Quantum Phase Transitions in the Triangular-Lattice Bilayer Heisenberg Model

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We study the triangular-lattice bilayer Heisenberg model with antiferromagnetic interplane coupling $J_\perp$ and nearest-neighbor intraplane coupling $J = \lambda J_\perp$ by expansions in λ. For negative λ a phase transition is found to an ordered phase at a $\lambda_c = -0.2636 \pm 0.0001$, which is in the 3D classical Heisenberg universality class. For $\lambda > 0$, we find a transition at a rather large $\lambda_c \approx 1.2$. The universality class of the transition is consistent with that of Kawamura's 3D antiferromagnetic stacked triangular lattice. The spectral weight for the triplet excitations, at the ordering wave vector, remains finite at the transition, suggesting that a phase with free spinons does not exist in this model. [S0031-9007(98)07709-6]

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In recent years much interest has focused on the nature of quantum disordered phases of the Heisenberg antiferromagnets, where the combination of low dimensionality, low spin, and frustration cause the ground state of the system to be disordered [1,2]. The case of one-spatial dimension is relatively well studied and understood. Two dimensional systems have received particularly large attention, due to their relevance to high temperature superconductivity. However, despite much effort, quantum disordered phases are not fully understood in $d = 2$.

A special situation is those types of quantum disordered phases where the ground state is to a good approximation a product of local singlets over even-spin clusters. This can arise due to explicitly dimerized (or clustered) Hamiltonians; a situation that appears to be relevant for the material CaV_4O_9 [3]. Another scenario is the spontaneous breaking of translational symmetry, as found in large-N theories and also suspected in several frustrated models, which leads to dimerization [4–6]. In all these systems, the elementary excitations are triplets with a finite excitation energy.

In contrast to these, a different class of quantum disordered phases would be one where the elementary excitations are free spin-half objects or spinons. Such phases, for $d = 2$, have been predicted in systems where the classical ground state is noncolinear [7] and their properties have been investigated by field-theoretic methods [8]. However, no lattice models are known where such a behavior is realized. One potential candidate system for such a behavior is the Kagome-lattice antiferromagnet, where the ground state is widely believed to be magnetically disordered [9,10].

Here we study the triangular-lattice bilayer Heisenberg model. The model consists of two layers of triangular lattices, one on top of the other, with an intralayer nearest-neighbor Heisenberg coupling J, which could be ferromagnetic or antiferromagnetic, and an antiferromagnetic interlayer nearest-neighbor coupling $J_\perp$, between the spins on top of each other. Varying the ratio $\lambda = J/J_\perp$ allows one to investigate the quantum phase transition between the ordered and disordered phases of the model. The corresponding square-lattice Heisenberg bilayer has been extensively studied by many authors [11]. It was found that with increasing λ the triplet excitations at the ordering wave vector soften and at a critical λ the gap closes and there is a continuous quantum phase transition to a magnetically ordered phase. This transition lies in the universality class of the 3D classical Heisenberg model. Not surprisingly, we obtain similar results for ferromagnetic in-plane couplings in the triangular-lattice bilayer model.

More interesting, however, is the case of antiferromagnetic in-plane couplings. In this case the classical ground state is noncolinear. Thus, it represents a candidate system to look for free spinons, when the ground state is disordered by quantum fluctuations. The bilayer coupling can be viewed as reducing the effective spin of the 2D quantum system, thus leading to a disordered ground state. Furthermore, this system presents a possibility to find novel quantum critical points, different from the universality class of the 3D classical Heisenberg model. It has been shown [7,8] that when there is a transition from a noncolinear classical phase to a phase with unbound spinons, the universality class of the transition is that of the three-dimensional O(4) model. Furthermore, one expects that in this case the triplet excitations would decay into the two-spinon continuum and not remain well defined. The alternative possibility is that such a phase with free spinons does not exist and there is a direct transition from a magnetically ordered phase to one with massive triplet excitations. In this case the quantum phase transition may lie in the universality class of the classical stacked triangular-lattice Heisenberg model, first found by Kawamura [12].

We study the model by a strong coupling expansion in the parameter $\lambda = J/J_\perp$, calculating the ordering susceptibility, the triplet excitation spectrum, and its spectral weight. Our analysis of the susceptibility and the inverse gap series shows evidence for a phase transition at $\lambda_c \approx 1.2$ with exponents $\nu \approx 0.53$ and $\gamma \approx 1.1$. These results are consistent with the universality class discussed by Kawamura [12] for the stacked triangular Heisenberg antiferromagnet and not consistent with the 3D classical O(4) model.

Furthermore, we find that as λ is increased in the model and the minimum of the triplet spectrum becomes more pronounced, the spectral weight of the triplets is reduced over much of the Brillouin zone but it stays finite and grows with λ in the vicinity of the ordering wave vector. This implies that the triplets stay well defined excitations, near the minimum, even at the transition to the ordered phase. Together with the estimates for the critical exponents at the transition, this suggests that free spinons do not exist in this model. The divergence of the magnetic susceptibility and the closing of the triplet gap at the ordering wave vector of the triangular lattice also implies that for $\lambda > \lambda_c$, the system is magnetically ordered. Thus, our results provide further support for the existence of antiferromagnetic order in the single-plane triangular-lattice antiferromagnet [10,13,14].

The triangular-lattice bilayer Heisenberg model is given by the Hamiltonian:

$$\mathcal{H} = J_\perp \sum_i \mathbf{S}_{A,i} \cdot \mathbf{S}_{B,i} + J \sum_{\langle i,j \rangle} [\mathbf{S}_{A,i} \cdot \mathbf{S}_{A,j} + \mathbf{S}_{B,i} \cdot \mathbf{S}_{B,j}], \qquad (1)$$

where A and B refer to the two layers of the triangular lattice and $\langle i,j \rangle$ are nearest neighbors in a given layer of the lattice. The triangular lattice sites are spanned by the two nonorthogonal primitive vectors

$$\mathbf{e_1} = (1,0) \quad \text{and} \quad \mathbf{e_2} = \frac{1}{2}(-1, \sqrt{3}).$$

For $J = 0$, spins are coupled only in pairs and the ground state is a direct product of singlets over these pairs. The excitations are isolated triplets localized at some site i. For finite values of $\lambda = J/J_\perp$ an effective Hamiltonian $\mathcal{H}^{\text{eff}}(\mathbf{R}_{i,j})$ describing the interaction between these localized degenerate triplet states can be derived by a systematic expansion in λ:

$$\mathcal{H}^{\text{eff}}(\mathbf{R}) = \sum_n \lambda^n h_n(\mathbf{R}).$$

The methods for calculating $\mathcal{H}^{\text{eff}}$ in powers of $\lambda = J/J_\perp$ are well developed and discussed in the literature [15]. The excitation spectrum is given by the eigenvalues of the effective Hamiltonian $\mathcal{H}(\mathbf{R})$, where $\mathbf{R}_{i,j} = \mathbf{r}_i - \mathbf{r}_j$ is the vector connecting sites i and j. It can easily be diagonalized by a Fourier transform. We have calculated these quantities complete to 10th order.

TABLE I. Series for the triplet energies $E(\mathbf{q})$.

	$\mathbf{q} = 0$	$\mathbf{q} = \mathbf{Q}_{\text{AF}}$
0	1.0	1.0
1	3.0	−1.5
2	−1.5	1.875
3	−0.75	−1.875
4	−4.125	0.4453125
5	15.632 8125	−1.488 28125
6	−26.944 335 937 5	14.685 058 593 75
7	56.977 294 921 875	−43.228 454 589 843 7
8	−244.898 391 723 633	84.745 834 350 585 9
9	794.878 423 690 796	−241.322 682 380 676
10	−2301.242 520 332 34	911.485 698 580 742

In Table I, the expansion coefficients for $E(\mathbf{q})$ with $\mathbf{q} = 0$ and $\mathbf{Q}_{\text{AF}} = 4\pi/3\ \mathbf{e_1}$ are presented, corresponding to the ordering wave vectors for the ferromagnetic and the antiferromagnetic systems. The expansion coefficients for the magnetic susceptibilities at the same two wave vectors [11,16], calculated to 10th order are given in Table II.

In addition to the wave vector dependent susceptibilities and the excitation spectra, we also calculate series for the spectral weights associated with the excitations. The spectral weights are defined by the delta-function piece of the dynamical correlation function,

$$S(\mathbf{q}, \omega) = A(\mathbf{q})\delta[\epsilon(\mathbf{q}) - \omega] + B(\mathbf{q}, \omega).$$

They are calculated via the spin-spin correlation functions, where the intermediate states are restricted to the elementary triplet excitations [17]. These latter calculations are more difficult and are only done to 6th order.

For ferromagnetic intraplane couplings, the critical point occurs at small values of $\lambda < 0$, so even with relatively short series we can determine the critical point quite well and also get reasonable estimates for the critical exponents. For the susceptibility series, the d-log Pade approximants

TABLE II. Susceptibility series $\chi(\mathbf{q})$.

	$\mathbf{q} = 0$	$\mathbf{q} = \mathbf{Q}_{\text{AF}}$
0	0.250 000 000 000 00	0.250 000 000 000 00
1	−1.500 000 000 000 0	0.750 000 000 000 00
2	7.125 000 000 000 0	0.937 500 000 000 00
3	−30.750 000 000 000	0.609 375 000 000 00
4	128.476 562 501 74	−0.101 562 498 263 4
5	−528.799 479 161 14	1.974 934 901 323 7
6	2148.051 106 780 6	0.240 885 426 764 74
7	−8631.954 499 400 9	−1.081 393 189 130 7
8	34 434.857 183 080	−13.218 768 766 815
9	−136 648.824 764 77	59.415 134 251 052
10	539 861.353 042 63	−93.997 993 646 134

TABLE III. Critical exponents.

Universality class	ν	γ
Ising [18]	0.6300 ± 0.0008	1.2402 ± 0.0009
xy [18]	0.6693 ± 0.0010	1.3160 ± 0.0012
Heisenberg [18]	0.7054 ± 0.0011	1.3866 ± 0.0012
O(4) [20]	0.74	1.47
Chiral [12]	0.55	1.1
This work	$\approx$0.53	$\approx$1.1

lead to estimates

$$\lambda_c = -0.263\,62 \pm 0.000\,09, \qquad \gamma = 1.407 \pm 0.004\,.$$

Here the uncertainties reflect the spread between different Pade estimates. Applying d-log Pade approximants to the inverse of the energy-gap series, one obtains

$$\lambda_c = -0.2641 \pm 0.0005, \qquad \nu = 0.73 \pm 0.01\,.$$

Here, the estimates for the critical points and exponents from individual approximants are correlated and the more negative the critical point estimates, the larger is the exponent. Given the length of our series, these numbers are in quite good agreement with the 3D classical Heisenberg university class, where the best current estimates come from field theory: $\gamma = 1.3866 \pm 0.0012$, $\nu = 0.7054 \pm 0.0011$ [18]. That the series analysis gives slightly higher estimates for the exponents is common to many models and is primarily due to corrections to scaling [19].

We now consider the analysis for $\lambda > 0$, which corresponds to antiferromagnetic intraplane couplings. We analyzed the inverse of the energy gap and the ordering susceptibility series using d-log Pade approximants and differential approximants. In this case, the convergence was much poorer as the critical point occurs at much larger λ_c. The estimates for the critical points and the exponents show tremendous scatter. Assuming that the two series have the same critical point, the most consistent estimate for λ_c is in the range 1.18–1.29. In that range there are four approximants for the susceptibility series, which give (λ_c, γ) values of (1.19,1.10),(1.19,1.08), (1.21,1.06),(1.26,1.32), and four approximants for the inverse gap series, which lead to (λ_c, ν) values of (1.18,0.45),(1.22,0.51),(1.25,0.59),(1.29,0.57). These lead us to conclude that $\lambda_c \approx 1.2$ and that $\nu \approx 0.53$ and $\gamma \approx 1.1$. These exponents are also obtained if the approximants are biased to have the critical point near $\lambda_c = 1.2$. These results are consistent with Kawamura's universality class for the stacked triangular-lattice Heisenberg model, where he found $\nu \approx 0.55$ and $\gamma \approx 1.1$ [12], and not consistent with the O(4) universality class, which has $\nu \approx 0.74$ and $\gamma \approx 1.47$ [20]. The difference between the critical exponents for Kawamura's universality class and those of other 3D classical models is highlighted in Table III. Following Chubukov, Sachdev, and Senthil [7], Kawamura's universality class should arise in this model only if there is a direct transition from the disordered phase without free spinons to the 3-sublattice ordered phase.

Another way to explore the existence of an intermediate phase with free spinons is to study the spectral weights for the triplets and see if it vanishes as λ is increased. When the spinons become the elementary excitations, the triplets can break up into a pair of spinons and thus will not remain sharp excitations. To analyze the series for the triplet spectra, we use Euler transforms and Pade approximants. In Fig. 1, we show the Brillouin zone of the triangular lattice. In Fig. 2, the excitation spectra for $\lambda = 0.2$, 0.4, and 1.0 are shown along selected contours. In Fig. 3, the spectral weights estimated by the [3/3] Pade are shown along the same contours. It is evident from these plots that as λ is increased, the triplet dispersion develops a sharp minimum at the ordering wave vector of the triangular-lattice Heisenberg model. The spectral weight associated with the triplets is rapidly reduced over much of the Brillouin zone, however, in the vicinity of the ordering wave vector, the spectral weights continue

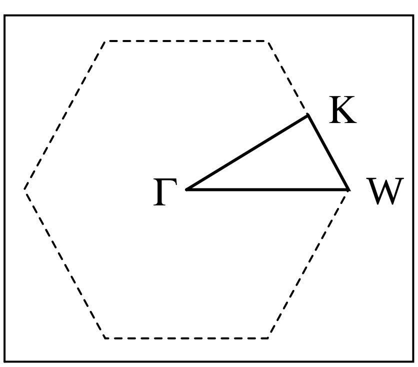

FIG. 1. Brillouin zone of the triangular lattice.

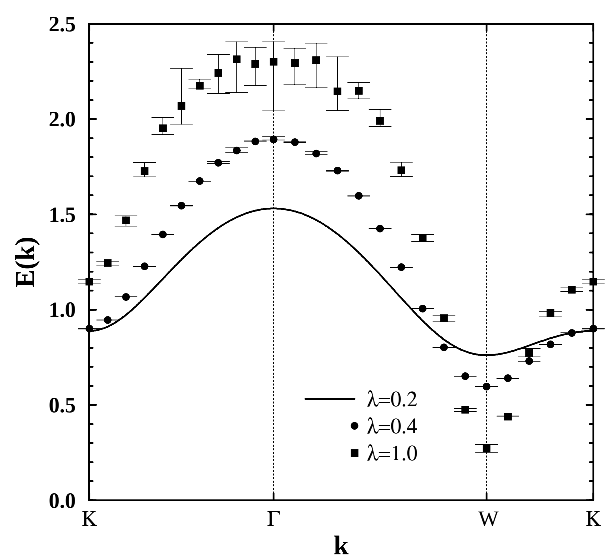

FIG. 2. Dispersion of the triplet excitations.

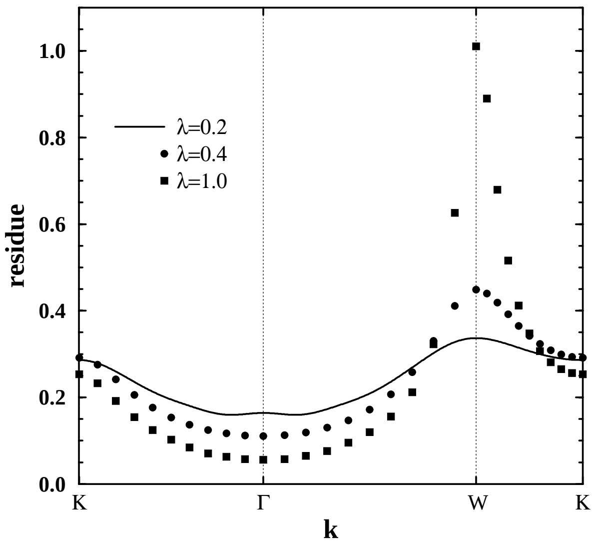

FIG. 3. Spectral weights along selected contours.

to increase with λ, and the triplet excitations remain sharp. This provides further evidence for the absence of an intermediate phase in this model, and a direct transition from the disordered phase with massive triplet excitations to the magnetically ordered phase.

In conclusion, in this paper we have studied the quantum phase transitions in the bilayer triangular-lattice Heisenberg models in a strong coupling expansion. For ferromagnetic intralayer coupling, the transition to the ordered phase is found to be in the 3D classical Heisenberg universality class. The antiferromagnetic intraplane coupling case appears to be quite different. We find evidence that there is a transition to an ordered phase at much larger values of λ and the transition is in the universality class of the stacked triangular lattice. This, together with the result that the triplet spectral weight near the ordering wave vector continues to grow with λ suggests that in this model, a phase with free spinons does not exist and there is a direct transition from the disordered phase with massive triplet excitations to the three-sublattice ordered phase. This study lends further support to the idea that the single-plane spin-half triangular-lattice Heisenberg model is ordered.

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