Quantum phase transitions in the Triangular-lattice Bilayer Heisenberg Model

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(January 2, 2014)

We study the triangular-lattice bilayer Heisenberg model with antiferromagnetic interplane coupling $J_\perp$ and nearest-neighbor intraplane coupling $J = \lambda J_\perp$, which could be ferro- or antiferromagnetic, by expansions in $\lambda$. For negative $\lambda$ 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 wavevector, remains finite at the transition, suggesting that a phase with with free spinons does not exist in this model.

PACS: 75.10.Jm, 75.40.Cx, 75.40.Mg, 75.50.-y, 75.50.Ee

In recent years much interest has focussed 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. A special situation is that 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 are 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$_4$O$_9$. 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. 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 non-collinear and their properties have been investigated by field-theoretic methods. 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.

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 ferro- or antiferromagnetic, and an antiferromagnetic interlayer nearest neighbor coupling $J_\perp$, between the spins on top of each other. This model maybe relevant to bilayer quantum-hall systems and to layers of He$^3$. The corresponding square-lattice Heisenberg bilayer has been extensively studied by many authors. It was found that with increasing $\lambda$ the triplet excitations at the ordering wavevector soften and at a critical $\lambda \approx 0.40$ the gap closes and there is a continuous quantum phase transition to a magnetically ordered phase. It should be mentioned that the same scenario is found for ferromagnetic intralayer coupling $\lambda < 0$ with a critical point at $\lambda_c \approx -0.44$, which, to our knowledge, has not been reported in the literature before.

We study the triangular-bilayer model by a strong coupling expansion in the parameter $\lambda = J/J_\perp$. At $\lambda = 0$, the ground state consists of products of singlets over pairs of spins and the elementary excitations are isolated triplets. We focus on the ordering susceptibility, the triplet excitation spectrum and its spectral weight as a function of $\lambda$. For ferromagnetic intralayer couplings, the model exhibits a continuous quantum phase transition to an ordered phase at a critical coupling $\lambda_c \approx -0.2636$. Our results for the critical exponents associated with the closing of the triplet gap and the divergence of the magnetic susceptibility are consistent with those of the 3D classical Heisenberg model.

For the antiferromagnetic intralayer coupling, it is more difficult to reliably estimate the critical $\lambda_c$, at which the gap vanishes, as $\lambda_c$ is large and the convergence of the series not very good at these values of $\lambda$. Unbiased analysis for the susceptibility and the inverse of the gap series shows evidence for a transition at $\lambda_c \approx 1.2$ with an exponent $\nu \approx 0.53$ and $\gamma \approx 1.1$. These results are also confirmed by biasing the critical point in the series analysis. These results are consistent with the universality class discussed by Kawamura for the stacked triangular Heisenberg antiferromagnet.

These results also appear to rule out a phase in the model, at intermediate values of $\lambda$, where there is still...
a gap in the spectrum but unbound spinons become the elementary excitations. It has been shown\[9\] that in this case the order-disorder transition will lie in the universality class of the 3-dimensional $O(4)$ model. One might also expect that in this case the triplet excitations would decay into the two-spinon continuum and not have a well defined energy momentum relation. However, we find that as $\lambda$ 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 $\lambda$ in the vicinity of the ordering wavevector. Together with the estimates for the critical exponents at the transition, this suggests that free spinons do not exist in this model. Our results provide further support for existence of antiferromagnetic order in the single-plane triangular-lattice antiferromagnet.\[10\]\[11\]\[12\]

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

$$H = J_\perp \sum_i S_{A,i} \cdot S_{B,i} + J \sum_{<i,j>} [S_{A,i} \cdot S_{A,j} + S_{B,i} \cdot S_{B,j}],$$

where $A$ and $B$ refer to the two layers of the triangular lattice and $<i,j>$ are nearest neighbours 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 consists of product of singlets over these pairs. The excitations are isolated triplets localised at some site $i$. For finite values of $\lambda = J/J_\perp$ an effective hamiltonian $H^\text{eff}(\mathbf{R}_{i,j})$ describing the interaction between these localised degenerate triplet states can be derived by a systematic expansion in $\lambda$:

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

The methods for calculating $H^\text{eff}$ in powers of $\lambda = J/J_\perp$ are well developed and discussed in the literature\[13\]. The excitation spectrum is given by the eigenvalues of the effective Hamiltonian $H(\mathbf{R})$, where $\mathbf{R}_{i,j} = \mathbf{r}_i - \mathbf{r}_j$ is the vector connecting sites $i$ and $j$. It can easily be diagonalised by a Fourier transform. We have calculated these quantities complete to 10-th order.

In table I, the expansion coefficients for $E(\mathbf{q})$ with $\mathbf{q} = 0$ and $Q_{AF} = 4\pi/3 \mathbf{e}_1$ are presented, corresponding to the ordering wavevectors for the ferromagnetic and the antiferromagnetic systems. The expansion coefficients for the magnetic susceptibilities at the same two wavevectors, are calculated to 10-th order are given in the table II.

In addition to the wavevector 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.\[14\] 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 dlog Pade approximants lead to estimates

$$\lambda_c = -0.26362 \pm 0.00009, \quad \gamma = 1.407 \pm 0.004.$$
numbers are in quite good agreement with the 3d classical Heisenberg university class, where the best current estimates come from field-theory $\gamma = 1.3866 \pm 0.0012$, $\nu = 0.7054 \pm 0.0011$. That the series analysis gives slightly higher estimates for the exponents is common to many models and is primarily due to corrections to scaling.

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 $\lambda_c$. 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 $\lambda_c$ is in the range $1.18 - 1.29$. In that range there are four approximants for the susceptibility series, which give $(\lambda_c, \gamma)$ 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 $(\lambda_c, \nu)$ 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 $\gamma \approx 1.1$ and not consistent with the O(4) universality class, which has $\nu \approx 0.74$ and $\gamma \approx 1.47$. Following Chubukov, Sachdev and Senthil such a behavior is to be expected 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 $\lambda$ 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 $\lambda$ is increased, the triplet dispersion develops a sharp minimum at the ordering wavevector 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 wavevector, the spectral weights continue to increase with $\lambda$, 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 local-singlet phase to the magnetically ordered phase.

These results provide further confirmation that the single-plane triangular-lattice antiferromagnet is ordered. However, the ratio of the ferromagnetic to antiferromagnetic critical points is almost an order of magnitude smaller for the triangular lattice than for the square-lattice. This, together with previous perturbative studies of the triangular lattice Heisenberg model, shows that the antiferromagnetic ordering in the triangular-lattice model is much less robust.

In conclusion, in this paper we have studied the quan-
tum 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 $\lambda$ 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 wavevector continues to grow with $\lambda$ suggest that in this model, a phase with free spinons does not exist and there is a direct transition from the local singlet phase to the 3-sublattice ordered phase. This study lends further support to the idea that the single-plane spin-half triangular-lattice Heisenberg model is ordered, but that this ordering is much less robust than for the square-lattice.

Acknowledgements: We would like to thank Subir Sachdev and Oleg Starykh for valuable discussions. This work is supported in part by the US National Science Foundation under Grants No. DMR-96-16574.

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