Two-particle Bound States in the S=1/2 Heisenberg Bilayer Model

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The spectrum of two-particle states in the dimerized S=1/2 Heisenberg bilayer model is explored, using 'triplet wave' and series expansion techniques. Near the Néel point $\mathbf{k}=(\pi,\pi)$ bound states of two triplons are found in the S=0 and S=1 channels, and antibound states in the S=2 channel, as for other dimerized antiferromagnetic systems.

1. Introduction

Modern probes of material properties, such as the new inelastic neutron scattering facilities, are reaching such unprecedented sensitivity that they can measure the spectrum not only of a single quasiparticle excitation, but even two-particle excitations [1]. These quasiparticles can collide, scatter, or form bound states just like elementary particles in free space. The spectrum of the multiparticle excitations is a crucial indicator of the underlying dynamics of the system.

One of the principal theoretical means of predicting the excitation spectrum is the method of high-order perturbation series expansions [2]. We have previously used a 'linked-cluster' approach to generate series expansions for 2-particle states in 1-dimensional models [3], but for 2-dimensional models the only calculations carried out so far have been those of Uhrig's group in Germany [4], using the 'continuous unitary transformation' (CUTS) method, which is of only limited applicability. Our original aim here was to extend the linked-cluster approach to 2-dimensional models, starting with the bilayer model as a simple example.

The S=1/2 Heisenberg bilayer model is one of the simplest two-dimensional systems to treat theoretically, and is of particular interest because it displays a dimerized valence-bond-solid ground state. It has also attracted continuing interest from experimentalists because many of the cuprate superconductors contain pairs of weakly coupled copper oxide layers [5]. Recently, the organic material piperazinium hexachlorodicuprate has also been found to have a bilayer structure [6].

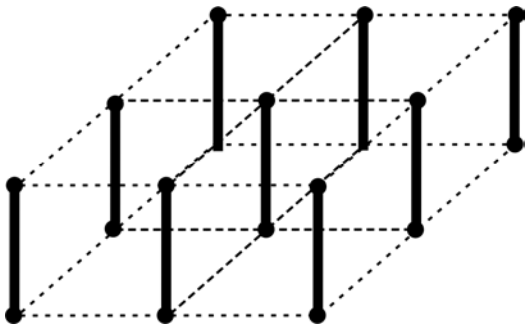

Fig. 1. The bilayer structure. At $\lambda = 0$, each pair of spins on the dashed interlayer bonds forms a dimer with S = 0.

The model is shown in Figure 1. It consists of two planes of S = 1/2 spins on a square lattice, with antiferromagnetic interactions on the bonds of the lattice:

$$H = \sum_i S_{1i} \cdot S_{2i} + \lambda \sum_{l=1,2} \sum_{\langle ij \rangle} S_{li} \cdot S_{lj}$$

where l=1,2 labels the two planes of the bilayer, and <i,j> nearest-neighbour sites within a layer. The physics of the system then depends on the coupling λ. At $\lambda = 0$, only the interlayer bonds remain, and the ground state consists simply of an S = 0 dimer on each bond between the two layers, while excitations are composed of S = 1 `triplon' states on one or more bonds. At large $\lambda$, where the intralayer interaction is dominant, the ground state will be a standard Nėel state, with S = 1 `magnon' excitations. At some intermediate critical value λ_c, a phase transition will occur between these two phases. It is believed that this transition is of second order, and is accompanied by a Bose-Einstein condensation of triplons/magnons in the ground state.

Theorists have discussed this model using series expansion methods [7], quantum Monte Carlo simulations at small temperatures, Schwinger-boson mean-field theory, and spin-wave theory [8]. The series analysis of Zheng [7] put the critical point at $\lambda_c = 0.394(1)$, with a critical index $\nu \approx 0.7$, in agreement with the O(3) nonlinear sigma model prediction. Early spin-wave estimates were well away from this position, but the improved Brueckner approach of Sushkov *et al.* [8] gave a remarkably accurate estimate of the critical point and critical index, and also the 1-particle dispersion in the model.

2. Methods

We have used two complementary theoretical methods to explore this model in the dimerized regime. The first is a 'triplet wave' treatment, analogous to the spin-wave techniques used in the antiferromagnetic regime. Sachdev and Bhatt [9] first proposed a 'bond operator' formalism for this purpose, but the constraint excluding two triplons from occupying the same site was hard to implement. Kotov et al. [8] introduced an infinite hard core repulsion for this purpose, while we [10] have preferred a projection operator technique. The spin operators $\mathbf{S}_{1,2}$ are represented in terms of triplet operators $\mathbf{t}$ by:

$$S_{1\alpha} = \tfrac{1}{2} [t^*_\alpha(1-t^*_\gamma t_\gamma) + (1-t^*_\gamma t_\gamma) t_\alpha - i\varepsilon_{\alpha\beta\gamma} t^*_\beta t_\gamma]$$

$$S_{2\alpha} = \tfrac{1}{2} [-t^*_\alpha(1-t^*_\gamma t_\gamma) - (1-t^*_\gamma t_\gamma) t_\alpha - i\varepsilon_{\alpha\beta\gamma} t^*_\beta t_\gamma]$$

The usual Fourier transform and Bogoliubov transform are then used to produce a triplet Hamiltonian diagonal through second order in momentum space.

This formalism leads to a Bethe-Salpeter equation for the two-particle states, which at leading order in λ, and at the specific momentum $\mathbf{k} = (\pi,\pi)$, has a simple solution corresponding to a pair of triplon excitations on nearest-neighbour sites, with energies

$$E^{S=0} = 2-\lambda, \quad E^{S=1} = 2-\lambda/2, \quad E^{S=2} = 2+\lambda/2,$$

compared to the continuum energy of exactly 2. Thus a pair of bound states are predicted for the singlet and triplet channels, and antibound states for the quintuplet channel. Further details will be given in a forthcoming paper [11].

The second method is the linked-cluster series expansion approach, reviewed in the book by Oitmaa *et al.* [2]. This approach has been used to calculate two-particle states in one-dimensional models such as the alternating Heisenberg chain (AHC) [3], but not for two-dimensional models, to our knowledge. We have applied a dimer series expansion, where the interlayer interaction term with the dimerized ground state is taken as the unperturbed Hamiltonian H_0, and the remainder as the perturbation λV. We have generalized the computer codes to deal with this two-dimensional bilayer system, but only results up to 3rd order in λ are available as yet.

3. Results

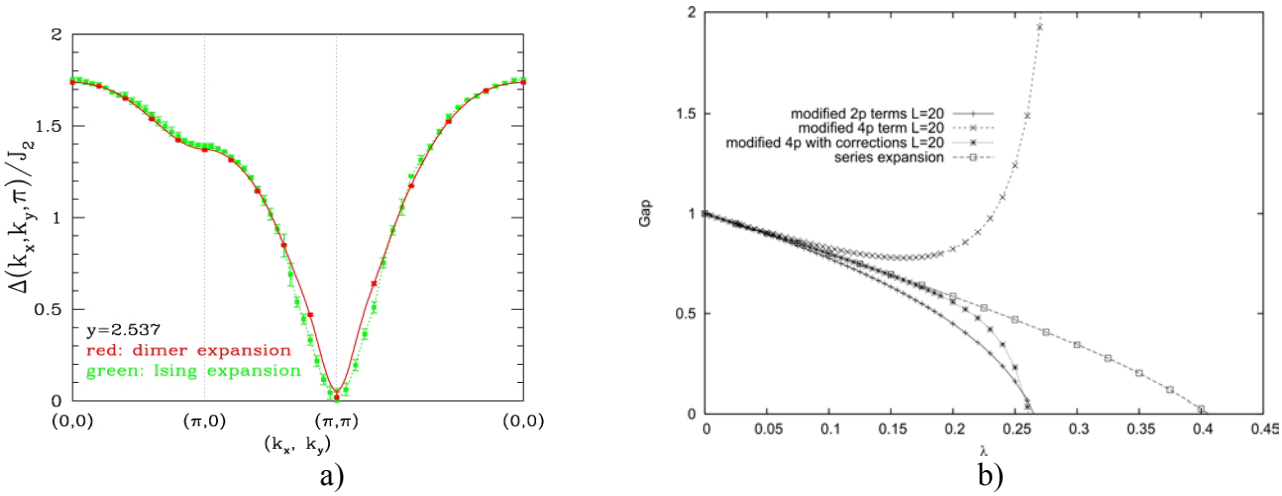

Fig. 2. a) Dispersion relation for one-triplon states (y = 1/λ). b) Energy gap at **k** =(π,π) for various triplet-wave expansions. The triplet wave expansions are plotted against the series estimate.

The dispersion of the one-triplon energy as a function of momentum or wave number along symmetric cuts in the Brillouin zone is illustrated in Figure 2a). It can be seen that the energy gap is least at the Néel point **k** =(π,π), and in fact vanishes at the critical λ. The energy gap at **k** =(π,π) is graphed against λ in Figure 2b), where it can be seen how the gap decreases towards the critical coupling $\lambda_c = 0.394(1)$, where Néel ordering sets in. These series data were obtained previously by Zheng [7], using terms up to $O(\lambda^{11})$, and extrapolated using naïve Pade approximants. The triplet-wave predictions have only been calculated completely through $O(\lambda^2)$, and do not match the series results beyond about λ ≈ 0.2, even with leading diagrammatic corrections added in. The self-consistent Born approximation of Kotov et al. [8] does much better in this regard.

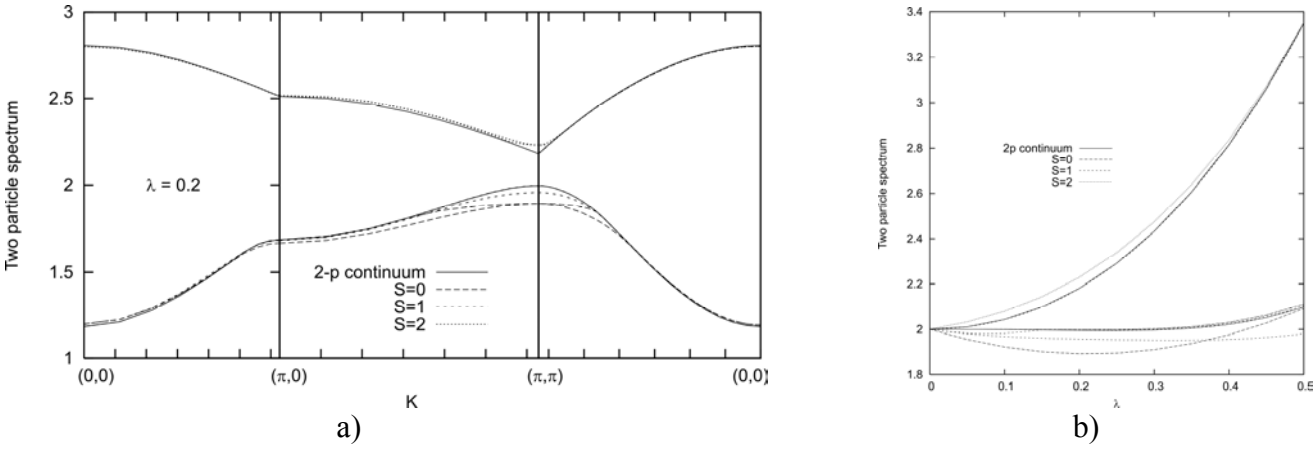

Fig.3. a) Two-particle dispersion curves at λ = 0.2. The solid lines delimit the continuum. b) Two-particle energies as functions of λ at **k** =(π,π).

We turn now to the two-triplon spectrum. Figure 3a) shows the dispersion of the 2-particle spectrum at λ = 0.2, calculated from series expansions. It can be seen that S = 0 singlet and S = 1 triplet bound states emerge below the continuum near **k** =(π,π), and S = 2 quintuplet antibound states appear above the continuum, as predicted by the triplet-wave theory. Each of these states is doubly degenerate, or nearly so, at **k** =(π,π). These states merge with the continuum at some finite

momentum point **k**, and for the most part they appear to merge at a tangent, as in the one-dimensional case [3].

The 2-particle energy gaps at $\mathbf{k} = (\pi,\pi)$ are shown as functions of λ in Figure 3b). The singlet bound state is the lowest, as predicted. Our preliminary results show it rising again after an initial decrease; but only low-order results are available as yet. For the AHC, the binding energies vanished at the critical endpoint of the dimerized phase. It is possible that the same thing is happening here.

4. Discussion

The pattern of 2-particle bound and antibound states found here is very similar to that found in dimerized antiferromagnetic systems in one dimension, such as the AHC [3]. The main difference is that these states are doubled in the two-dimensional model. Also, in the two-dimensional case the lowest singlet bound state vanishes at finite **k**, whereas in the AHC it exists at all **k**, only touching the continuum at $\mathbf{k} = 0$. The bound states appear to merge with the continuum at a tangent, much as in the one-dimensional case [3].

In future work we plan to push the calculations to higher order, in order to get a better idea of the behaviour near the critical point, and to see whether there are multiple bound states in the model. Later on, we hope to perform similar calculations for other two-dimensional models, such as the simple Heisenberg model on the square lattice, and the Shastry-Sutherland model, which has already been studied by Uhrig et al. [4]

Acknowledgments

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