Linked-tetrahedra spin chain: Exact ground state and excitations

Martin P. Gelfand
Department of Physics, University of California, Los Angeles, Los Angeles, California 90024
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A particular quasi-one-dimensional Heisenberg antiferromagnet, which falls into a large and well-known class of models with simple dimerized ground states, is shown to have some especially appealing properties. For $S = \frac{1}{2}$ spins, all excited states are strictly localized, and may be identified with the states of collections of finite, open, $S = 1$ chains.

There is a large class of antiferromagnetic Heisenberg models that are known to have ground states with the particularly simple form of products over singlet pairs. The first example was discovered by Majumdar and Ghosh,[1,2] and it consisted of a $S = \frac{1}{2}$ chain with nearest- and next-nearest-neighbor couplings in the ratio 2:1. In this case the ground state is doubly degenerate. If we represent the singlet combination of spins S_i and S_j by $[i, j]$, then the ground states are $\cdots[-2,-1][0,1][2,3]\cdots$ and $\cdots[-1,0][1,2][3,4]\cdots$. Later work expanded the class of models with such ground states (or ground states with similar features) to include higher dimensions, yet further-neighbor (and multispin) interactions, higher spin, randomness, and other qualities.[3-10] Progress was also made in describing at least some of the excited states for such models, and particularly the original Majumdar-Ghosh model.[11,12]

Consider now the spin Hamiltonian represented by Fig. 1, where the bonds represent isotropic antiferromagnetic couplings of strength J_1, if they are vertical, or J_2, for all others. This does not fall into the class of one-dimensional models with singlet-pair ground states described by Caspers;[6] if the spins were ordered linearly, the resulting interactions would not be fully translationally invariant. However, it is apparent that the Hamiltonian can be partitioned into a sum over interactions within elementary triangles, and by using exactly the argument of, e.g., Shastry and Sutherland,[3] it follows that a sufficient condition for the ground state to consist of the product over singlets on all the vertical bonds is given by

$$J_2/J_1 \equiv r \leq \begin{cases} \frac{1}{2}, & \text{for } S = \frac{1}{2}, \\ [2(S+1)]^{-1}, & \text{for } S \geq 1. \end{cases} \tag{1}$$

This model has two properties which make it of particular interest.

First, the model might be realizable in some physical system. If one takes alternate vertical bonds in Fig. 1 and rotates them about their midpoints so that they lie out of the plane of the page, the resulting geometrical structure is a chain of tetrahedra with shared edges. All the J_2 bonds now correspond to the same distance in space. Fine tuning of parameters is not required, because the singlet-pair ground state is stable for a range of J_2/J_1; but this ratio could conceivably be changed, if desired, by application of uniaxial stress. The singlet-pair ground state is also stable with respect to small magnetic fields, so long as both spins within every vertical pair are subject to the same field, though different pairs can be subject to different fields. Since there is a gap to excited states, we should expect small interchain couplings to have only small effects, as in the case of the quasi-one-dimensional $S = 1$ antiferromagnets.[13] For an example of a magnetic material consisting of tetrahedral units (but joined at corners rather than edges, and with three- rather than one-dimensional arrangement), see Ref. 14.

Second, for $S = \frac{1}{2}$ spins one can say quite a bit more about the solution of the model than the result (1). Let r_c denote the critical value for the stability of the singlet-pair ground state. For $r < r_c$, the elementary excitations are strictly localized (in the sense that all but a finite number of the vertical pairs remain singlets) and may be identified with the states of finite, open, $S = 1$ chains.[15] In consequence, r_c can be accurately determined, and a level-crossing transition for the lowest excited state can be identified.

It is convenient to employ the eigenstates of the system with $J_2 = 0$ as the basis states for the present purposes. Let s_i denote the singlet state on the ith vertical bond, and t_i^-, t_i^0, and t_i^+ (generically, t_i) the triplet states. Decompose the Hamiltonian into terms of the form $J_1\mathcal{S}_i$, for the ith vertical coupling, and $J_2\mathcal{T}_i$, which consists of the four terms that couple the spins of the ith vertical bond to those of the $(i+1)$st. One finds by direct calculation

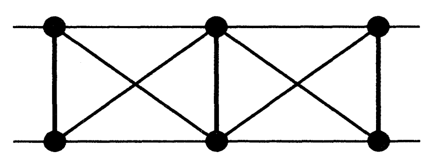

FIG. 1. The quasi-one-dimensional lattice of spins (vertices) and antiferromagnetic couplings (bonds) of present interest. The vertical bonds represent couplings of strength J_1, while all others represent couplings of strength J_2.

that $\mathcal{T}$ "annihilates" singlet states, that is,

$$\mathcal{T}_i|\ldots,s_i,\ldots\rangle = 0, \tag{2}$$

$$\mathcal{T}_i|\ldots,s_{i+1},\ldots\rangle = 0. \tag{3}$$

The action of $\mathcal{T}_i$ on triplet states t_i and t_{i+1} is also simply stated: it is identical to the action of $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$, where the $\mathbf{S}_i$ are spin-*one* operators, and t_i^+ corresponds to a $S_z = 1$ state, etc.

It is now evident that all the eigenstates of the model, for any value of r, may be classified by identifying which sets of vertical neighbors form singlet pairs. To explicitly identify the states within each class one must diagonalize $S = 1$ chains with open boundary conditions for lengths corresponding to the numbers of consecutive vertical pairs which are not singlets. Note that the eigenstates *do not depend* on r, and the eigenvalues vary linearly. (In the nomenclature of Sutherland and Shastry,[4] all eigenstates are superstable with respect to variation of J_2; we discuss the "region of superstability as a ground state" for the singlet-pair state below.)

If the ground state is assumed to be the fully singlet-paired state, the elementary excitations consist of a single triplet pair, with energy J_1 above the ground state; two adjacent triplets, with energies $2J_1 - J_2$, $2J_1$, and $2J_1 + 2J_2$ (and total spin 0, 1, and 2, respectively); and so on. The condition of stability with respect to the formation of two consecutive triplets yields the condition $r_c < 2$, which is rather weaker than (1). For N consecutive triplets, the lowest-lying state has energy $J_1(N + rE_N)$, where E_N denotes the ground state of the N-spin, spin-one chain $\sum_{i=1}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}$; the corresponding stability criterion is $r_c < -N/E_N$. Numerical studies[16] indicate that $-N/E_N$ approaches its $N \to \infty$ limit from above, so that calculations of the energy per spin in chains subject to periodic boundary conditions,[17] extrapolated to $N \to \infty$, may be used to estimate

$$r_c = 0.7135 \pm 0.0003. \tag{4}$$

As r is increased from 0, the character of the lowest-lying excitations changes from isolated triplets to sets of *four* consecutive triplets at $r_4 \approx 0.645\,75$. [It turns out that $r_4 = -(E_4 + 4)$ to machine precision, so the exact value of r_4 is apparently $\sqrt{7}-2$.] On the basis of the data up to $N = 14$, there appear to be no further transitions of this sort between r_4 and r_c, and thus the gap approaches the value $0.6853 J_1$ as $r \to r_c$ from below.

It would to be interesting to find out if nonanalytic behavior of the gap at some $r < r_c$ continues to hold in the presence of experimentally relevant perturbations. For $r > r_c$, the value of the gap is grJ_1 with[17] $g \approx 0.41$; thus as the character of the ground state changes at r_c there is also a discontinuity in the gap, which drops by a factor of ≈ 0.43 upon passing though r_c from below.

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