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Inequalities between ground-state energies of Heisenberg models

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HIGHLIGHTS

- Lieb–Schupp inequality has been numerically examined for families of Heisenberg systems.
- Precision of inequalities has been computed for some families of 1-d systems.
- They turned out to be related to the speed of correlation fall-off.
- We have formulated as a conjecture the quantified form of this relation.

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ABSTRACT

The Lieb–Schupp inequality is the inequality between ground state energies of certain antiferromagnetic Heisenberg spin systems. In our paper, the numerical value of energy difference given by Lieb–Schupp inequality has been tested for spin systems in various geometries: chains, ladders and quasi-two-dimensional lattices. It turned out that this energy difference was strongly dependent on the class of the system. The relation between this difference and a fall-off of a correlation function has been empirically found and formulated as a conjecture.

1. Introduction

The list of general results on the area of quantum spin systems is not too large. Among them, there is a result due to Schupp [1], establishing the inequality between a ground-state energies of an antiferromagnetic Heisenberg chains. (The simplest example is the difference $2E_{m+n}$ and $E_{2n} + E_{2m}$, where E_k is the ground state energy of the Heisenberg chain with k sites). Later on, this inequality has been extended to more general class of Heisenberg models [2].

These inequalities are rigorous ones. They are based on the matrix inequality proved by Kennedy, Lieb and Shastry (KLS) [3]. Authors applied this inequality to prove the existence of the Long Range Order in a class of anisotropic Reflection-Positive $d \geq 2$ quantum Heisenberg models. The KLS inequality has also been applied to establish certain properties of ground states of Hubbard models [4–6] as well as to prove the absence of orderings in Heisenberg models on pyrochlore lattices [7,8].

Although the Schupp inequalities between ground-state energies of Heisenberg models are rigorous, they do not give any information about the actual value of this difference. It would be very interesting to test how close to each other are both sides of the inequality. This was one of the goals of our paper: *To test a numerical value of the difference between the both sides of the inequality.*

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We have tested this difference numerically. We used exact diagonalization procedure and in some cases the DMRG method. The ARPACK++ and ALPS packages have been used [9,10]. We considered systems in various geometries: chains, ladders, and rectangles, up to 27–28 sites[2] (exact diagonalization) and 200–256 sites (DMRG). As a rule, the differences between both sides of inequality were *very small*. More quantitative considerations allowed us to pose certain conjecture between strength of spin correlations in the system and the difference between both sides of inequality.

The outline of the paper is as follows.

In Section 2, the ground-state energy inequalities have been formulated.

In Section 3, the differences between both sides of inequality for various systems have been numerically tested. The chains, ladders, and rectangles in various geometries: square, pyrochlore and squares with crossing bonds, have been analysed. The results and their implications (both rigorous and conjectural) have been presented.

Section 4 contains summary, conclusions as well as perspectives for future research.

2. Formulation of inequalities

2.1. Structure of the system

We consider finite lattice spin systems with all spins being finite, so all spaces are finite-dimensional and operator are matrices. We assume that all spins are identical (this assumption can be relaxed).

We consider system which can be divided into two subsystems: L (‘left’) and R (‘right’) parts. Corresponding division of the total Hilbert space $\mathcal{H}$ is:

$$\mathcal{H} = \mathcal{H}_L \otimes \mathcal{H}_R, \tag{1}$$

where $\mathcal{H}_L$ and $\mathcal{H}_R$ are Hilbert spaces for the L and R subsystems, respectively. Let H_L be the Hamiltonian of the L subsystem acting on $\mathcal{H}_L$, and analogously H_R the Hamiltonian of the R subsystem acting on $\mathcal{H}_R$. They can be lifted to operators acting on the whole $\mathcal{H}$:

$$H_L \to H_L \otimes \mathrm{Id}_R, \qquad H_R \to \mathrm{Id}_L \otimes H_R. \tag{2}$$

Then, the Hamiltonian is of the following general form:

$$H = H_L \otimes \mathrm{Id}_R + \mathrm{Id}_L \otimes H_R + H_I, \tag{3}$$

where H_I is the ‘interaction’ Hamiltonian, acting on $\mathcal{H}$.

2.2. Assumptions on Hamiltonian

Hamiltonians H_L and H_R are arbitrary spin-interaction Hamiltonians. The crucial assumption is the one concerning the interaction Hamiltonian H_I.

We assume [1] that it is the sum of *antiferromagnetic Heisenberg interactions*. More precisely:

Let $A \subset L$ be some m-site subset of L: $m = |A|$. Let us write: $A = \{i_1, i_2, \dots, i_m\}$. Let us define $\mathbf{S}_A$ being operator acting on $\mathcal{H}_L$: $\mathbf{S}_A = \sum_{k=1}^m J_k \mathbf{s}_{i_k}$, where coefficients J_k are *real*, and $\mathbf{s}$ is total spin operator: $\mathbf{s} = (s^x, s^y, s^z)$. Let $A' \subset R$ be some subset of R, let $m = |A'|$, let $A' = \{i'_1, i'_2, \dots, i'_m\}$, and define $\mathbf{S}_{A'}$—an operator acting on $\mathcal{H}_R$: $\mathbf{S}_{A'} = \sum_{k=1}^m J_k \mathbf{s}_{i'_k}$. (So, we can say that $\mathbf{S}_{A'}$ is a ‘mirror image’ of $\mathbf{S}_A$; but we *do not* assume that the L system is a mirror image of R system.) Then we assume that the interaction Hamiltonian is of the form

$$H_I = \sum_A \mathbf{S}_A \cdot \mathbf{S}_{A'}. \tag{4}$$

The simplest example of A is one site; it leads to ordinary Heisenberg AF interaction. For A being two-site set, an example is the pyrochlore lattice. We will consider these two sorts of interactions. See Figs. 1 and 2.

2.3. Formulation of the main inequality

Consider now the following Hilbert spaces and systems (‘LL’ and ‘RR’ ones):

$$\mathcal{H}_{LL} = \mathcal{H}_L \otimes \mathcal{H}_L, \qquad \mathcal{H}_{RR} = \mathcal{H}_R \otimes \mathcal{H}_R; \tag{5}$$

and Hamiltonians:

$$H_{LL} = H_L \otimes \mathrm{Id}_L + \mathrm{Id}_L \otimes H_L + \sum_A \mathbf{S}_A \cdot \mathbf{S}_A, \tag{6}$$

$$H_{RR} = H_R \otimes \mathrm{Id}_R + \mathrm{Id}_R \otimes H_R + \sum_{A'} \mathbf{S}_{A'} \cdot \mathbf{S}_{A'}. \tag{7}$$

[2] Depending on the lattice type.