Excitation Spectrum of a Dimerized Next-Neighbor Antiferromagnetic Chain

B. Sriram Shastry[a] and Bill Sutherland
Department of Physics, University of Utah, Salt Lake City, Utah 84112
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The excitation spectrum of an antiferromagnetic chain exhibiting the effects of both dimerization and frustration is studied. The method used is based on an exact solution for the doubly degenerate ground state, and views the excitations as propagating defect boundaries between the two exact ground states. These excitations are analogous to "solitons," and can bind into a second type of excitation, analogous to "breathers."

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In this Letter we consider a one-dimensional model for magnetism which includes two distinct phenomena of great current interest. First, the model exhibits frustration through the competition of nearest- and next-nearest-neighbor interactions. Second, the model is dimerized through the introduction of nearest-neighbor interactions alternating in strength. This resulting model is of sufficient generality to include several recent models considered by others in the literature, and in particular we locate and consider in detail the singular point corresponding to a model first treated by Majumdar. This model is a special class of models in two and three dimensions treated recently.

The system we consider is a linear-chain antiferromagnet of $2M$ spins described by the Hamiltonian

$$H=\sum_{1\le i\le M}[2\alpha h_{2i-1,2i}+2\beta h_{2i,2i+1}+\gamma(h_{2i-1,2i+1}+h_{2i,2i+2})]. \tag{1}$$

We impose periodic boundary conditions so that $i+2M=i$, and assume $\alpha,\beta,\gamma\ge 0$. The two-spin Hamiltonian h_{jk} is

$$h_{jk}=J_x S_j{}^x S_k{}^x+J_y S_j{}^y S_k{}^y+J_z S_j{}^z S_k{}^z, \tag{2}$$

with $J_x, J_y, J_z \ge 0$, and $|\vec{S}_i|=S$. The parameter space of this model is shown in Fig. 1, where we normalize so that $\alpha+\beta+\gamma=3$. This is a useful representation to exhibit various special cases which have been previously studied in the literature, and for which exact or approximate results are known for the ground state (g.s.) and elementary excitations (EE). However, we first remark the symmetry under exchange of α and β.

The points $B=(3,0,0)$ and $C=(0,3,0)$ are, of course, known exactly for all models, being simply a two-spin problem. For $S=\frac{1}{2}$ the points $A=(0,0,3)$ and $\bar{A}=(\frac{3}{2},\frac{3}{2},0)$ correspond to the nearest-neighbor X-Y-Z model which has been extensively studied by using generalized versions of Bethe's *Ansatz*. The symmetric point $O=(1,1,1)$ and the line $AO\bar{A}$ were first considered by Majumdar and co-workers[1] for the isotropic, $S=\frac{1}{2}$ case, and several exact and numerical results are available. The line $B\bar{A}C$ has been investigated numerically by Fields, Blote, and Bonner for the isotropic, $S=\frac{1}{2}$ case.[2] These results indicate that the symmetric point $\bar{A}$ is a singular point. Physical realizations of the model are available at several values of the parameters and provide an additional impetus for its study.

In this Letter we focus attention on the lines BO ($\beta=\gamma$) and CO ($\alpha=\gamma$), and in particular, concentrate on the point O ($\alpha=\beta=\gamma$) and its vicinity. Among other results, we extend Majumdar's investigation to determine the exact g.s. energy for the general situation of arbitrary spin and anisotropy along portions of the line BOC. For the popular isotropic, $S=\frac{1}{2}$ case, we determine the g.s. energy for the whole line BOC, and establish that the point O is a singular point of the g.s. energy corresponding to a first-order transition.

The main results reported in this Letter concern the excitation spectrum and low-temperature thermodynamics of the model at the point O ($\alpha=\beta=\gamma=1$). Here, the g.s. is doubly degenerate

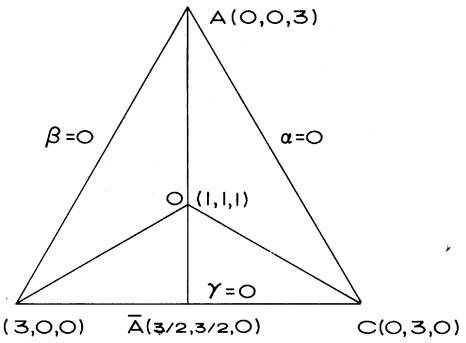

FIG. 1. Parameter space of the Hamiltonian.

and we show that it first exhibits long-range order in the four-spin correlation function. We have developed a simple physical picture for the EE in terms of propagating defects or boundaries between the nonequivalent ground states and present our variational results for the ensuing quantum lumps (or solitons) and the bound state of pairs (a "breather" bound state of a soliton-antisoliton pair). We also present a simple and yet accurate theory for the low-temperature thermodynamics based on these independent quantum lumps. Our picture of the excitations bears some resemblance to that recently proposed in connection with other linear-chain systems[3].

Let us confine ourselves henceforth to BO and further set $\beta=\gamma=1$. Consider the state

$$|\psi_1\rangle=[1,2][3,4][5,6]\cdots[2M-1,2M], \quad (3)$$

where $[i,j]$ denotes the normalized singlet combination of spin i and j. It is easy to see that $|\psi_1\rangle$ is an eigenstate of H by using the relation $(S_i^{\alpha}+S_j^{\alpha})[i,j]=0$ $(\alpha=x,y,z)$. The eigenvalue is $E_0=2MW$, where

$$W=-\tfrac{1}{3}\alpha S(S+1)(J_x+J_y+J_z). \quad (4)$$

We next show that E_0 saturates a lower bound to H for appropriate values of parameters, and hence $|\psi_1\rangle$ is the exact ground state. To see this, we decompose $H=\sum H_t$, where the sum is over the $2M$ triangles (each triangle consists of two nearest-neighbor bonds and one next-nearest-neighbor bond). The Hamiltonian H_t is of the form

$$H_t=\alpha h_{i,i+1}+h_{i-1,i}+h_{i-1,i+1}. \quad (5)$$

The Rayleigh-Ritz variational principle implies $E_{\text{g.s.}}=\langle\psi_{\text{g.s.}}|\sum_t H_t|\psi_{\text{g.s.}}\rangle\geq 2Me_t$, where e_t is the g.s. energy of H_t. We have shown that e_t equals W and, hence, $|\psi_1\rangle$ is the g.s. provided $\alpha\geq\alpha_b$, where the bounding value in two cases of special interest is (a) $\alpha_b=1$ for $S=\frac{1}{2}$, and for arbitrary J_x, J_y, and J_z; (b) $\alpha_b=1+S$ for $S\geq 1$ in the isotropic limit $J_x=J_y=J_z$. Other cases can likewise be evaluated. These conditions are identical to the ones discussed recently in connection with the two- and three-dimensional problem solved by us.[4]

We now show that α_b is, in fact, a critical value of the parameter in the case $S=\frac{1}{2}$, and for $\alpha<\alpha_b$ the nature of the ground state is different, implying a (first-order) level-crossing phase transition. To see this, consider the state

$$|\psi_2\rangle=[2M,1][2,3][4,5]\cdots[2M-2,2M-1]. \quad (6)$$

Choosing $|\psi_2\rangle$ as a trial state we find $E_{\text{trial}}=-\frac{1}{4}(J_x+J_y+J_z)2M$, and hence $E_{\text{trial}}<E_0$, implying that $|\psi_1\rangle$ cannot be the ground state for $\alpha<1$. For $S>\frac{1}{2}$, $|\psi_2\rangle$ is not a better variational state in the range $1\leq\alpha\leq 1+S$ and hence the above does not constitute a proof, but we expect that α_b is probably a critical value in that case too. For $\alpha>\alpha_b$, the nature of ground-state correlations is short ranged and "liquidlike" and, hence, we may term the phase a "quantum spin liquid." In the remainder of the Letter we consider mainly the case $S=\frac{1}{2}$, and the point O $(\alpha=\beta=\gamma=1)$.

At the point O, the Hamiltonian possesses (lattice) translation invariance (invariance under $i\to i+1$) but the state $|\psi_1\rangle$ does not. However, it is easy to see that the state $|\psi_2\rangle$ is also an eigenstate of H with the same eigenvalue, Eq. (4). Hence, for $S=\frac{1}{2}$, the model has two nonequivalent ground state $|\psi_1\rangle$ and $|\psi_2\rangle$ at the point O. (The two states are orthogonal in the limit $M\to\infty$.) The breaking of translation invariance leads to the existence of long-range order in the four-spin correlation function. We construct a state $|O\rangle=(1/\sqrt{2})(|\psi_1\rangle+|\psi_2\rangle)$ which is clearly an eigenstate of H with eigenvalue Eq. (4) and is also a zero-momentum state and, hence, may be regarded as a physically acceptable ground state. We find the two-spin correlation function $K^{(2)}(ij)\equiv\langle O|S_i^z S_j^z|O\rangle=\frac{1}{4}\delta_{ij}-\frac{1}{8}\delta_{|i-j|,1}$. The four-spin correlation function $K^{(4)}(ij;lm)\equiv\langle O|S_i^x S_j^x S_l^y S_m^y|O\rangle$ can also be easily calculated and we find for $|i+j|\gg|l+m|$

$$K^{(4)}(ij;lm)-K^{(2)}(ij)K^{(2)}(lm)\simeq+\tfrac{1}{64}\delta_{|i-j|,1}\delta_{|l-m|,1}\exp[i(\pi/2)(i+j-l-m)]. \quad (7)$$

In order to construct the excited states at the point O, we restrict ourselves to the isotropic limit $(J_x=J_y=J_z)$ and $S=\frac{1}{2}$. In this case we have two ground states $|\psi_1\rangle$ (say phase A) and $|\psi_2\rangle$ (say phase B) and it is natural to think of excitations as consisting of the two phases separated by a defect. Therefore we consider the basic defect states

$$\psi(p,m)=[2p-3,2p-2]\alpha_{2p-1}[2p+1,2p+2]\cdots[2m-2,2m-1]\alpha_{2m}[2m+1,2m+2], \quad (8)$$

where α_j is an up-spin Pauli spinor. In Eq. (8) we have two defects since periodic boundary conditions

preclude an odd number, and the two defect sites have been assigned spin up. There are three other spin assignments possible and, hence, we have a total of four defect states for a given p and m (the total number of states is therefore $4M^2$). The set of two-defect states does not form a complete set of spin-1 states and hence our results, which are restricted to the above space, are variational in nature rather than exact. We expect, however, that the error involved should be small in view of the optimal nature of the functions.

We introduce the momentum-space wave function

$$\psi_{k_1+k_2}(k_1-k_2) \equiv \frac{1}{\sqrt{M}} \sum_{1\le p,m\le M} \exp[i(2pk_1+2mk_2)]\psi(p,m), \tag{9}$$

where k_1+k_2 is the total momentum and periodic boundary conditions determine k_1 and k_2. The overlap matrix of ψ's in momentum space can be worked out and after considerable algebra we get

$$(\psi_{Q'}(k'), \psi_Q(k)) = \delta_{Q,Q'}[(3J/4\omega_+)(3J/4\omega_-)M\,\delta_{k,k'} + \chi_Q(k,k')], \tag{10}$$

$$\chi_Q(k,k') = \frac{3J^4}{8\omega_+\omega_-\omega_+'\omega_-'}(\cos k+\cos k'+\tfrac{5}{2}\cos Q)[\tfrac{5}{4}(e^{ik}+e^{-ik'})+\cos Q\, t(k,k')], \tag{11}$$

where $t(k,k') = 1+e^{ik-k'}$, $\omega_\pm = \omega((Q\pm k)/2)$, $\omega_\pm' = \omega((Q\pm k')/2)$, and $\omega(p) = J(\frac{5}{4}+\cos 2p)$. In a similar fashion, we compute the matrix element of the Hamiltonian in momentum space where

$$(\psi_{Q'}(k'), (H-E_0)\psi_Q(k)) = \delta_{Q,Q'}[M\,\delta_{k,k'}(3J/4\omega_+)(3J/4\omega_-)(\omega_++\omega_-)+h_Q(k,k')], \tag{12}$$

$$h_Q(k,k') = \tfrac{1}{2}t(k,k')+\tfrac{3}{8}[t(k,k')+\tfrac{5}{4}(e^{i(Q+k)}+e^{-i(Q+k')})]/\omega_+\omega_+' + \tfrac{3}{8}[t(k,k')+\tfrac{5}{4}(e^{i(Q-k')}+e^{i(k-Q)})]/\omega_-\omega_-'. \tag{13}$$

We construct a wave function $\sum_k f_Q(k)\psi_Q(k)$ and demand that it be an eigenstate of H (within the defect subspace) with eigenvalue $E_0+\epsilon_Q$, which leads to the Schrödinger equation

$$(\epsilon_Q-\omega_+-\omega_-)f_Q(k) = (16/9M)\omega_+\omega_-\sum_{k'} f_Q(k')[h_Q(k',k)-\epsilon_Q\chi_Q(k',k)]. \tag{14}$$

The scattering states are obtained by ignoring the right-hand side and the bottom of the scattering continuum is given by $J(\frac{5}{2}-2|\cos Q|)$ leading to a gap in the spectrum at $Q=0$ of magnitude $J/2$. The wave functions for the scattering states correspond to weakly interacting defects and hence the spectrum has a fourfold degeneracy (three states of spin one and one singlet). We have also studied the possibility of bound states in Eq. (14) numerically. The result of the computation is shown in Fig. 2. It is seen that the bound state emerges from the continuum at $Q \cong 0.36\pi$ and reenters at $Q \simeq 0.64\pi$. The dotted line corresponds to a variational estimate[1] of the fourfold degenerate bound state $\epsilon = 2J_Q$ (indepen-

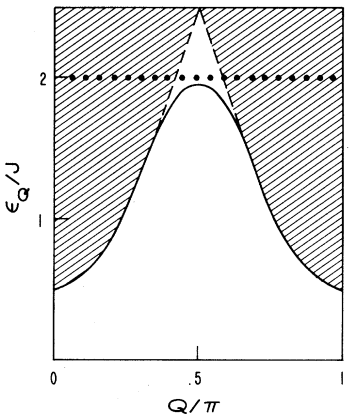

FIG. 2. Excitation spectrum at the point O. Shaded region is the scattering continuum. The dotted line is the variational bound state and the dashed line is the continuation of the scattering continuum threshold.

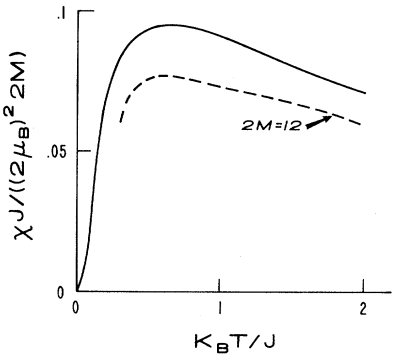

FIG. 3. Low-temperature susceptibility compared with the result of a twelve-spin chain.

dent of Q).

At sufficiently low temperatures, we expect the EE to play an important role in determining the thermodynamic properties. The bound state occurs at energies above the gap and, hence, we may expect the scattering states to dominate the response. We thus assume that we may create $2, 4, 6, \ldots$ propagating and noninteracting well-separated defects at finite temperatures. In the presence of a magnetic field the defects behave as essentially free spin-$\frac{1}{2}$ particles and, hence, their energy is $\omega(k) - bs^z$, where $b = 2\mu_B H_{ext}$ (μ_B is the Bohr magneton). A simple calculation gives the susceptibility χ in terms of Y ($\equiv J/k_B T$) as

$$\chi J/8M\mu_B{}^2 = (0.25Y)\exp(-1.25Y)I_0(Y), \qquad (15)$$

where I_0 is a Bessel function. In Fig. 3, we compare Eq. (15) with the numerical results on finite chains of twelve spins.

It is clear from Fig. 3 that the theory presented in this Letter provides a quantitative explanation for the numerical results based on an appealing physical picture. It has been suggested previously[1] that this system may support gapless modes. We feel, however, that the evidence points towards a finite gap; in fact, the gap we find ($J/2$) seems to lie lower than the lowest spin-one states for a twelve-spin chain. Also, the finite-chain susceptibility resembles that of the anisotropic Heisenberg chain rather than the isotropic (gapless) case. Finally we observe that the defect picture is applicable to the lines OB and OC too but in this case the defects interact (and presumably bind) strongly (one-dimensional Coulomb-like).

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[a]Address after March 1982: Theory Group, Tata Institute of Fundamental Research, Bombay 400005, India.

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