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CORRESPONDENCE

Lower bound to the ground-state energy of the Heisenberg Hamiltonian on a triangular lattice

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ABSTRACT

A lower bound to the ground-state energy E_0 of the Heisenberg Hamiltonian with longitudinal anisotropy

$$H=\tfrac{1}{2}J\sum_{\langle i,j\rangle}[s_i^z s_j^z+\gamma(s_i^x s_j^x+s_i^y s_j^y)]$$

on the triangular lattice is found to be given by

$$E_0/NJ \geqslant -0{\cdot}25-0{\cdot}400\,\gamma-0{\cdot}037\,\gamma^2$$

for $0\leqslant\gamma\leqslant 1$.

Anderson (1973) and Fazekas and Anderson (1974) discussed the problem of the ground state of the anisotropic Heisenberg Hamiltonian on the triangular lattice, and found that the resonance valence bond functions gave a lower energy than the spin wave theory. For the isotropic case the value obtained is $-0{\cdot}54\,NJ$ as compared with the spin wave value $-0{\cdot}436\,NJ$. For the anisotropic case they express the energy as

$$E_0/NJ \simeq -0{\cdot}25-a\gamma-b\gamma^2, \tag{1}$$

where they estimated $0{\cdot}125 \lesssim a \lesssim 0{\cdot}25$ and $0{\cdot}08 \lesssim b \lesssim 0{\cdot}15$ (γ is defined in (2) below). One way of examining how close this is to the true ground state is to have lower bounds to the ground-state energy E_0. Such lower bounds have been calculated by the method of divide and conquer, that is, the total Hamiltonian is decomposed into sub-Hamiltonians and the lower bound is obtained by observing that the true ground-state wavefunction is a variational function for each of the sub-Hamiltonians. The method has already been used by Anderson (1951) in a similar problem.

The Hamiltonian is written as

$$H=\tfrac{1}{2}J\sum_{\langle i,j\rangle}[s_i^z s_j^z+\gamma(s_i^x s_j^x+s_i^y s_j^y)], \tag{2}$$

$J>0$. The sum goes over i and j, $i\neq j$, the angular brackets indicate that i and j have to be nearest neighbours on the triangular lattice, and γ is the longitudinal anisotropy parameter, $0\leqslant\gamma\leqslant 1$. A simple lower bound is obtained by noting that the triangular lattice contains $2N$ independent triangles, each having the Hamiltonian

$$H_t=\tfrac{1}{2}J\sum_{123}[s_1^z s_2^z+\gamma(s_1^x s_2^x+s_1^y s_2^y)], \tag{3}$$

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the sum going over the three terms obtained by the cyclic permutations of (123). The lowest eigenvalue of (3) is $\frac{1}{2}J(-\frac{1}{4}-\frac{1}{2}\gamma)$ and thus for E_0 of (2)

$$E_0/NJ \geqslant -0{\cdot}25-0{\cdot}5\gamma. \tag{4}$$

The lattice may be divided into N parallelograms, each containing one diagonal bond in addition to the four sides. This gives exactly the same bound as (4).

An improved lower bound is obtained by decomposing the triangular lattice into $\frac{1}{3}N$ hexagons. Each hexagon contains a seven-particle unit, six on the boundary in a ring and the central seventh spin interacting with each of the six spins on the boundary. The Hamiltonian describing this unit is

$$\begin{aligned} H_{\mathrm{h}} = \tfrac{1}{2}J\{ & s_1{}^z s_2{}^z + \tfrac{1}{2}\gamma(s_1{}^+ s_2{}^- + s_1{}^- s_2{}^+) \\ & + s_2{}^z s_3{}^z + \tfrac{1}{2}\gamma(s_2{}^+ s_3{}^- + s_2{}^- s_3{}^+) \\ & + \ldots \\ & + s_6{}^z s_1{}^z + \tfrac{1}{2}\gamma(s_6{}^+ s_1{}^- + s_6{}^- s_1{}^+)\} \\ + J[& s_7{}^z S_6{}^z + \tfrac{1}{2}\gamma(s_7{}^+ S_6{}^- + s_7{}^- S_6{}^+)], \end{aligned} \tag{5}$$

where

$$\mathbf{S}_6 = \sum_{i=1}^{6} \mathbf{s}_i. \tag{6}$$

It will be noted that the coupling of the seventh spin with others is twice as large as that between the spins on the boundary of the hexagon because each bond on the boundary is counted twice as it is shared by two hexagons.

The ground-state energy of (5) for arbitrary γ can be found by well-known methods (Bonner and Fisher 1964, Majumdar, Mabayi and Jain 1973). For the isotropic case ($\gamma=1$) it is very simple. Equation (5) can be written as

$$H_{\mathrm{h}} = \tfrac{1}{2}J\{\mathbf{s}_1 \cdot \mathbf{s}_2 + \ldots + \mathbf{s}_6 \cdot \mathbf{s}_1\} + J\mathbf{s}_7 \cdot \mathbf{S}_6. \tag{7}$$

The terms in braces for the six-membered Heisenberg ring and all its eigenvalues are already known (Orbach 1959). The total spin $\mathbf{S}=\mathbf{S}_6+\mathbf{s}_7$ being a constant of motion, it follows from (7) that

$$H_{\mathrm{h}} = \tfrac{1}{2}J[\mathbf{s}_1 \cdot \mathbf{s}_2 + \ldots + \mathbf{s}_6 \cdot \mathbf{s}_1 + \mathbf{S}^2 - \tfrac{3}{4} - \mathbf{S}_6{}^2]. \tag{8}$$

The ground state belongs to $|\mathbf{S}|=\frac{1}{2}$ and is obtained from the lowest $|\mathbf{S}_6|=1$ state of the ring by combining it with $\mathbf{s}_7$. This gives

$$E_0(\gamma=1) \geqslant -0{\cdot}68634\, NJ. \tag{9}$$

For $\gamma \neq 1$, it should be noted that the total z-component of spin, S^z, is a constant of motion. States in each S^z subspace can be classified according to the representations of an intransitive permutation group of seven objects, which is isomorphic to the dihedral group of the hexagon. The Hamiltonian matrices in these bases can be diagonalized by Householder's method. The table lists the actual lower bound E_{L} to the ground-state energy for various γ. These numbers can be represented with reasonable accuracy by a formula similar to (1):

$$E_0/NJ \geqslant -0{\cdot}25-0{\cdot}400\,\gamma-0{\cdot}037\,\gamma^2. \tag{10}$$

It is interesting that the wavefunctions of the ground states of the clusters show no marked preference for a specific direction of magnetization and can be called ' liquid-like '. However, the nature of the ordering in the true ground state may not be fully reflected in small clusters.

Lower bound for various γ.

γ	E_L/NJ	γ	E_L/NJ
0·0	−0·25000	0·6	−0·50479
0·1	−0·28879	0·7	−0·54981
0·2	−0·32985	0·8	−0·59513
0·3	−0·37238	0·9	−0·64065
0·4	−0·41589	1·0	−0·68634
0·5	−0·46009		

Currently available computer programmes can handle up to 14 spin-$\frac{1}{2}$ particles for the Heisenberg Hamiltonian, and in other kinds of lattices a procedure similar to that used above can be utilized to obtain lower bounds. For the three-dimensional simple cube, $E_0 \geqslant -1{\cdot}205\ NJ$ (Ghosh, Majumdar and Rajagopal 1969) compared with the upper bound $E_0 \leqslant -0{\cdot}9022\ NJ$ (Marshall 1955).

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