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Exact lower bounds to the ground-state energy of spin systems: The two-dimensional $S=\frac{1}{2}$ antiferromagnetic Heisenberg model

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We present a very simple but fairly unknown method to obtain exact lower bounds to the ground-state energy of any Hamiltonian that can be partitioned into a sum of sub-Hamiltonians. The technique is applied, in particular, to the two-dimensional spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model. Reasonably good results are easily obtained and the extension of the method to other systems is straightforward.

The discovery of high-temperature superconductors[1] has induced a renewed interest in models that describe strongly correlated systems, in particular, in the two-dimensional (2D) spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model[2]

$$H_H = J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \,, \tag{1}$$

where $\mathbf{S}_i$ and $\mathbf{S}_j$ are spin operators on sites i and j, the sum is over nearest neighbors (NN), and $J>0$.

Exact results of the spectrum of the Hamiltonian have been obtained for the regular 1D problem[3] and for small finite systems where diagonalization is computationally feasible. A great amount of work has been done for the 2D model, but only numerical ground-state-energy results are known.[4] The best energy value (upper bound) has been obtained variationally by Liang, Douçot, and Anderson[5] ($-0.6688J$/site). In order to supplement the usual variational methods that lead to upper bounds, we present a fairly unknown method that provides exact lower bounds to the ground-state energy of any Hamiltonian that can be partitioned into a sum of subHamiltonians, and apply it, as an example, to the Heisenberg model.

The method is based on a theorem that states that given a Hamiltonian H that can be decomposed into n elementary Hamiltonians H_i, $i=1,2,\ldots,n$:

$$H=\sum_{i=1}^{n} H_i \,, \tag{2}$$

where normally,

$$[H_i,H_j]\neq 0, \quad i\neq j \,, \tag{3}$$

then,

$$E_0 \geq \sum_{i=1}^{n} E_{0i} \,, \tag{4}$$

where E_0 and E_{0i} are, respectively, the ground-state energies of the total Hamiltonian H and of each one of the H_i's. Whenever the H_i commute among them, the equal sign holds.

The proof of this theorem is very simple,

$$H=\sum_{i=1}^{n}\sum_{s} E_{is}\,|i,s\rangle\langle i,s| \,, \tag{5}$$

and

$$I_i=\sum_{s}|i,s\rangle\langle i,s| \tag{6}$$

is the identity in the space of H_i. The index i denotes the subsystems in which the Hamiltonian has been divided $i=1,2,\ldots,n$ (notice that the corresponding subspaces are in general overlapping). s is the index that sums over the whole spectrum of H_i, and E_{is} are the corresponding energies with

$$E_{i0}\leq E_{i1}\leq \cdots \leq E_{is}\leq \cdots \leq E_{in} \,. \tag{7}$$

Then,

$$\sum_{i=1}^{n}\sum_{s} E_{is}\,|i,s\rangle\langle i,s| \geq \sum_{i=1}^{n} E_{i0}\sum_{s}|i,s\rangle\langle i,s| = \sum_{i=1}^{n} E_{i0} I_i \,, \tag{8}$$

from which (4) follows.

Once a particular decomposition is chosen, it only remains to obtain the ground-state energies of H_i, which usually are such that they do not depend on i, or at most fall into a few classes. The efficiency of the method will strongly depend on the choice of the H_i's.

We have applied this technique to the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model (1) on the square lattice.

The square lattice can be partitioned into different pieces: lines, squares, crosses, etc. From all elementary partitions, i.e., those where H_i is trivially diagonalized, the best has proved to be into crosses. The ground-state energy corresponding to a cross is easily computed. We have [see Fig. 1(a)]

$$\begin{aligned} H_a &= J(\mathbf{S}_1\cdot\mathbf{S}_2+\mathbf{S}_1\cdot\mathbf{S}_3+\mathbf{S}_1\cdot\mathbf{S}_4+\mathbf{S}_1\cdot\mathbf{S}_5) \\ &= J/2[\mathbf{S}_{12345}^2-\mathbf{S}_1^2-\mathbf{S}_{2345}^2] \,, \end{aligned} \tag{9}$$

where $\mathbf{S}_{12345}\equiv \mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3+\mathbf{S}_4+\mathbf{S}_5$, etc. Therefore,

$$E_a = J/2[S(S+1)-\tfrac{3}{4}-\mathrm{S}_{2345}(\mathrm{S}_{2345}+1)] \,, \tag{10}$$

with $S=S_{12345}$ the total spin.

By the Lieb and Mattis theorem for bipartite lattices,[6] the ground state will have total spin $S=\frac{3}{2}$. Furthermore,

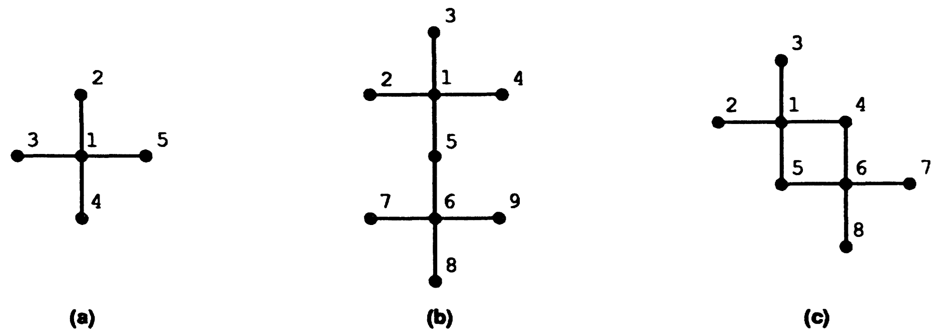

FIG. 1. Elementary Hamiltonians considered.

$S_{2345} = 2$. Then,

$$E_{a0} = -1.5J . \tag{11}$$

The next step consists of doing the proper combination of these H_a in order to recover H. In the square lattice, two bonds are assigned to each site; when covering the lattice with crosses centered at all sites, four bonds are introduced per site. Then, the following lower bound to the ground-state energy of the whole system is obtained:

$$E^{(a)}/\text{site} = E_{a0} \times \tfrac{2}{4} = -0.75J . \tag{12}$$

This is an exact lower bound to the ground-state energy of the square lattice which has been obtained with no effort. Any other elementary partition, which incidentally all have a lower ground-state spin, leads to a worse bound.

An improvement of this result can be obtained by defining new H_i's which are combinations of the previous elemental H_i's.

In our case, the new H_i's correspond to combinations of crosses. The same theorem (4) assures that these H_i's will provide a better lower bound to the ground-state energy of the whole system.

Only two different combinations of two crosses exist [see Figs. 1(b) and 1(c)]. Their Hamiltonians can be written as

$$H_b = J/2[\mathbf{S}^2_{1234} - \mathbf{S}^2_1 - \mathbf{S}^2_{234} + \mathbf{S}^2_{6789} - \mathbf{S}^2_6 - \mathbf{S}^2_{789}] + J\mathbf{S}_5(\mathbf{S}_1 + \mathbf{S}_6) , \tag{13}$$

and

$$H_c = J/2[\mathbf{S}^2_{1234} - \mathbf{S}^2_1 - \mathbf{S}^2_{234} + \mathbf{S}^2_{6789} - \mathbf{S}^2_6 - \mathbf{S}^2_{789}] + J(\mathbf{S}_1 \cdot \mathbf{S}_5 + \mathbf{S}_4 \cdot \mathbf{S}_6) . \tag{14}$$

For H_b the ground-state spin is[6] $S = \frac{5}{2}$. Now, as

$$[H_b, \mathbf{S}^2_{234}] = [H_b, \mathbf{S}^2_{789}] = 0 \tag{15}$$

the ground state also has well-defined values of S_{234} and S_{789}. It is a less straightforward consequence of the proof of the same theorem of Lieb and Mattis that $S_{234} = S_{789} = \frac{3}{2}$ (i.e., they take their maximum value as their spins belong to the same sublattice in the language of Ref. 6). The diagonalization of H_b which has to be performed in order to obtain E_{b0} thus boils down to consider its reduction to the 7D $S = \frac{5}{2}$, $S_{234} = S_{789} = \frac{3}{2}$ subspace. For H_c a similar argument based on

$$[H_c, S^2_{23}] = [H_c, S^2_{78}] = 0 \tag{16}$$

leads to the reduction of H_c in the 11D $S = 2$, $S_{23} = S_{78} = 1$ subspace. These matrices are easily diagonalized and the corresponding lower bounds come out to be

$$E^{(b)}/\text{site} = E_{b0} \times \tfrac{2}{8} = -0.7421J ,$$
$$E^{(c)}/\text{site} = E_{c0} \times \tfrac{2}{8} = -0.7391J . \tag{17}$$

This process can be further iterated, so that better lower bounds will be obtained defining new subsystems H_i, combination of the previous ones. The computations performed suffice, however, to show the efficiency and simplicity of the method.

In conclusion, we have presented a technique for obtaining exact lower bounds to the ground-state energy that provides reasonably good results with little computational effort and can be improved by applying the method iteratively.

The 2D Heisenberg Hamiltonian has been chosen as an example and fairly good results have been obtained (17).

This method can be applied to a wide variety of systems and Hamiltonians and its most relevant features are its simplicity and the fact that it limits energies from below.

Note added in proof. We have run a computer program by Allan H. MacDonald (Indiana University) with which we have obtained the ground-state energies for the Hamiltonian formed by four crosses in a 45° tilted square [twice Fig. 1(c), 13 sites]

$$E/\text{site} = E_0 \times \tfrac{2}{16} = -0.7224J$$

and for the Hamiltonian formed by six crosses in a 45° tilted rectangle [three times Fig. 1(c), 18 sites]

$$E/\text{site} = E_0 \times \tfrac{2}{24} = 0.7158J .$$

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