Energy spectrum of the two-magnon bound states in the Heisenberg-Ising antiferromagnet on the square lattice

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The energy spectra of the two-magnon bound states in the Heisenberg-Ising antiferromagnet on the square lattice are calculated using series expansion methods. The results confirm an earlier spin-wave prediction of Oguchi and Ishikawa that the bound states vanish into the continuum before the isotropic Heisenberg limit is reached.

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I. INTRODUCTION

We consider the anisotropic antiferromagnetic Heisenberg model on a bipartite lattice,

$$H = J\sum_{\langle ij\rangle} [S_i^z S_j^z + x(S_i^x S_j^x + S_i^y S_j^y)]$$
$$= J\sum_{\langle ij\rangle}\left[S_i^z S_j^z + \frac{x}{2}(S_i^+ S_j^- + S_i^- S_j^+)\right] \equiv H_0 + xV, \qquad (1)$$

with $S=1/2$ spins interacting with their nearest neighbors.

In the Ising limit $x=0$, the system is Néel ordered, with spins up ($S^z=+1/2$) on the A sublattice, let us say, and down ($S^z=-1/2$)) on the B sublattice. The one-particle "magnon" excitations correspond to a single flipped spin on either the A sublattice, with total spin $S^z=-1$, or on the B sublattice ($S^z=+1$). They have an excitation energy $zJ/2$, where z is the lattice coordination number.

Separated two-particle excitations then have energy zJ in this limit. But a two-particle excitation on neighboring A and B sites has energy only $(z-1)J$, with total spin $S^z=0$, forming a two-particle bound state.

When one takes the isotropic limit $x\to 1$, as is well known, the energy gap for the single-magnon states vanishes. The question then is: do the two-particle bound states survive in this limit?

It is well known that two-magnon bound states exist for the isotropic Heisenberg *ferromagnet*; see, for example, the textbook discussion by Mattis.[1] In recent years, there have also been considerable discussions of bound states in antiferromagnetic systems with frustration or anisotropy.[2,3] The question still remains, however, whether there might also be bound states in the simple, isotropic antiferromagnet. According to Mattis,[1] this remained an "unanswered question" in 1965 (Ref. 1, p. 166).

The question was investigated using spin-wave theory by Oguchi and Ishikawa[4] in 1973. They used linear spin-wave theory with some fourth-order interaction terms included. They found that the two-magnon bound states merge into the continuum as one goes from the Ising limit to the isotropic limit so that none survive. This calculation neglects many higher-order effects which might be important, however, so it cannot be taken as definitive. Some numerical calculations involving multimagnon states have also been carried out for the isotropic antiferromagnet on the square lattice. These include studies of the spectral weights using series expansions[5] and quantum Monte Carlo simulations[6] and a continuous unitary transformation (CUTS) study of the spectrum.[7] None of these works, however, have addressed the question of the bound states.

In this Brief Report we explore the fate of the two-magnon bound states for two particular cases: the one-dimensional chain and the two-dimensional square lattice. In one dimension, the model is exactly solvable, and the answer is already known: we simply review the results. In two dimensions, we use linked cluster methods[8] to obtain series expansions in x up to order $O(x^8)$ for the bound-state energies and extrapolate the results to $x=1$ using standard methods. In summary, our results agree quite well with the spin-wave predictions.[4] The bound states disappear into the two-particle continuum shortly before the isotropic limit $x\to 1$ is reached.

II. ONE-DIMENSIONAL CASE

The one-dimensional model, i.e., the linear chain, is a special case. The model can be solved exactly using the Bethe ansatz,[9] and exact expressions for the low-lying spectrum have been obtained.[10] The independent quasiparticles in this case are not $S^z=\pm 1$ magnons but $S^z=\pm 1/2$ "spinons," or domain walls. In the Ising limit $x=0$, for instance, the ground state consists of alternating spins $S^z=\pm 1/2$ on even or odd sites, respectively, or the reverse [Fig. 1(a)]. A spinon or domain wall consists of a neighboring pair of identical spins

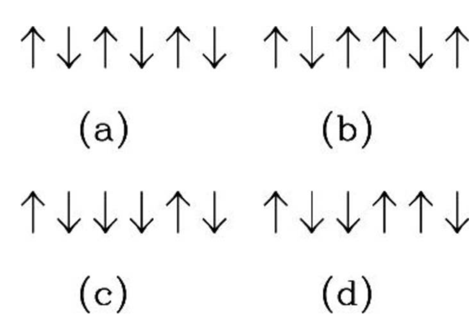

FIG. 1. Spin configurations on the linear chain in the Ising limit: (a) a Néel ground state; (b) a single spinon state; (c) two adjacent spinons or a single magnon; and (d) two spinons separated by one site or two adjacent magnons.

in an otherwise alternating chain [Fig. 1(b)]. For periodic or antiperiodic boundary conditions, spinons can only be created in pairs. Thus on an even lattice with periodic boundary conditions, say, the lowest-lying excitations above the ground state consist of a pair of spinons, which may be one lattice spacing apart [Fig. 1(c)], two spacings apart [Fig. 1(d)], or any number apart. Figure 1(c) then corresponds to a single spin flip, Fig. 1(d) to two neighboring spin flips, and so on. The excitation energy in this limit, however, is $\Delta E = J$, independent of the spacing.

Johnson *et al.*[10] obtained an exact expression for the low-lying excitation energy at all x,

$$\Delta E = \frac{2K \sinh \nu}{\pi \cosh \nu}[(1 - k^2 \cos^2 q_1)^{1/2} + (1 - k^2 \cos^2 q_2)^{1/2}], \tag{2}$$

where $\cosh \nu = 1/x$, K is a complete elliptic integral of the first kind whose nome is $q = e^{-\nu}$ and modulus k, and $0 \le q_1, q_2 < \pi$ are two free parameters corresponding to the momenta of the two domain walls in each sector. This spectrum is the same in the $S^z = \pm 1$ and the (doubly degenerate) $S^z = 0$ sectors so that the two $S = 1/2$ spinons combine to form a degenerate $S = 1$ triplet and $S = 0$ singlet at all couplings x in the range. So in this case, the state with two neighboring flipped spins merely forms part of the two-spinon continuum.

III. SQUARE LATTICE

As the prime example of a bipartite system in two dimensions, we consider the model on a square lattice. In this case no exact solution is known, and so we have calculated numerical estimates for the energy of the two-magnon state using series methods.[8] We perform an Ising expansion, taking the Ising Hamiltonian H_0 in Eq. (1) as our unperturbed starting point, when the bound state consists simply of a pair of flipped spins on neighboring sites, as discussed above. A perturbation series expansion in x is then calculated for the bound-state energy, with V in Eq. (1) as the perturbation operator. As a technical point, we note that the bound state lies in the same sector as the ground state, and hence a "multiblock" diagonalization algorithm[8] must be employed.

Note also that there is one bound-state configuration for each lattice bond, making a total of four times as many configurations as for either of the single-magnon states. Correspondingly, we obtain results for four different paths $\Gamma_1, \ldots, \Gamma_4$ in the Brillouin zone, as shown in Fig. 2, whereas only the Γ_1 mode is independent for the single-magnon state.

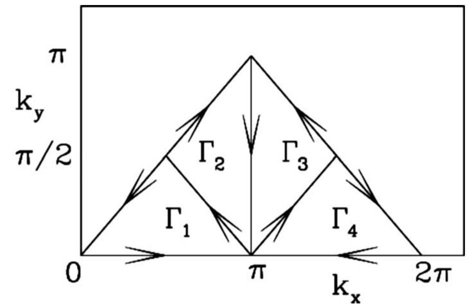

FIG. 2. Cuts through the Brillouin zone Γ_1-Γ_4 corresponding to the four two-magnon bound states.

The calculations have been carried out through $O(x^8)$. Since only even-order terms appear, this corresponds to only five series coefficients at any fixed momentum. The leading order terms in the dispersion relation for the bound-state excitation energy are

$$\epsilon(\mathbf{k}) = 3 - x^2\left[\frac{1}{4} + \frac{2}{3}\cos\frac{k_x}{2}\cos\frac{k_y}{2} + \frac{1}{12}(\cos k_x + \cos k_y) + \frac{1}{6}\left(\cos\frac{k_x}{2}\cos\frac{3}{2}k_y + \cos\frac{3}{2}k_x \cos\frac{k_y}{2}\right) + \frac{1}{6}\cos k_x \cos k_y + \frac{1}{24}(\cos 2k_x + \cos 2k_y)\right]. \tag{3}$$

The complete series coefficients at selected momenta are listed in Table I.

Estimates of the bound-state energy as a function of x were now obtained using Padé approximants to extrapolate the series. The estimated errors in the extrapolated values are always somewhat subjective.[11] From the table of Padé approximants, the outliers with obvious "defects" are excluded, where a defect consists of a spurious pole with low residue at a small coupling value. The remaining approximants are then weighted to favor the higher-order approximants, and the error is estimated from the scatter among the remaining weighted estimates.

Since the number of coefficients is small, the accuracy of the extrapolation is also low. At smaller values of x, nevertheless, quite good estimates are possible. For example, Fig. 3 shows dispersion relations for the four bound-state modes at $x = 0.8$, as compared with the lower bound of the two-particle continuum. It can be seen that all four modes remain

TABLE I. Ising expansion series coefficients in powers of x for the excitation energy ΔE of the two-particle bound state at selected momenta $\mathbf{k} = (k_x, k_y)$.

(k_x, k_y)	(0,0)	$(\pi/2, 0)$	$(\pi, 0)$	$(\pi/2, \pi/2)$	(π, π)
0	3.00000000000000	3.00000000000000	3.00000000000000	3.00000000000000	3.00000000000000
2	−1.66666666666667	−0.804737854124365	−0.166666666666666	−0.333333333333334	−0.333333333333333
4	0.299074074074084	0.412245678974668	−0.0712962962962898	0.403819444444453	−0.727546296296289
6	−2.21500154321004	−0.955337158046685	−0.371659167631400	−0.517003970550667	−0.576196887860336
8	5.95191488216504	2.06716252423366	0.237274308271624	0.738026171850790	−0.604532331023972

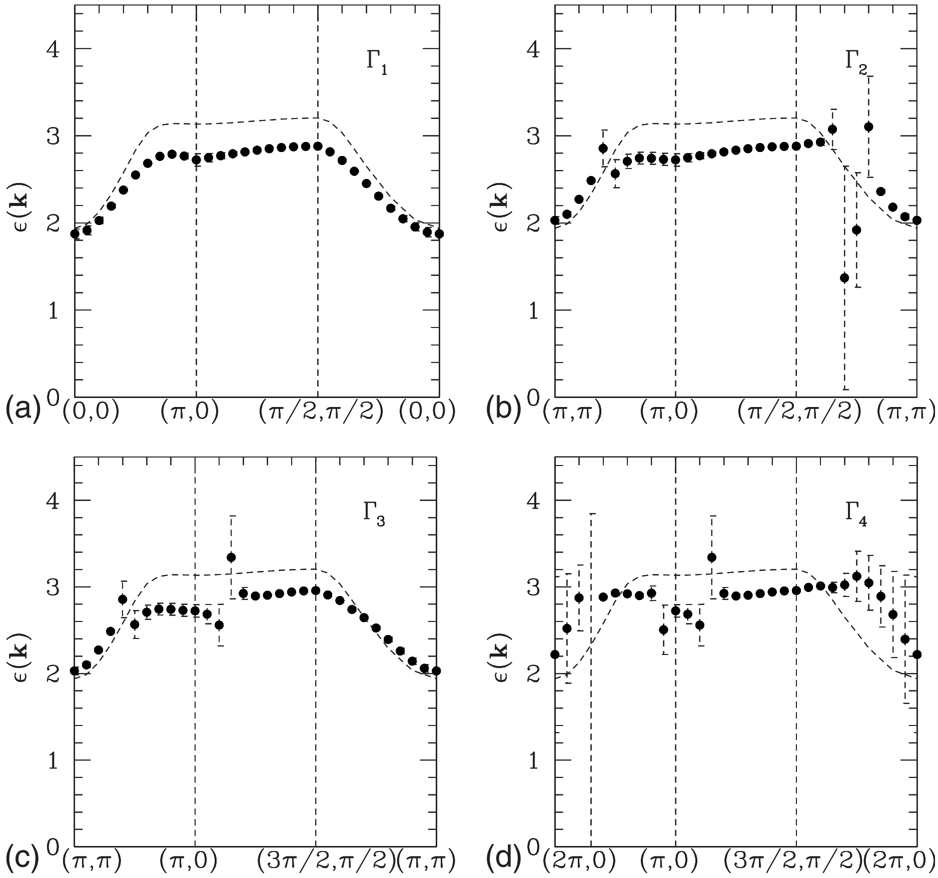

FIG. 3. Spectrum of the two-particle bound states Γ_1-Γ_4 at $x=0.8$. The dashed lines mark the lower edge of the two-particle continuum.

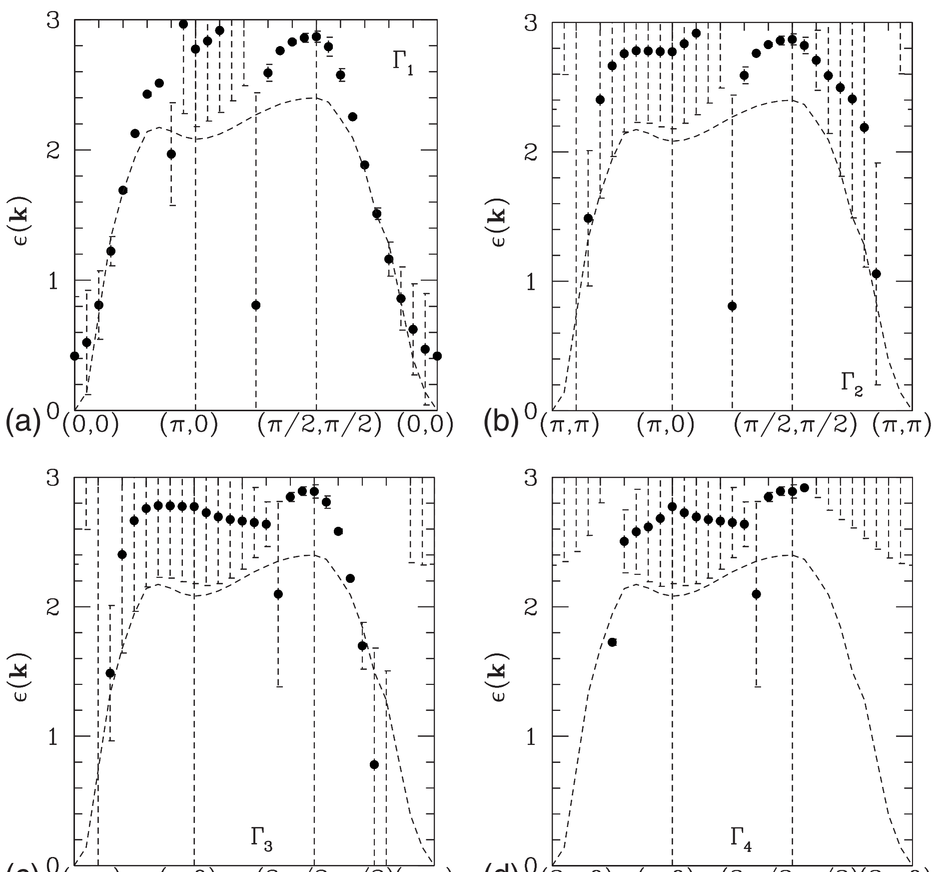

FIG. 4. Spectrum of the two-particle bound states Γ_1-Γ_4 at $x=1.0$. The dashed lines mark the lower edge of the two-particle continuum.

bound below the intermediate plateau of the continuum, and only near $\mathbf{k}=0$ do three out of the four modes merge into the continuum. The first mode appears to remain bound at all momenta.

At $x=1.0$ it is a different story, as shown in Fig. 4. In short, it appears that none of the four modes remain bound at any momentum. The nominal error bars are much larger in this case first because x is larger but also because we may expect some sort of singular behavior where the bound state merges with the continuum. The clearest picture is obtained for the first mode, where near $\mathbf{k}=0$ the estimates lie on the lower edge of the continuum, within errors. A Huse transform[12] was performed before the extrapolation, but there is still an apparent leveling off at very small momenta: this may be attributed to the small number of terms in the series. At larger momenta, the estimates generally lie well above the continuum lower bound.

These results may be compared with the spin-wave results of Oguchi and Ishikawa,[4] who calculated the bound-state energies as functions of x for two specific momenta. At $\mathbf{k}=(0,0)$, they found that the bound states merged with the continuum in the range $0.7 \leq x \leq 0.95$; we find only one bound state remaining at $x=0.8$, in agreement with their results. At $\mathbf{k}=(\pi/2,\pi/2)$, they found the merger to occur at somewhat larger values $0.96 \leq x \leq 0.98$; we find that all four states remain bound at $x=0.8$ but have vanished by $x=1.0$, once more in agreement with their results. Of course, the actual values for the energies have changed as higher-order terms are added in but not by a large amount.

IV. CONCLUSIONS

We have used series expansion methods to calculate the energy of two-magnon bound states in the anisotropic Heisenberg-Ising antiferromagnet on the square lattice. We find that the bound states do not survive in the isotropic limit, in agreement with the spin-wave predictions of Oguchi and Ishikawa.[4] There are no bound states in the linear chain model either. Hence one may extrapolate that there will be no bound states in the isotropic Heisenberg antiferromagnet on any bipartite lattice, in sharp distinction to the ferromagnetic case. Oguchi and Ishikawa[4] gave some qualitative arguments why this might be so.

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