Restoration of Symmetry in the Spectrum of the Bilayer Heisenberg Antiferromagnet

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The longitudinal mode in the Heisenberg model on a bilayer square lattice is studied using series expansion methods. It is demonstrated numerically that the longitudinal mode becomes degenerate with the magnon modes at the quantum phase transition between Néel and dimerized phases, thus forming a spin-1 multiplet in accord with the restoration of SU(2) symmetry. It is also shown that the magnon mode becomes degenerate with the triplet mode in the dimerized phase at the critical point, showing continuity of the excitation spectrum across the critical point.

1. Introduction

The physics of quantum phase transitions is a topic of ongoing interest. One question concerns the behaviour of the excitation spectrum. For an order-disorder transition, for example, we expect that in the disordered phase the excitations will fall into multiplet representations of the full symmetry group of the system, whereas in an ordered phase where the symmetry is spontaneously broken, only the remnant, unbroken symmetry is evident in the spectrum. How does this change manifest itself at the transition point?

Another question concerns the continuity of the excitation spectrum across the transition point. At a first-order phase transition where the bulk properties of the system change discontinuously, one would expect the excitation spectrum to change discontinuously also. At a continuous phase transition, however, only the long-range properties of the system change in a singular fashion, and one would expect the properties of local excitations to remain continuous across the transition. Can this be verified numerically?

In this paper, we provide numerical results to answer these questions in the case of the spin-½ Heisenberg antiferromagnet on a square lattice bilayer. The bilayer system has attracted considerable interest in recent years. One reason is the experimental observation that some of the high-T_c superconductors contain pairs of CuO_2 layers separated by a charge reservoir. Another is the fact that the bilayer is perhaps the simplest 2D spin system to display an order-disorder transition in the O(3) universality class, without the complication of any frustrating interactions.

2. Method

The Hamiltonian of the system is

$$H = J_1 \sum_{\alpha=1,2} \sum_{<i,j>} \mathbf{S}_{\alpha,i} \cdot \mathbf{S}_{\alpha,j} + J_2 \sum_{i} \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i}$$

where α = 1,2 labels the two planes of the bilayer, and the sum <i,j> runs over nearest-neighbour pairs of sites within a plane. The physics of this system depends on the ratio $y = J_2/J_1$. At small J_2, the system is Néel ordered, with alternate spins pointing in opposite directions along what we define as the *z* axis (Fig. 1(a)). Thus the SU(2) symmetry of the

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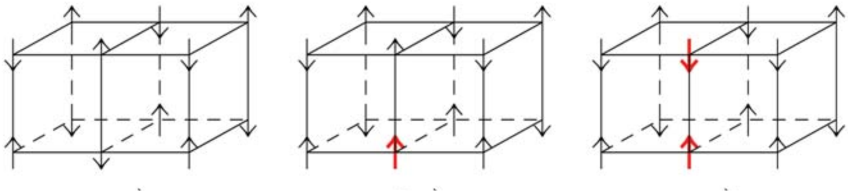

(a) (b) (c)

Fig. 1. Spin configurations in the Ising limit for (a) the vacuum state; (b) a single flipped spin; (c) two flipped spins on the same rung.

original model is spontaneously broken. Then the lowest-lying excitations are the two Goldstone modes, consisting in the Ising limit of a single flipped spin, with $S_z = \pm 1$, depending on the sub-lattice (Fig. 1(b)). For large J_2, on the other hand, the system is in a dimerized (disordered) state, with the pair of spins on each bond between the bilayers forming a singlet dimer, so as to minimize the energy on that bond. Then the SU(2) symmetry remains unbroken, and the lowest-lying (gapped) excitations are the spin-1 triplet excitations on a single bond.

How is the symmetry restored as one moves from the Néel phase to the critical point? The two Goldstone modes with $S_z = \pm 1$ must become degenerate with a longitudinal $S_z = 0$ mode, so as to form a triplet. This has been recently observed in the material $TlCuCl_3$ [1]. It is clear that this longitudinal mode must originate in the Ising limit from the third possible excitation on a single bond, namely that with *both* spins flipped (Fig. 1(c)), which does have $S_z = 0$. We shall study this mode in what follows.

Theorists have discussed this model using series expansion methods, quantum Monte Carlo (QMC) simulations at low temperatures, Schwinger-boson mean-field theory, and bond-operator theory. The exponent-biased series analysis of Zheng [2] put the critical point at $y_c = 2.54(2)$, while the accurate stochastic series-expansion study by Wang *et al*. [3] gave $y_c = 2.5220(2)$, with a critical index $\nu = 0.7106(9)$ to be compared with the best estimate from the classical three-dimensional Heisenberg model of $\nu = 0.7112(5)$, showing universality of the bilayer system with the Heisenberg model.

Conventional spin wave and Schwinger boson approaches, while very successful for the single layer $S = \pm$ antiferromagnet, give poor results for the bilayer system, predicting a critical value y_c nearly twice too large. Chubukov and Morr [4] showed that this was due to the neglect of longitudinal spin fluctuations, which are large and indispensable near the critical point, but become very small as $y \sim 0$. Within the bond-operator formalism, Sommer *et al*. [5] showed how the longitudinal mode becomes degenerate with the magnon modes at the critical point.

Here we use series expansion methods to perform a numerical study of the behaviour of the longitudinal mode in the Néel phase, using an expansion about the Ising limit for the system. We introduce an anisotropy parameter *x*, and write the Hamiltonian for a Heisenberg-Ising model as

$$H/J_1 = H_0 + xV$$

where

$$H_0 = \sum_{\alpha=1,2} \sum_{\langle i,j\rangle} S^z_{\alpha,i} S^z_{\alpha,j} + y \sum_i S^z_{1,i} S^z_{2,i}$$

$$V = \sum_{\alpha=1,2} \sum_{\langle i,j\rangle} (S^x_{\alpha,i} S^x_{\alpha,j} + S^y_{\alpha,i} S^y_{\alpha,j}) + y \sum_i (S^x_{1,i} S^x_{2,i} + S^y_{1,i} S^y_{2,i})$$

The limits $x = 0$ and $x = 1$ correspond to the Ising model and the isotropic Heisenberg model

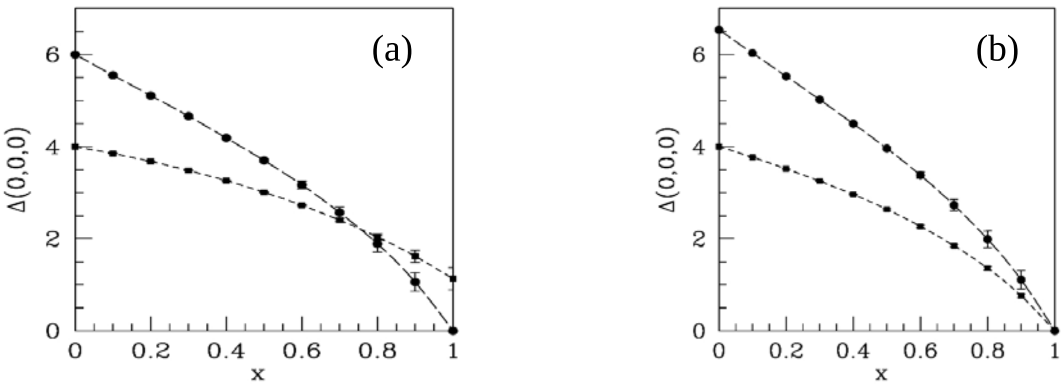

Fig. 2. A graph of the excitation energy of the longitudinal mode at **k** = (0,0,0) versus x (squares), compared with the continuum limit (circles), at (a) y = 2.0, and (b) y = 2.527.

respectively. The operator H_0 is taken as the unperturbed Hamiltonian, with the unperturbed ground state being the usual Néel state. The operator V is treated as a perturbation, where the 2-site operators flip a pair of spins on neighbouring sites.

Series have previously been calculated by Zheng [2] for the single-particle magnon excitation spectrum $\Delta(k_x,k_y,k_z)$ for several coupling ratios y. The series were calculated using the linked cluster expansion method [6]. We have added to these results a calculation of series for the energy spectrum $\Delta_L(k_x,k_y,k_z)$ of the longitudinal mode. The series have been calculated to order x^{10}, requiring 2678838 clusters of up to 12 sites. Given the series expansions in the variable x, extrapolations have been made using standard Pade approximant methods to obtain estimates of the excitation energies at finite values of x up to the isotropic value x = 1.

3. Results

Fig. 2 shows the estimated values for the energy of the longitudinal mode at **k** = (0,0,0) as a function of x, compared with the expected lower edge of the 2-particle continuum limit, equal to twice the magnon energy at **k** = (0,0,0). The magnon energy should have a Goldstone zero at the isotropic point x = 1, which is difficult to reproduce using such a short series, so to obtain our best estimates we have used a 2-point Pade approximant technique for this series, constraining the energy to vanish at the isotropic point. Fig. 2(a) shows values at y = 2, which is inside the Néel phase for the isotropic Heisenberg model. It can be seen that the longitudinal mode remains a bound state out to approximately x = 0.75, where it enters the continuum and becomes unstable.

Fig. 2(b) shows a similar plot at y = 2.537, which is close enough to the critical point for our purposes. In this case, 2-point Pade approximants have been used to estimate both curves, because the longitudinal mode is also expected to vanish at the critical point [5]. The series is compatible with this expectation, but too short to provide accurate verification. The graph then indicates that the longitudinal mode remains bound at all x < 1, and only becomes degenerate with the continuum right at the isotropic point x = 1. Of course, this evidence is not conclusive, because of the constraints placed on the extrapolations.

More dramatic evidence is provided in Fig. 3, which shows dispersion relations along symmetry lines in the Brillouin zone for both states at y = 2 and y = 2.537. The top two curves in Fig. 3 show the dispersion relations at y = 2, in the Néel phase, and it can be seen that the energy of the longitudinal mode remains clearly separate from and above that of the magnon mode. The bottom two curves show the corresponding data at y = 2.537, the critical point, and they are very nearly identical. They leave little room for doubt that the states become degenerate at the critical point, corresponding to the restoration of SU(2) symmetry in the spectrum at this point.

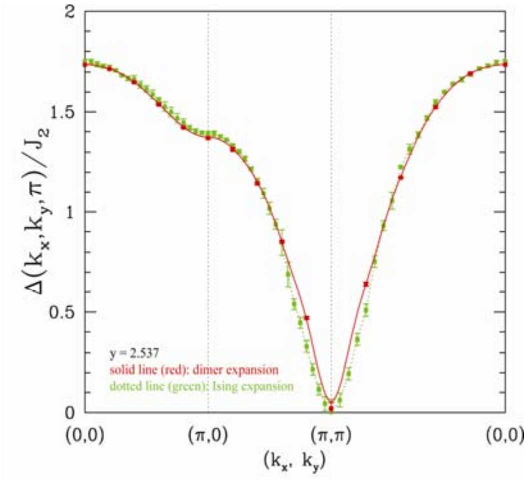

Fig. 3. A comparison of dispersion relations along symmetry lines in the Brillouin zone for the single-magnon mode (SW) and the longitudinal mode (LM) at two different values y = 2.0 and y = 2.537.

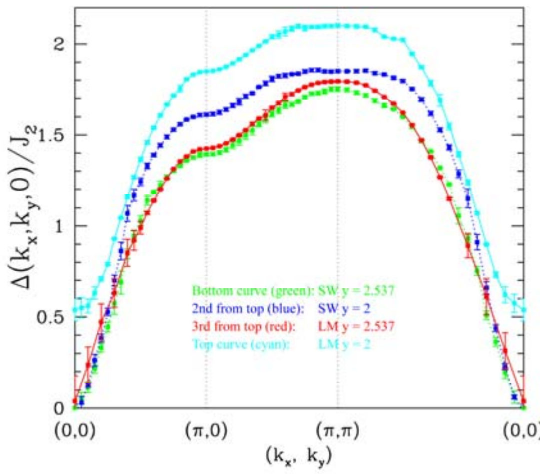

Fig. 4. A comparison of the dispersion relations for the single-magnon mode in the Néel phase, obtained from an Ising expansion (green), and the triplet mode in the dimerized phase, obtained from a dimer expansion (red), both at y = 2.537.

Finally, we show Fig. 4, which compares the dispersion relations at the critical point for the single magnon state obtained from an Ising expansion, with that for the lowest triplet dimer state obtained from a dimer expansion in the dimer phase (note that there is a symmetry between points **k** = (0,0,0) and **k** = (π,π,π) in the bilayer model). Again there is a remarkable match, illustrating how the dispersion relation for the triplet excitation remains continuous across the boundary between the Néel phase and the dimerized phase.

4. Conclusions

We have used series expansion methods to demonstrate that while the longitudinal mode is a bound state in the Ising limit, it enters the continuum and becomes unstable as the isotropic Heisenberg limit is approached in the Néel phase. At the critical point, the spectrum of the longitudinal mode becomes degenerate with that of the single-magnon modes, forming a spin-1 triplet of states in accord with the restoration of full SU(2) symmetry at that point. We have also shown that the spectrum of the single-magnon state in the Néel phase becomes degenerate with that of the triplet mode in the dimerized phase at the critical point, illustrating the continuity of the excitation spectrum across a continuous quantum phase transition.

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