $S(S + 1)$. Both results are readily understood. In the dimer phase the lowest spin-$S$ state is essentially composed of $S$ triplet excitations. In the magnetically ordered phases the situation is rather different. In the bulk, arbitrarily low-energy excitations of any size of spins are possible, but for large but finite clusters the excitations amount to finite angular momentum states of the staggered moment (for which the corresponding moment of inertia is the uniform susceptibility) which accounts for the $S(S + 1)$ scaling. The crossover between the two different behaviors is impossible to pin down.
the critical points precisely in a system as small as the one we have considered, but the critical points obtained from the series analysis are clearly in the range where the crossover is taking place, see Fig. 7 (a).

Finally let us present further results obtained from the series expansions regarding properties along the boundary of the dimer phase. The spin-wave velocity on the dimer-$(\pi, \pi; \pi)$ and dimer-$(0, 0; \pi)$ critical lines was determined using the method described in Ref. 4). In Fig. 8, we show how the quantum renormalization factor of the critical spin-wave velocity defined by

$$Z_c(\theta) = c / c_{LSWT}$$

depends on $\theta$, where $c_{LSWT}$ is the spin-wave velocity within linear spin-wave theory whose value was given earlier. To a good approximation we find that $Z_c(\theta)$ is independent of $\theta$ along the dimer-$(0, 0; \pi)$ boundary. This seems to be consistent with the fact that the phase boundary itself can be well described by $J_1 + J_2 = \text{const.}$

Fig. 8. Quantum renormalization factor of the critical spin-wave velocity $Z_c(\theta)$ along continuous transition boundaries as a function of $\theta$.

One can also extrapolate the excitation spectra for values of $q$ far from the characteristic momenta $(0, 0)$ or $(\pi, \pi)$, where one expects direct Padé approximants to provide accurate estimates. Estimates of the dispersion relations along selected lines in the Brillouin zone are presented for several $\theta$ values in Fig. 9.
§4. Summary and Discussion

We have investigated the ground state properties and phase diagram of bilayer Heisenberg model on the square-lattice with general nearest-neighbor intralayer couplings. The ground state phase diagram of the model has been first examined in the classical limit in order to get an insight to its asymptotic behaviors. Then the effects of quantum fluctuations are studied on the basis of several methods; dimer mean-field theory, small cluster diagonalization, and high-order perturbation theory about the interlayer dimer limit. We have found four phases for the model with $S = 1/2$: one “spin liquid” (dimer) phase which is the analytic continuation of the interlayer dimer Hamiltonian, two antiferromagnetically ordered $[(π, π; π)$ and $(0, 0; π)]$ phases, and one phase with weak magnetization stabilized by competing interactions between layers (WF). The transitions between the dimer phase and the antiferromagnetically ordered phases are continuous (and belong to the classical $d = 3$ Heisenberg model universality class), while the character of the dimer-WF transitions could not be reliably determined. Concerning the dimer-$π; π)$ and dimer-$0, 0; π)$ transitions, it appears that quantum fluctuations play a more important role in the former, and lead to a rather intriguing result that Néel order is suppressed more strongly when the intralayer couplings are evenly distributed between the layers than when they are concentrated in one layer.

The case $(θ = 0)$ is especially interesting. In this case, the spins are antiferromagnetically coupled in one of layers and not coupled at all in the other. This model corresponds to symmetric Hubbard-Kondo square-lattice model in the large-$U$ limit. Provided $t \to \infty$ and $U \to \infty$ with
4t^2/U = J_s = constant (the intralayer coupling) and the on-site Kondo coupling (the interlayer coupling) is \( J_K \), we have found that there is a transition to a magnetically ordered state when \( J_s \) is increased up to approximately 0.71\( J_K \). This leads to the result for the critical \( t \) mentioned in the Introduction.

The one-dimensional version of the Hamiltonian (1.1), with general intrachain couplings, has been attracting interest recently in connection with the spin-ladder materials\(^{24}\). In particular, Tsukano and Takahashi\(^ {25} \) studied the one-dimensional model with \( J_2 = -J_1 (\theta = -\pi/4) \) and found a continuous transition between the dimer phase and a magnetically ordered phase, supporting continuous transition scenario of the dimer-WF transition.

Finally, Sachdev and Senthil\(^ {17} \) have studied a rather general quantum rotor model for which, in the large-\( S \) limit, there is a direct mapping to the model (1.1). It is interesting to see which features of their model persist for \( S = 1/2 \), and which do not. The mean-field analysis of the rotor model finds a “gapped quantum paramagnet,” equivalent to the dimer phase in the spin model, a Néel phase, a “quantized ferromagnet” phase, and a canted phase, equivalent to the WF phase in the spin model. They suggest that, quite generally, continuous phase transitions into the canted phase, where there is nonzero magnetization, are only possible from phases with gapless excitations. Consequently, continuous phase transitions between the dimer phase and the WF phase should not be possible. (In the section of the phase diagram for the rotor model which is presented by Sachdev and Senthil, not even first order transitions between the gapped quantum paramagnet and canted phases are exhibited, but there is no reason to believe that holds for all choices of parameters\(^ {23} \).) Our numerical studies were not able to establish the nature of the dimer-WF transition, and so our results are not in direct disagreement with the general principle espoused by Sachdev and Senthil even though they do not provide any support for it, either. However, there is one significant difference between the phase diagrams of the rotor model and of the spin model. For \( S = 1/2 \), the Hamiltonian (1.1) does not exhibit an analog of the quantized ferromagnet phase. Ferromagnetically coupled bilayers of \( S = 1/2 \) spins could exhibit such a phase, since in the absence of intralayer coupling the interlayer dimers would have angular momentum 1. In contrast to the rotor model, however, it does not appear possible to go to such a phase directly from the dimer phase by varying the intralayer couplings.

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\(^{1}\) A. J. Millis and H. Monien: Phys. Rev. Lett. 70 (1993) 2810; H. Monien and A. W. Sandvik: J. Low. Temp.
Phys. 99 (1995) 343.

2) A. W. Sandvik and D. J. Scalapino: Phys. Rev. Lett. 72 (1994) 2777.
3) K. Hida: J. Phys. Soc. Jpn. 61 (1991) 1013.
4) M. P. Gelfand: Phys. Rev. B 53 (1996) 11309.
5) Z. Wei-hong: Phys. Rev. B 55 (1997) 12267.
6) T. Matsuda and K. Hida: J. Phys. Soc. Jpn. 59 (1990) 2223.
7) K. K. Ng, F. C. Zhang and M. Ma: Phys. Rev. B 53 (1996) 12196.
8) A. V. Chubukov and D. K. Morr: Phys. Rev. B 52 (1995) 3521.
9) S. Chakravarty, B. I. Halperin and D. R. Nelson: Phys. Rev. B 39 (1989) 2344.
10) S. Doniach: Physica B 91 (1977) 231.
11) J. Igarashi, T. Tonegawa, M. Kaburagi and P. Fulde: Phys. Rev. B 51 (1995) 5814.
12) N. Shibata, T. Nishino, K. Ueda and C. Ishii: Phys. Rev. B 53 (1996) R8828.
13) Z. P. Shi, R. R. P. Singh, M. P. Gelfand and Z. Wang, Phys. Rev. B 51 (1995) 15630.
14) However, in recent studies of the Kondo lattice model away from half-filling the direct intersite Heisenberg coupling plays an important role in the analysis; see A. E. Sikkema, I. Affleck and S. R. White: preprint [cond-mat/9702143]
15) C. K. Majumdar and D. K. Ghosh: J. Math. Phys. 10 (1969) 1399.
16) A. P. Ramirez: Annu. Rev. Mater. Sci. 24 (1994) 453.
17) S. Sachdev and T. Senthil: Ann. Phys. 251 (1996) 76.
18) The numerical calculations were done with the use of the program TITPACK Version 2 developed by H. Nishimori at the Tokyo Institute of Technology.
19) M. P. Gelfand, R. R. P. Singh and D. A. Huse: J. Stat. Phys. 59 (1990) 1093.
20) M. E. Fisher and H. Au-Yang: J. Phys. A 12 (1979) 1677; D. L. Hunter and G. A. Baker, Jr.: Phys. Rev. B 19 (1979) 3808. To carry out the calculations we have used the package DA written by Keith Briggs at the University of Adelaide.
21) M. Ferer and A. Hamid-Aidinejad: Phys. Rev. B 34 (1986) 6481; and references cited therein.
22) H. Kawamura: J. Phys. Soc. Jpn. 56 (1987) 474.
23) B. Bernu, C. Lhuillier and L. Pierre: Phys. Rev. Lett. 69 (1992) 2590; A. Parola, S. Sorella and Q. F. Zhong: Phys. Rev. Lett. 71 (1993) 4393.
24) E. Dagotto and T. M. Rice: Science, 271 (1996) 618.
25) M. Tsukano and M. Takahashi: J. Phys. Soc. Jpn. 66 (1997) 1153.
26) S. Sachdev: private communication.
\[
\begin{align*}
1/J_1 + 1/J_2 &= -8 \\
1/J_1 + 1/J_2 &= 8
\end{align*}
\]

\((\&P, \&P; \&P)\)
Dimer

WF

$J_1$

$J_2$

$(0,0;\&P)$

$(\&P,\&P;\&P)$
(c)
