Some properties of frustrated spin systems: extensions and applications of Lieb-Schupp approach

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Abstract. Lieb and Schupp have obtained a number of ground-state properties for frustrated Heisenberg models. The basic tool used was certain version of "spin-reflection positivity" method. One group of these results is related to singlet nature of ground state. It needs an assumption of reflection symmetry present in the system. In this paper, it is shown that analogous results hold also for other symmetries (inversion etc.). The second Lieb-Schupp result is matrix inequality, which imply inequalities between ground-state energies of certain systems. In the paper, the Lieb-Schupp inequality is applied to relate ground-state energies of various systems: spin chains, ladders and multidimensional lattices.

PACS. 75.10.Jm Quantized spin models – 75.50.Ee Antiferromagnetics – 05.50.+q Lattice theory and statistics (Ising, Potts, etc.)

1 Introduction

Geometric frustration takes place, when no arrangement of spins on the lattice is possible in such a way that all interactions minimize their energy. The canonical example is an antiferromagnetic Ising model on triangular lattice [1] (see Fig. 1). Another systems where the geometric frustration is particularly strong, are antiferromagnetic systems on kagomé, pyrochlore, or (in $d = 3$) fcc cubic lattices.

Frustrated systems are very interesting and hard to analyse, both in classical version and especially in the quantum case. The source of these difficulties traces back to the large ground-state degeneracy in the classical version. Such systems are very sensitive to perturbations. A consequence is possibility of very complicated phase diagram at finite temperatures. The canonical example of such beahviour is an ANNNI model [3], where such phenomena as the presence of infinite number of phases, devil's staircase etc. appear. Besides of numerous efforts and important results, [2–4], (for reviews, see [5,6,8]), full treatment of such systems is not worked out so far.

The situation for quantum frustrated antiferromagnets is even less clear. It is generally suspected that the ground state emerging as a linear combination of many classical configurations is a featureless, "spin liquid" state, i.e. the state without long-range ordering, where correlation functions fall off exponentially [9]. However, another scenario are also possible: it is "order by disorder" – exotic ordering(s) absent in a classical version of these models. It is difficult to predict which type of scenario will take
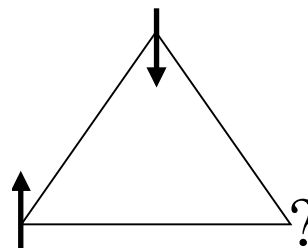

Fig. 1. Example of frustrated spin system.

place in given concrete system. (For a review, see for instance [7].) To my best knowledge, no general definite conclusions have been obtained so far.

Most informations obtained comes from an analysis using approximate methods, such as guessing of ground-state wave functions, numerical diagonalization of small systems, spin waves, semiclassical (i.e. large-S) approximations. However, it is difficult to estimate how reliable are these approximations. For this reason, exact results are very desirable. Unfortunately, they are very exceptional.

In such a situation, exact results obtained by Lieb and Schupp [10,11] (summarized also in [12]) for fully frustrate systems are of first importance. They are interesting both as themselves and moreover, they can serve as a test of validity of approximate methods. Results obtained in [10,11] can be divided into two groups. The first one concern ground-state properties for such systems and it can be summarized as follows: ground states are singlets; zero-field magnetization is zero; susceptibility is bounded by certain constant. One of assumptions of these theorems

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is *reflection symmetry*. It was apparent that this method could work also for another kind of symmetry, not necessarily reflection one. Such a generalization turned out to be possible, and this is the first result of the paper.

The second collection of results [11] concern comparison of ground state energies for spin rings. It turned out that similar results hold for more complicated systems (multidimensional lattices). This is second result of the paper.

The outlook of the paper is as follows. In Section 2, the basic ingredients of Lieb and Schupp technique are presented. Some systems of physical interest, for which the results of [10,11] can be applied, are listed. After that, the Lieb-Schupp technique is adapted to systems exhibiting symmetry other than reflection one (rotation or inversion). In Section 3, Lieb and Schupp results concerning comparison of ground-state energies for spin rings with the use of certain matrix inequality are described. Then it is discussed how this technique can be applied to other systems – for instance ground-state energies of systems on different lattices. Section 4 contains short summary and conclusions. The Appendix contains proof of Lieb-Schupp inequality, which is fundamental for Section 3.

2 Lieb-Schupp approach and generalizations for spin systems with symmetries

2.1 Reflection-symmetric systems

2.1.1 Assumptions

We make the following assumptions concerning systems under consideration.

1. We consider Heisenberg models for arbitrary spin. (Below we consider mainly the $s = 1/2$ case, but generalization to other spin values is straightforward.)
2. The system is invariant with respect to the reflection with respect to the O axis ($d - 1$ plane for d-dimensional system). The system consist of two parts ("Left" and "Right" ones), which are interchanged under reflection (see Fig. 2). The Hilbert space $\mathcal{H}$ of the system is a tensor product of Hilbert spaces $\mathcal{H}_L, \mathcal{H}_R$ of the corresponding subsystems; $\mathcal{H}_L$ and $\mathcal{H}_R$ are isomorphic. The Hamiltonian is a sum of three parts: H_L, H_R and H_C; H_L acts only on the left part (i.e. $H_L = h \otimes \mathbf{1}$), whereas H_R acts on the right one (i.e. $H_R = \mathbf{1} \otimes h$). H_C is the Hamiltonian for "crossing bonds" (i.e. for bonds which intersect the symmetry line). It has the form:
$$H_C = \sum_{y \in L, \, y' \in R} j_{y,y'} \hat{\mathbf{s}}_y \cdot \hat{\mathbf{s}}_{y'} \qquad (1)$$
where $j_{y,y'}$ is a diagonal matrix with non-negative diagonal elements. The object $\hat{\mathbf{s}}_y$ can be a single spin or more generally, it can be a linear combination of them: $\hat{\mathbf{s}}_y = \sum_{\alpha \in L} j_{i;\alpha} \mathbf{s}_\alpha$, where $j_{i;\alpha}$ are real coefficients. The objects $\hat{\mathbf{s}}_y$ need not be all identical for all indices y. Under reflection operation, H_L is transformed to H_R and vice versa, whereas H_C transforms into itself.
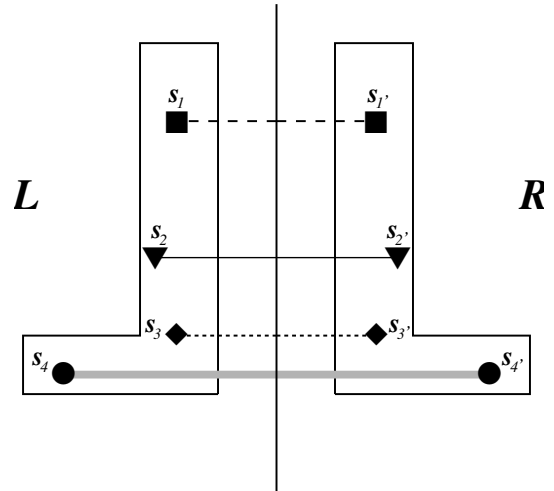

Fig. 2. System exhibiting reflection symmetry.

3. H_L and H_R are (almost) arbitrary: the only limitations are: both commute with the total spin operator, and
4. moreover, all operators: H_L, H_R and H_C are *real* in the S^3 basis. More precisely, it means that their matrices are real in the base built up from tensor products of S^3 eigenstates of every spin.

2.1.2 Ground state properties

Every state of the system can be expressed as a linear combination:
$$\psi = \sum_{\alpha,\beta} c_{\alpha\beta} \psi_\alpha^L \otimes (\psi_\beta^R)_{\text{rot}}, \qquad (2)$$

where states ψ_α^L form a real orthonormal base of S^3 eigenstates for the left subsystem, whereas $(\psi_\beta^R)_{\text{rot}}$ are corresponding *rotated* states for the right subsystem. (The rotation – meant as an operation in the spin space – acting for the state: $|s, m\rangle$ produces the state $(-1)^{s-m}|s, -m\rangle$.)

The eigenvalue problem: $H\psi = E\psi$ can be written as a matrix equation for c matrix:

$$h_L c + c(h_R)^T - \sum_{i=1}^{3} \sum_y t_y^{(i)} c (t_y^{(i)})^T = Ec, \qquad (3)$$

where $(h_L)_{\alpha\beta}$ and $(h_R)_{\alpha\beta}$ are real, symmetric matrices for corresponding terms of the Hamiltonian, whereas $t_y^{(i)}$ are *real* matrices, defined for spin operator $\hat{\mathbf{s}}_y = \sum_{\alpha \in L} j_{i;\alpha} \mathbf{s}_\alpha$ (in the yth "bond") by: $t_{y;\alpha\beta}^{(1,3)} = \langle \psi_\alpha^L | \hat{s}_y^{(1,3)} | \psi_\beta^L \rangle$ and $t_{y;\alpha\beta}^{(2)} = i\langle \psi_\alpha^L | \hat{s}_y^{(2)} | \psi_\beta^L \rangle$. Notice the total "minus" sign before third term in expression (3); it is so because replacement of $\hat{\mathbf{s}}_y$ by $\hat{\mathbf{s}}_{y'}$ produces sign change for components 1 and 3, whereas the i factor in definition of $t^{(2)}$ produces minus sign for component 2.

The energy expectation value, expressed in term of the c matrix, is

$$\langle\psi|H|\psi\rangle = \mathrm{Tr}\,(cc^\dagger h_L) + \mathrm{Tr}\,(c^\dagger ch_R)$$
$$- \sum_{i=1}^{3}\sum_{y} \mathrm{Tr}\,c^\dagger t_y^{(i)}c(t_y^{(i)})^\dagger. \quad (4)$$

Lieb and Schupp have established a number ground-state properties for reflection-symmetric systems. There are:

1. The c matrix is hermitian, i.e. without loss of generality we can express eigenstates of H by *hermitian* matrix $c = c^\dagger$. (It is proved using the left-right symmetry in expression (4) for energy.)
2. Let the c matrix corresponds to the ground state; then, also the $|c|$ matrix corresponds to the ground state. Here $|c| = \sqrt{c^2}$; we take the unique positive square root. (It is proved by writing down (4) in the diagonal basis.)
3. Properties above imply that we can choose the base for ground states as a collection of functions of the form (2), where $c_{\alpha\beta}$ are positive semi-definite (p.s.d.) coefficient matrices.
4. The overlap of the ground state with canonical spin-zero state (given by unit matrix in a basis of $S^{(3)}$ eigenstates in either subsystem) is non-zero.
5. This property implies that there exist ground state with spin zero, and moreover, that coefficient matrix for this state is positive semidefinite. It follows from the inequality: $E_b \geq E_0$ (E_b is an energy of the system in the magnetic field b), which in turn is proved using the matrix inequality (8).
6. We have "ice rule" for frustrated units, i.e. for collection of spins appearing in the expression $\hat{\mathbf{s}}_y \cdot \hat{\mathbf{s}}_{y'}$ for every index y. More precisely, if we denote: $\hat{\mathbf{s}}_y = \sum_{\alpha \in L} j_\alpha \mathbf{s}_\alpha$, then the expectation of the third component of sites in each crossing bond vanishes for any ground state $|\psi_0\rangle$:

$$\langle\psi_0|\hat{\mathbf{s}}_y + \hat{\mathbf{s}}_{y'}|\psi_0\rangle.$$

Let us note that it is a "local" property, valid for every "bond" separately. It is rather obvious if we know that the ground state is singlet. However it is fulfilled also in *all* ground states, where we have no warranty that all ground states are singlets.

Under additional assumptions, these results can be made stronger. For instance, if the system has periodic boundary condition in at least one direction, then – using the "ice rule" property – one shows ([10,11]) that *all* ground states are singlets. Moreover, the magnetic susceptibility is bounded from above, both in the ground state and in positive temperatures.

Remark. Lieb and Schupp in [10] and [11] have developed general method and (almost) haven't given examples of systems where their method could apply; the only example discussed is the checkerboard pyrochlore lattice. Some further examples of physical interest, where their results are applicable, are:
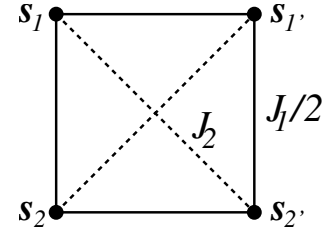
Fig. 3. Spin enumeration on square plaquette.

1. $J_1 - J_2$ 2d Heisenberg model:

$$H = J_1 \sum_{n.n.} \mathbf{s}_i \cdot \mathbf{s}_j + J_2 \sum_{n.n.n.} \mathbf{s}_i \cdot \mathbf{s}_j \quad (5)$$

(we consider antiferromagnetic case, i.e. $J_1, J_2 > 0$). It was considered by numerous authors – see, for instance, [13] and references therein. This model exhibits very interesting behaviour: when the quotient J_2/J_1 is varied, the ground state undergoes a transition from ordered, antiferromagnetic state to the 'glassy', non-magnetic, spin-liquid-like one. (Such a picture emerged as a result of investigations with the use of approximate methods). Lieb and Schupp results apply for $J_2 \leq \frac{1}{2}J_1$. This condition is rather easy corollary from results of [11] (in [10] less general result appear, namely, $J_2 = \frac{1}{2}J_1$). As this stronger result does not appear explicitly in [11], the short derivation will be given: The Hamiltonian (5) can be written in "plaquette" form:

$$H = \sum h_\square,$$

where

$$h_\square = \frac{1}{2}J_1(\mathbf{s}_1 \cdot \mathbf{s}_{1'} + \mathbf{s}_2 \cdot \mathbf{s}_{2'} + \mathbf{s}_1 \cdot \mathbf{s}_2 + \mathbf{s}_{1'} \cdot \mathbf{s}_{2'})$$
$$+ J_2(\mathbf{s}_1 \cdot \mathbf{s}_{2'} + \mathbf{s}_{1'} \cdot \mathbf{s}_2);$$

(see Fig. 3); this expression can be written as

$$h_\square = J_2\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}' + \left(\frac{1}{2}J_1 - J_2\right)\left(\mathbf{s}_1 \cdot \mathbf{s}_{1'} + \mathbf{s}_2 \cdot \mathbf{s}_{2'}\right)$$
$$+ \frac{1}{2}J_1(\mathbf{s}_1 \cdot \mathbf{s}_2 + \mathbf{s}_{1'} \cdot \mathbf{s}_{2'}) \quad (6)$$

where $\hat{\mathbf{s}} = \mathbf{s}_1 + \mathbf{s}_2$, $\hat{\mathbf{s}}' = \mathbf{s}_{1'} + \mathbf{s}_{2'}$. Consider $h_\square$ as "crossing bond". Then, the third term in (6) is irrelevant, as it contains terms belonging to the left and right subsystems only. The second term is antiferromagnetic if $J_2 \leq J_1/2$. In such a case, first and second terms are of desired form (1). Note that spins $\mathbf{s}_i$ and $\hat{\mathbf{s}}$ are of different nature. Note also that all conclusions above are still valid, if we consider the anisotropic version of the Hamiltonian (5):

$$H = J_v \sum_{v.n.n.} \mathbf{s}_i \cdot \mathbf{s}_j + J_h \sum_{h.n.n.} \mathbf{s}_i \cdot \mathbf{s}_j + J_2 \sum_{n.n.n.} \mathbf{s}_i \cdot \mathbf{s}_j \quad (7)$$

where $v.n.n$ denotes vertical nearest neighbour and $h.n.n$ denotes horizontal nearest neighbours. For

the Hamiltonian (7) Lieb-Schupp results hold for $J_2 \le J_h/2$, whereas J_v can be arbitrary (even ferromagnetic).

Most of approximate methods of analysis of (5) *assume* that its ground state is singlet. Lieb and Schupp' results can be used to justify this assumption. Moreover, it can serve also as a test of these methods by supplying rigorous upper bounds for susceptibility.

2. Axial Next-Nearest-Neighbour Heisenberg (ANNNH) model [5]. This is Heisenberg model with two coupling constants; we have isotropic coupling J_1 between nearest neighbours, and moreover, there is coupling J_2 between second neighbours along one of the axes (say, z axis). Such models have been used to describe helical and incommensurate configurations, and Lifshitz points in magnets ([5] and references therein). Lieb-Schupp results can be applied when both constants are antiferromagnetic, or when J_1 is antiferromagnetic and J_2 is ferromagnetic (in this case, one should take the reflection plane to be parallel to the line formed by J_2 couplings).

2.2 Generalization to other symmetries

In the course of proofs in the previous section, geometric properties of systems exhibiting reflection symmetry were *not* employed. Only assumption which was used was that h_L transforms into h_R and vice versa; particular nature of this transformation was not essential. It suggests that more general symmetry operations than reflection are allowed. It is the case; more precise formulation is as follows.

We make assumptions identical as 1., 3. and 4. in Section 2.1.1; the assumption 2. is changed into the following one.

2'. The system again can be divided by two identical parts "L" and "R", each of them is described by the Hamiltonians $H_L = h \otimes \mathbf{1}$ and $H_L = \mathbf{1} \otimes h$, respectively. H_C is the Hamiltonian for "bonds" between spins in L and R subsystems. It has the form:

$$H_C = \sum_{i \in L, i' \in R} \gamma_{i,i'} \mathbf{s}_i \cdot \mathbf{s}_{i'}$$

where the symmetric $\gamma_{i,i'}$ matrix is positive definite. One can view on this property as a demand that H_C has to be "globally antiferromagnetic", i.e. some coupling constants $\gamma_{i,i'}$ can be negative (ferromagnetic), however, the whole matrix γ has to be positive definite. The whole system is invariant with respect to the some symmetry operation $\mathbf{T}$, such that $\mathbf{T}^2 = \mathbf{1}$ ($\mathbf{1}$ is identity operator); $\mathbf{T}$ transforms the "L" subsystem into "R" one and vice versa. The following operations: reflection, C_2 rotation (see Fig. 4), or inversion can serve as examples of such operation. Under action of $\mathbf{T}$, H_L transforms into H_R, H_R into H_L and H_C into itself.

The system described above can be easily transformed into form equivalent to the one considered in the previous subsection. Let us notice that H_C is *bilinear* in $\mathbf{s}_i, \mathbf{s}_{i'}$.
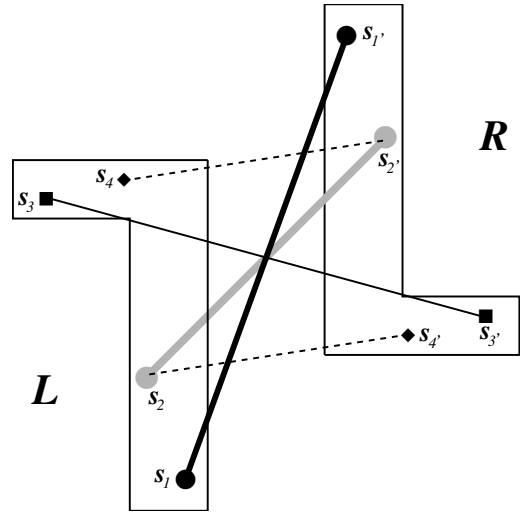

Fig. 4. System exhibiting inversion symmetry.

Then, the form: $H_C = \sum_{i \in L, i' \in R} \gamma_{i,i'} \mathbf{s}_i \cdot \mathbf{s}_{i'}$ can be diagonalized by suitable linear transformation in the spin variables on "L" and the same transformation on "R". After diagonalization, H_C takes the form

$$H_C = \sum_{I \in L, I' \in R} J_{I,I'} \sigma_I \cdot \sigma_{I'}$$

where the matrix $J_{I,I'}$ is diagonal and has only nonnegative elements. Then, we have system in the form analogous as (1) and one can repeat all considerations from previous subsection, obtaining analogous results. One should only remember that the "ice rule" concern spin variables after diagonalizing transformation, i.e. we have

$$\langle \psi_0 | \sigma_I + \sigma_{I'} | \psi_0 \rangle = 0.$$

3 Trace inequality and comparison of ground-state energies for various systems

Lieb and Schupp have proved beautiful inequality for traces of matrices. It is crucial in further considerations.

Theorem ([11,12]). Let M, N – square matrices of dimensions $m \times m$ and $n \times n$ respectively, and c – rectangular $m \times n$ matrix. Then the following inequality holds:

$$|\mathrm{Tr}\, c^\dagger M c N^\dagger| \le \frac{1}{2}(\mathrm{Tr}\, c_L M c_L M^\dagger + \mathrm{Tr}\, c_R N c_R N^\dagger), \quad (8)$$

where $c_R = \sqrt{c^\dagger c}$, $c_L = \sqrt{cc^\dagger}$ are unique (positive) square roots from positive definite matrices $c^\dagger c$ and $cc^\dagger$.

For the convenience of reader, the proof is supplied in Appendix A.

Now, let us consider the system *without* reflection symmetry, which however still consists of the "left" subsystem L described by H_L and the "right" subsystem R described by H_R. The Hilbert space $\mathcal{H}$ of the system is a tensor product of Hilbert spaces $\mathcal{H}_L, \mathcal{H}_R$ of the corresponding subsystems; however, $\mathcal{H}_L$ and $\mathcal{H}_R$ don't have

to be isomorphic. The full system will be denoted by $L-R$, and its Hamiltonian H_{L-R} contains also the "crossing bond" term H_C, describing "interaction" of these two parts: $H_{L-R} = H_L + H_R + H_C$. Every state of the system can be written in the form (2). We change slightly the notation and write an analogon of (2) as:

$$\psi = \sum_{\alpha, \beta'} c_{\alpha\beta'} \psi^L_\alpha \otimes (\psi^R_{\beta'})_{\text{rot}}, \qquad (9)$$

to distinguish between indices referring to the L part (unprimed) and R (primed ones). Remember that the c matrix is now, in general, the *rectangular* one.

Consider first the situation, where H_C corresponds to only *one* bond coupling both subsystems:

$$H_C = \mathbf{s} \cdot \mathbf{S},$$

where $\mathbf{s}$ belongs to L and $\mathbf{S}$ belongs to R. One can write expression for the mean value of energy in the manner analogous as equation (4):

$$E_{L-R} = \text{Tr}\, cc^\dagger h_L + \text{Tr}\, c^\dagger c h_R - \sum_{\mu=1}^3 \text{Tr}\left[c^\dagger t^{(\mu)} c (T^{(\mu)})^\dagger\right], \tag{10}$$

where: h_L, h_R are matrices of corresponding Hamiltonians. t refers to the left subsystem, whereas T to the right one; t, T matrices are given by: $t^{(1,3)}_{\alpha\beta} = \langle\psi^L_\alpha|s^{(1,3)}|\psi^L_\beta\rangle$, $t^{(2)}_{\alpha\beta} = i\langle\psi^L_\alpha|s^{(2)}|\psi^L_\beta\rangle$, and similarly for T: $T^{(1,3)}_{\alpha'\beta'} = \langle\psi^R_{\alpha'}|S^{(1,3)}|\psi^R_{\beta'}\rangle$, $T^{(2)}_{\alpha'\beta'} = i\langle\psi^R_{\alpha'}|S^{(2)}|\psi^R_{\beta'}\rangle$.

Inequality (8) applied to the last term of (10) gives:

$$-\sum_{\mu=1}^3 \text{Tr}\, c^\dagger t^{(\mu)} c (T^{(\mu)})^\dagger \geq$$
$$-\frac{1}{2}\sum_{\mu=1}^3\left(\text{Tr}\, c_L t^{(\mu)} c_L (t^{(\mu)})^\dagger + \text{Tr}\, c_R T^{(\mu)} c_R (T^{(\mu)})^\dagger\right).$$

Then, we can write:

$$E_{L-R} \geq \text{Tr}\, cc^\dagger h_L + \text{Tr}\, c^\dagger c h_R$$
$$-\frac{1}{2}\sum_{\mu=1}^3\left(\text{Tr}\, c_L t^{(\mu)} c_L (t^{(\mu)})^\dagger + \text{Tr}\, c_R T^{(\mu)} c_R (T^{(\mu)})^\dagger\right)$$
$$= \text{Tr}\, c_L c_L h_L + \text{Tr}\, c_R c_R h_R$$
$$-\frac{1}{2}\sum_{\mu=1}^3\left(\text{Tr}\, c_L t^{(\mu)} c_L (t^{(\mu)})^\dagger + \text{Tr}\, c_R T^{(\mu)} c_R (T^{(\mu)})^\dagger\right)$$
$$= \frac{1}{2}\left(\text{Tr}\, c_L c_L^\dagger h_L + \text{Tr}\, c_L^\dagger c_L h_L - \sum_{\mu=1}^3 \text{Tr}\, c_L^\dagger t^{(\mu)} c_L (t^{(\mu)})^\dagger\right) \tag{11}$$
$$+ \frac{1}{2}\left(\text{Tr}\, c_R c_R^\dagger h_R + \text{Tr}\, c_R^\dagger c_R h_R - \sum_{\mu=1}^3 \text{Tr}\, c_R^\dagger T^{(\mu)} c_R (T^{(\mu)})^\dagger\right). \tag{12}$$
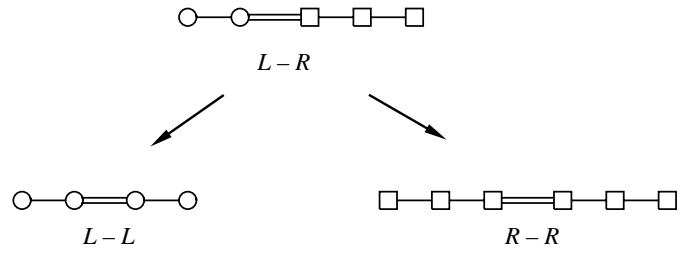

Fig. 5. Illustration of inequality (14) in the case of spin chains for $n=2, m=3$.

How can we interpret two last expressions? They resemble very much ground-state energies for the following systems: the first one consists of two copies of L subsystem with "interaction" Hamiltonian $H_C = \mathbf{s} \cdot \mathbf{s}'$, where $\mathbf{s}$ belongs to L, whereas $\mathbf{s}'$ to its twin copy (let's denote it as the $L-L$ system). The second one consists of two copies of R subsystem with $H_C = \mathbf{S} \cdot \mathbf{S}'$ (it will be denoted as $R-R$ system). More precisely, they are energies of trial functions, built up from matrices c_L and c_R, respectively. From variational principle, they are not less than true ground-state energies, so we have the general inequality for ground-state energies for three systems $L-R, L-L, R-R$:

$$2E_{L-R} \geq E_{L-L} + E_{R-R}. \tag{13}$$

Considerations above concerned the situation, where "interaction" part was the only "bond" $\mathbf{s} \cdot \mathbf{S}$ coupling both subsystems. Generalization to multi-bond case is immediate. Let's have general "interaction" Hamiltonian:

$$H_C = \sum_{i\in L}\sum_{j'\in R} J_{ij'} \mathbf{s}_i \cdot \mathbf{S}_{j'},$$

where we assume that $J_{ij'}$ are positive numbers. Then, the inequality (13) is still true for systems $L-L$ and $R-R$ with "interaction" Hamiltonians: $H_C = \sum_{i\in L}\left(\sum_{j'\in R} J_{ij'}\right)\mathbf{s}_i \cdot \mathbf{s}'_i$ for the $L-L$ system, and $H_C = \sum_{j'\in R}\left(\sum_{i\in L} J_{ij'}\right)\mathbf{S}_{j'} \cdot \mathbf{S}'_{j'}$ for $R-R$ system.

Lieb and Schupp have applied inequality (13) to spin rings, getting the following relation between ground-state energies E_k for rings with k spins:

$$2E_{n+m} \geq E_{2n} + E_{2m}.$$

However, it seems that it can be used in much more general situations, if we consider the multi-bond case.

Examples.

1. For spin chains (Fig. 5), we have analogous inequality:

$$2E_{n+m} \geq E_{2n} + E_{2m}. \tag{14}$$

2. Rather obvious is generalization of this result for systems defined on subsets of $\mathbb{Z}^d$ for $d > 1$ (rectangles, parallelepipeds etc.) ($d = 2$ case is illustrated in Fig. 6); as a result, we again have inequality (14), where m, n are lengths of systems in direction perpendicular to reflection line (plane for $d = 3$).
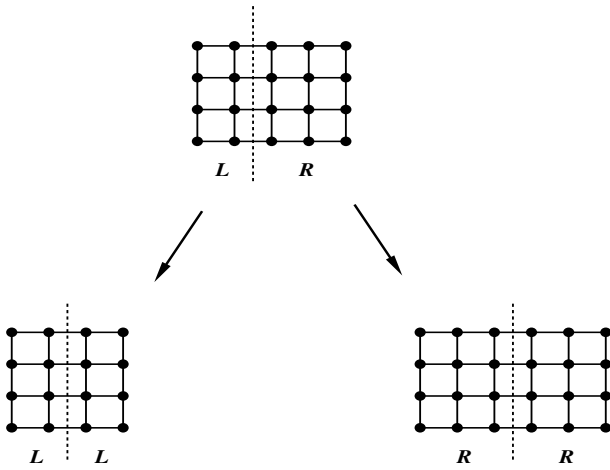
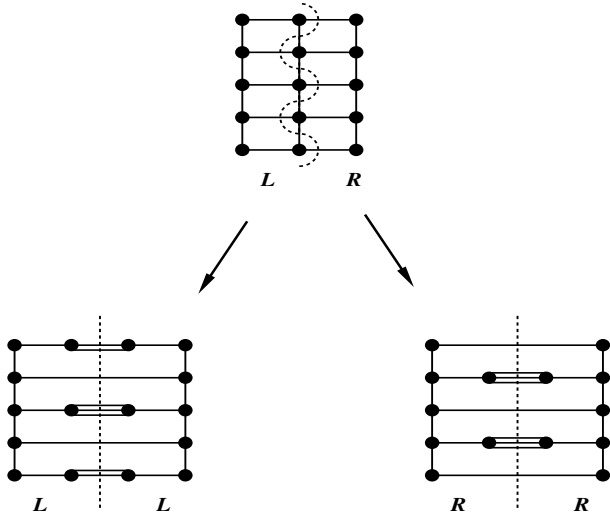**Fig. 6.** Illustration of inequality (14) for 2d lattices; $m = 2, n = 3$.

Fig. 7. Division of the system defined on a rectangular subset of square lattice into L and R subsets by "snaky" line. Single lines denote coupling constants equal to J, double lines correspond to $2J$ couplings, and triple ones – to $3J$. The same convention is used on two following pictures.
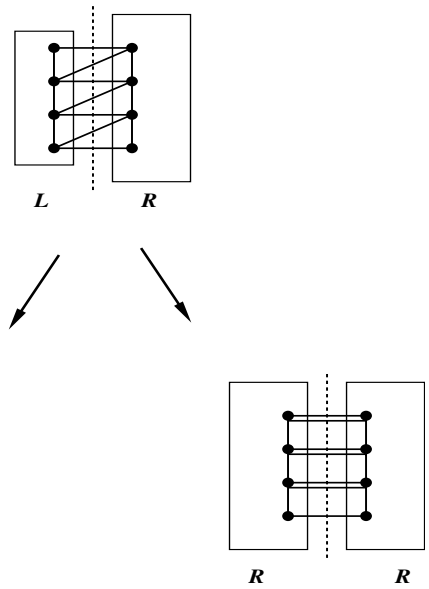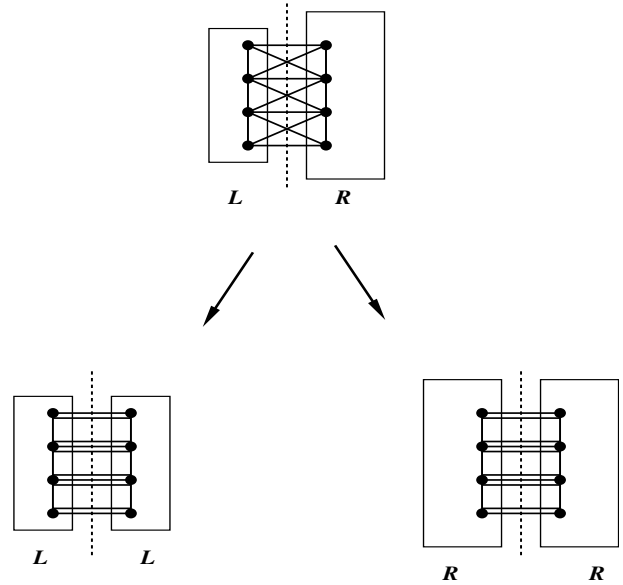

Fig. 8. "Zig-zag" and ordinary ladders.

Fig. 9. "Pyrochlore" and ordinary ladders.

3. Consider system defined on a rectangular subset of square lattice (see Fig. 7). Divide it into L and R part in nonsymmetric manner (in this example, this division is realized by the "snaky" line). Then, we obtain the inequality (13) for systems as pictured in Figure 7.

4. Consider "zig-zag ladder" (see Fig. 8). Divide it into parts L and R by the line going through the middle of the ladder and parallel to it. Then, the inequality (13) gives relation between ground-state energies of the "zig-zag" ladder and ordinary one, with suitable relation between coupling constants (see Fig. 8).

5. The same construction can be applied to the "pyrochlore" ladder (see Fig. 9).

6. Ground-state energy relations for systems described in Example 4 can be repeatedly used to obtain the inequality between systems defined on triangular and rectangular lattices. Namely, consider the system defined on isotropic triangular lattice with coupling constant J and with periodic boundary condition in both ("horizontal" and "vertical") directions. Assume, moreover, that we have 2^k sites in the horizontal direction and M sites in the horizontal one (k, M are arbitrary). Let us assume that the division of the

system onto L and R parts is realized by "vertical" plane in such a way that both parts contain equal number of sites. Then, by subsequent use of inequality (13), we obtain relation between ground state energies of systems on triangular lattice E_{tr} and on rectangular one E_{rect}:

$$E_{\text{tr}} \geq E_{\text{rect}}$$

where system on rectangular lattice has coupling constants equal J in the vertical direction and $2J$ in the horizontal one.

7. Analogous construction can be applied to obtain the ground-state energy inequality between systems defined on lattices: isotropic pyrochlore one (E_{pyro}) and rectangular one (E_{rect}):

$$E_{\text{pyro}} \geq E_{\text{rect}}$$

where system on pyrochlore lattice has coupling constants all equal to J, whereas system on rectangular lattice has couplings J in the vertical direction and $3J$ in the horizontal one.

4 Summary

In the course of paper, some extension and applications of Lieb-Schupp approach have been given. The first result concerns relaxing of demand of reflection symmetry, present in their papers. It turned out that also other kinds of symmetry are allowed (inversion, C_2 rotation). The second result is an application of Lieb-Schupp inequality, relating ground-state energies of various systems, to numerous new (to my best knowledge) situations. The relation between ground-state energies of models on triangular and rectangular lattices can serve as an example.

In the paper [12] Schupp wrote: "There is no doubt that the scheme can be further generalized". I consider my paper as a step in this direction, but of course possibilities of the Lieb-Schupp scheme seem to be far from exhaustion.

Appendix A

Here we supply proof of the inequality (8). Consider first the weaker form of this inequality, where all matrices are square ones.

Theorem ([11,12]). For any square matrices c, M, N it is true that

$$|\text{Tr}\, c^\dagger M c N^\dagger| \leq \frac{1}{2}(\text{Tr}\, c_L M c_L M^\dagger + \text{Tr}\, c_R N c_R N^\dagger), \quad \text{(A.1)}$$

where $c_R = \sqrt{c^\dagger c}$, $c_L = \sqrt{cc^\dagger}$ are unique (positive) square roots from positive definite matrices $c^\dagger c$ and $cc^\dagger$.

Proof: Using polar decomposition theorem, we can express the u matrix as: $c = uc_R$, where the u matrix is unitary. We have: $(uc_R u^\dagger)^2 = uc^\dagger cu^\dagger = (uc_R)(c_R u^\dagger) = (uc_R)(uc_R)^\dagger = cc^\dagger = c_L^2$, then, because the (positive)

square root is unique, we have: $uc_R u^\dagger = c_L$. Analogously, for arbitrary analytic function f defined on positive real numbers, we have: $uf(c_R)u^\dagger = f(c_L)$. In particular, $u\sqrt{c_R} = \sqrt{c_L}u$, which implies: $c = \sqrt{c_L}u\sqrt{c_R}$. Now, let: $P = u^\dagger\sqrt{c_L}M\sqrt{c_L}u$ and $Q := \sqrt{c_R}N^\dagger\sqrt{c_R}$; then, we have:

$$|\text{Tr}\, c^\dagger M c N^\dagger| = |\text{Tr}\, PQ| \leq \frac{1}{2}(\text{Tr}\, PP^\dagger + \text{Tr}\, QQ^\dagger)$$

$$= \frac{1}{2}(\text{Tr}\, c_L M c_L M^\dagger + \text{Tr}\, c_R N c_R N^\dagger), \quad \text{(A.2)}$$

where we have used Schwarz inequality for matrices:

$$|\text{Tr}\, PQ| = |\sum_{i,j} P_{ij}Q_{ji}| \leq \frac{1}{2}\sum_{i,j}(|P_{ij}|^2 + |Q_{ji}|^2)$$

$$= \frac{1}{2}(\text{Tr}\, PP^\dagger + \text{Tr}\, QQ^\dagger).$$

Now let us notice that the inequality (A.1) still remains valid if matrices c, M, N are not of the same dimension: If c is $m \times n$ matrix, then M is $m \times m$ matrix, N is $n \times n$ matrix, u is *partial* isometry, whereas c_L and c_R are positive matrices of dimension $m \times m$ and $n \times n$, respectively. We can repeat all considerations as above and – as a conclusion – we obtain the inequality (8).

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