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Singlets and reflection symmetric spin systems

Elliott H. Lieb* and Peter Schupp**

Department of Physics, Princeton University

Princeton, New Jersey 08544, USA

Abstract

We rigorously establish some exact properties of reflection symmetric spin systems with antiferromagnetic crossing bonds: At least one ground state has total spin zero and a positive semidefinite coefficient matrix. The crossing bonds obey an ice rule. This augments some previous results which were limited to bipartite spin systems and is of particular interest for frustrated spin systems.

E-mail: lieb@math.princeton.edu, schupp@theorie.physik.uni-muenchen.de

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**Present address: Sektion Physik der Universität München, Theresienstr. 37, 80333 München, Germany

1 Introduction

Total spin is often a useful quantum number to classify energy eigenstates of spin systems. An example is the antiferromagnetic Heisenberg Hamiltonian on a bipartite lattice, whose energy levels plotted versus total spin form towers of states. The spin-zero tower extends furthest down the energy scale, the spin-one tower has the next higher base, and so on, all the way up the spin ladder: $E(S+1) > E(S)$, where $E(S)$ denotes the lowest energy eigenvalue for total spin S [3]. The ground state, in particular, has total spin zero; it is a singlet. This fact had been suspected for a long time, but the first rigorous proof was probably given by Marshall [1] for a one-dimensional antiferromagnetic chain with an even number of sites, each with intrinsic spin-1/2 and with periodic boundary conditions. This system is bipartite, it can be split into two subsystems, each of which contains only every other site, so that all antiferromagnet bonds are *between* these subsystems. Marshall bases his proof on a theorem that he attributes to Peierls: Any ground state of the system, expanded in terms of $S^{(3)}$-eigenstates has coefficients with alternating signs that depend on the $S^{(3)}$-eigenvalue of one of the subsystems. After a canonical transformation, consisting of a rotation of one of the subsystems by π around the 2-axis in spin space, the theorem simply states that all coefficients of a ground state can be chosen to be positive. To show that this implies zero total spin, Marshall works in a subspace with $S^{(3)}$-eigenvalue $M = 0$ and uses translation invariance. His argument easily generalizes to higher dimensions and higher intrinsic spin. Lieb, Schultz and Mattis [2] point out that translational invariance is not really necessary, only reflection symmetry is needed to relate the two subsystems, and the ground state is unique in the connected case. Lieb and Mattis [3] ultimately remove the requirement of translation invariance or reflection symmetry and apply the M-subspace method to classify excited states. Like Peierls they use a Perron-Frobenius type argument to prove that in the $S^{(3)}$-basis the ground state wave function for the connected case is a positive vector and it is unique. Comparing this wave function with the positive wave function of a simple soluble model in an appropriate M-subspace [4] they conclude that the ground state has total spin $S = |S_A - S_B|$, where S_A and S_B are the maximum possible spins of the two subsystems. (In the antiferromagnetic case $S_A = S_B$ and the ground state has total spin zero.) In the present article we reintroduce reflection symmetry, but for other reasons: we want to exploit methods and ideas of "reflection positivity" (see [5] and references therein.) We do not require bipartiteness. The main application is to frustrated spin systems similar to the pyrochlore lattices discussed in [7].

2 Reflection symmetric spin system

We would like to consider a spin system that consists of two subsystems that are mirror images of one another, except for a rotation by π around the 2-axis in spin-space, and that has antiferromagnetic crossing bonds between corresponding sets of sites of the two subsystems. The spin Hamiltonian is

$$H = H_L + H_R + H_C, \tag{1}$$

and it acts on a tensor product of two identical copies of a Hilbert space that carries a representation of SU(2). "$H_L = \tilde{H}_R$" in the sense that $H_L = h \otimes 1$ and $H_R = 1 \otimes \tilde{h}$, where the tilde shall henceforth denote the rotation by π around the 2-axis in spin-space. We make no further assumptions about the nature of H_L and H_R, in particular we do *not* assume that these subsystems are antiferromagnetic. The crossing bonds are of anti-ferromagnetic type in the sense that $H_C = \sum_A \vec{S}_A \cdot \vec{S}_{A'}$, with $\vec{S}_A = \sum_{i \in A} j_i \, \vec{s}_i$ and $\vec{S}_{A'} = \sum_{i' \in A'} j_i \, \vec{s}_{i'}$, where A is a set of sites in the left subsystem, A' is the corresponding set of sites in the right subsystem, and j_i are *real* coefficients. The intrinsic spins s_i are arbitrary and can vary from site to site, as long as the whole system is reflection symmetric. We shall state explicitly when we make further assumptions, e.g., that the whole system is invariant under spin-rotations.

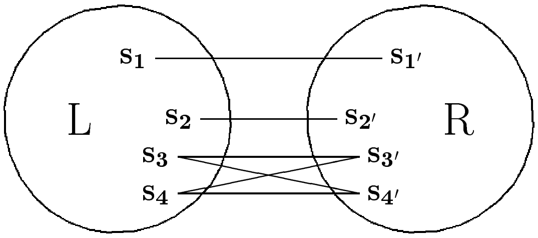

Figure 1: Some possible crossing bonds.

Any state of the system can be expanded in terms of a square matrix c,

$$\psi = \sum_{\alpha,\beta} c_{\alpha\beta}\psi_\alpha \otimes \widetilde{\psi}_\beta, \tag{2}$$

where $\{\psi_\alpha\}$ is a basis of $S^{(3)}$-eigenstates. (The indices α, β may contain additional non-spin quantum numbers, as needed, and the tilde on the second tensor factor denotes the spin rotation.) We shall assume that the state is normalized: $\langle\psi|\psi\rangle = \mathrm{tr}\, cc^\dagger = 1$. The energy expectation in terms of c is a matrix expression

$$\langle\psi|H|\psi\rangle = \mathrm{tr}\, cc^\dagger h + \mathrm{tr}(c^\dagger c)^T h - \sum_A \sum_{a=1}^{3} \mathrm{tr}\, c^\dagger S_A^{(a)} c (S_A^{(a)})^\dagger, \tag{3}$$

here $(h)_{\alpha\beta} = \langle\psi_\alpha|H_L|\psi_\beta\rangle = \langle\widetilde{\psi}_\alpha|H_R|\widetilde{\psi}_\beta\rangle$, $(S_A^{(a)})_{\alpha\beta} = \langle\psi_\alpha|\sum_{i\in A} j_i\, s_i^{(a)}|\psi_\beta\rangle$, and we have used $(\widetilde{S_A^{(a)}})^T = -(S_A^{(a)})^\dagger$. (For $a = 1, 3$ the minus sign comes from the spin rotation, for $a = 2$ it comes from complex conjugation. This can be seen by writing $S^{(1)}$ and $S^{(2)}$ in terms of the real matrices S^+ and S^-.) Note, that we do not assume $(h)_{\alpha\beta}$ to be real or symmetric, otherwise the following considerations would simplify considerably [7].

We see, by inspection, that the energy expectation value remains unchanged if we replace c by its transpose c^T, and, by linearity, if we replace it by $c + c^T$ or $c - c^T$. So, if c corresponds to a ground state, then we might as well assume for convenience that c is either symmetric or antisymmetric. Note, that in either case we have $(c_R)^T = c_L$, where $c_L \equiv \sqrt{cc^\dagger}$ and $c_R \equiv \sqrt{c^\dagger c}$. (Proof: $(c_R^2)^T = (c^\dagger c)^T = cc^\dagger = c_L^2$, if $c^T = \pm c$; now take the unique square root of this.) Using this we see that the first two terms in the energy expectation equal $2\,\mathrm{tr}\, c_L^2 h$ and thus depend on c only through the positive semidefinite matrix c_L. With the help of a trace inequality we will show that the third term does not increase if we replace c by the positive semidefinite matrix c_L.

3 Trace inequality

For any square matrices c, M, N it is true that [6]

$$|\,\mathrm{tr}\, c^\dagger M c N^\dagger| \leq \frac{1}{2}\left(\mathrm{tr}\, c_L M c_L M^\dagger + \mathrm{tr}\, c_R N c_R N^\dagger\right), \tag{4}$$

where $c_R = \sqrt{c^\dagger c}$, $c_L = \sqrt{cc^\dagger}$ are the unique square roots of the positive semidefinite matrices $c^\dagger c$ and $cc^\dagger$. For the convenience of the reader we shall repeat the proof here: By the polar decomposition theorem $c = uc_R$ with a unitary matrix u and $(uc_R u^\dagger)^2 = uc^\dagger c u^\dagger = cc^\dagger = c_L^2$, so by the uniqueness of the square root $uc_R u^\dagger = c_L$. Similarly, for any function f on the non-negative real line $uf(c_R)u^\dagger = f(c_L)$, and in particular $u\sqrt{c_R} = \sqrt{c_L}u$ and thus $c = \sqrt{c_L}u\sqrt{c_R}$. Let $P \equiv u^\dagger\sqrt{c_L}M\sqrt{c_L}u$ and $Q \equiv \sqrt{c_R}N^\dagger\sqrt{c_R}$, then

$$\begin{aligned} |\,\mathrm{tr}\, c^\dagger M c N^\dagger| &= |\,\mathrm{tr}\, PQ| \leq \frac{1}{2}(\mathrm{tr}\, PP^\dagger + \mathrm{tr}\, QQ^\dagger) \\ &= \frac{1}{2}\left(\mathrm{tr}\, c_L M c_L M^\dagger + \mathrm{tr}\, c_R N c_R N^\dagger\right), \end{aligned} \tag{5}$$

where the inequality is simply the geometric arithmetic mean inequality for matrices

$$|\operatorname{tr} PQ| = |\sum_{i,j} P_{ij}Q_{ji}| \leq \frac{1}{2}\sum_{i,j}(|P_{ij}|^2 + |Q_{ji}|^2) = \frac{1}{2}(\operatorname{tr} PP^\dagger + \operatorname{tr} QQ^\dagger).$$

4 Existence of a positive ground state

Consider any ground state of the system with coefficient matrix $c = \pm c^T$ and apply the trace inequality to the terms in $\langle\psi|H_C|\psi\rangle$:

$$-\operatorname{tr} c^\dagger S_A^{(a)} c (S_A^{(a)})^\dagger \geq -\frac{1}{2}\left(\operatorname{tr} c_L S_A^{(a)} c_L (S_A^{(a)})^\dagger + \operatorname{tr} c_R S_A^{(a)} c_R (S_A^{(a)})^\dagger\right),$$

but $(c_R S_A^{(a)} c_R (S_A^{(a)})^\dagger)^T = ((S_A^{(a)})^T)^\dagger c_L (S_A^{(a)})^T c_L = (S_A^{(a)})^\dagger c_L (S_A^{(a)}) c_L$, so in fact

$$-\operatorname{tr} c^\dagger S_A^{(a)} c (S_A^{(a)})^\dagger \geq -\operatorname{tr} c_L S_A^{(a)} c_L (S_A^{(a)})^\dagger.$$

Since the normalization of the state and the other terms in (3) are unchanged if we replace c by $c_L = \sqrt{cc^\dagger}$, and because we have assumed that c is the coefficient matrix of a ground state, it follows that the positive semidefinite matrix c_L must also be the coefficient matrix of a ground state.

5 Overlap with canonical spin zero state

Consider the (not normalized) canonical state with coefficient matrix given by the identity matrix in a basis of $S^{(3)}$-eigenstates of either subsystem

$$\begin{aligned} \Xi &= \sum_{k,k'}\sum_j \sum_{m=-j}^{j} \psi_{(j,m,k)} \otimes \widetilde{\psi}_{(j,m,k')} \qquad (6) \\ &= \sum_{k,k'}\sum_j \sum_{\tilde{m}=-j}^{j} \psi_{(j,m,k)} \otimes (-)^{j-m}\psi_{(j,-m,k')}. \end{aligned}$$

The states are labeled by the usual spin quantum numbers j, m and an additional symbolic quantum number k to lift remaining ambiguities. The state Ξ has total spin zero because of the spin rotation in the right subsystem: Its $S^{(3)}_{\rm tot}$-eigenvalue is zero and acting with either $S^{+}_{\rm tot}$ or $S^{-}_{\rm tot}$ on it gives zero. The overlap of any state with coefficient matrix c with the canonical state Ξ is simply the trace of c. In the previous section we found that the reflection symmetric spin system necessarily has a ground state with positive semidefinite, non-zero coefficient matrix, which, by definition, has a (non-zero) positive trace. Since the trace is proportional to the overlap with the canonical spin-zero state, we have now shown that there is always a ground state that contains a spin-zero part. Provided that total spin is a good quantum number, we can conclude further that our system always has a ground state with total spin zero, i.e., a singlet.

6 Projection onto spin zero

Consider any state $\psi = \sum c_{\alpha\beta}\psi_\alpha \otimes \widetilde{\psi}_\beta$ with positive semidefinite $c = |c|$. We have seen that this implies that ψ has a spin-zero component. If total spin is a good quantum number it is interesting to ask what happens to c when we project ψ onto its spin zero part

$$\psi^0 = \sum c^0_{\alpha\beta}\psi_\alpha \otimes \widetilde{\psi}_\beta. \tag{7}$$

We shall show that the coefficient matrix c^0 of ψ^0 is a partial trace of c and thus still positive semidefinite. A convenient parametrisation of the S^3 eigenstates ψ_α for this task is, as before, $\alpha = (j, m, k)$, where k labels spin-j multiplets $[j]_k$ in the decomposition of the Hilbert space of one subsystem into components of total spin. Note that $[j]_k \otimes [j']_{k'} = [j + j'] \oplus \ldots \oplus [|j - j'|]$, so $[j]_k \otimes [j']_{k'}$ contains a spin zero subspace only if $j = j'$, and for each k, k' that subspace is unique and generated by the normalized spin zero state

$$\xi_{k,k'} = (2j+1)^{-\frac{1}{2}} \sum_{\tilde{m}=-j}^{j} \psi_{(j,\tilde{m},k)} \otimes \widetilde{\psi}_{(j,\tilde{m},k')}. \tag{8}$$

(Recall that $\widetilde{\psi}_{(j,\tilde{m},k')} = (-)^{j-\tilde{m}} \psi_{(j,-\tilde{m},k')}$ is the rotation of $\psi_{(j,\tilde{m},k')}$ by π around the 2-axis in spin space.) The projection of ψ onto spin zero is thus amounts to replacing c with c^0, where

$$c^0_{(j,m,k)(j',m',k')} = \begin{cases} 0 \quad \text{if } j \neq j' \text{ or } m \neq m' \\ \dfrac{N}{2j+1} \displaystyle\sum_{\tilde{m}=-j}^{j} c_{(j,\tilde{m},k)(j,\tilde{m},k')} \quad \text{else.} \end{cases} \tag{9}$$

(N is a overall normalisation constant, independent of j, m, k.) Let us now show that this partial trace preserves positivity, i.e., $(v, c^0\ v) \geq 0$ for any vector $v = \left(v_{(j,m,k)}\right)$ of complex numbers. If we decompose v into a sum of vectors v_{jm} with definite j, m and use (9), we see

$$(v, c^0\ v) = \sum_{j,m} (v_{jm}, c^0\ v_{jm}) = \sum_{j,m,\tilde{m}} (\omega^m_{j\tilde{m}}, c\, \omega^m_{j\tilde{m}}) \geq 0, \tag{10}$$

where the $\omega^m_{j\tilde{m}}$ are new vectors with components $\omega^m_{(j,\tilde{m},k)} = v_{(j,m,k)}$, independent of $\tilde{m}$. Every term in the last sum is non-negative because c is positive semidefinite by assumption. This result implies in particular that a reflection symmetric spin system always has a ground state with total spin zero *and* positive semidefinite coefficient matrix – provided that total spin is a good quantum number.

7 Ice rule for crossing bonds

The expectation of the third spin component of the sites involved in each crossing bond B, weighted by their coefficients j_i, vanishes for *any* ground state ψ_0,

$$\langle \psi_0 | \sum_{i \in B} j_i (s_i^{(3)} + s_{i'}^{(3)}) | \psi_0 \rangle = 0, \tag{11}$$

provided that either the left and right subsystems are invariant under the spin rotation, $h = \tilde{h}$, or that their matrix elements are real (the latter is equivalent to the assumption $h = h^T$, since we know that $h = h^\dagger$ or otherwise the whole spin Hamiltonian would not be Hermitean). By symmetry (11) will also be true for the first spin component and, if we are dealing with a spin Hamiltonian that is invariant under spin rotations, it is also true for the second spin component. For ground states with symmetric or antisymmetric coefficient matrix we automatically have $\langle s_i^{(3)} + s_{i'}^{(3)} \rangle = 0$ for any pair of sites i and i', so in that case (11) is trivial.

For the proof we introduce a real parameter b in the spin Hamiltonian: $H(b) \equiv H - b(S_B^{(3)} + S_{B'}^{(3)}) + b^2/2$, where B is one of the sets of sites involved in the crossing bonds of the original Hamiltonian H. Let E_b be the ground state energy of $H(b)$ and E_0 the ground state energy of H. One can show that $E_b \geq E_0$ and (11) follows then by a variational argument:

$$\langle \psi_0 | H(b) | \psi_0 \rangle \geq E_b \geq E_0 = \langle \psi_0 | H | \psi_0 \rangle, \tag{12}$$

or, $\langle \psi_0 | b(S_B^{(3)} + S_{B'}^{(3)}) | \psi_0 \rangle \leq b^2/2$, which implies (11). Note, that we did not make any assumptions about the symmetry or antisymmetry of the coefficient matrix of ψ_0 here.

Sketch of the proof of $E_b \geq E_0$ (see also [6, 7]): $H(b) = H_L(b) + H_R(b) + H_C(b) + b^2/4$ with $H_{L,R}(b) = H_{L,R} - b/2 \cdot S_B^{(3)}$ and $H_C(b)$ equal to H_C except for the term $S_B^{(3)} \cdot S_{B'}^{(3)}$, which is replaced by $(S_B^{(3)} - b/2) \cdot (S_{B'}^{(3)} - b/2)$. If we now write the ground state energy expectation of $H(b)$ as a matrix expression like (3) and apply the trace inequality to it, we will find an equal or lower energy expectation not of $H(b)$, but rather of H: The trace inequality effectively removes the parameter b from the Hamiltonian. By the variational principle the true ground state energy of H is even lower and we conclude that $E_b \geq E_0$. Role of the technical assumptions mentioned above: If $h = h^T$, then the transpose in the second term in (3) vanishes, the matrix expression is symmetric in c_L and c_R (except for the sign of the parameter b), and the trace inequality gives $\langle H(b)\rangle_c \geq \frac{1}{2}\{\langle H\rangle_{c_L} + \langle H\rangle_{c_R}\}$. If $h = \tilde{h}$, then we should drop the spin rotation on the second term of the analog of expression (2) for ψ_b. The matrix expression for $\langle H(b)\rangle$ is then symmetric in c and c^T and we may assume $c = \pm c^T$ to prove $E_b \geq E_0$. The calculation is similar to the one in section 4. Note, that $c = \pm c^T$ only enters the proof of $E_b \geq E_0$, we still do not need to assume that the coefficient matrix of ψ_0 in (11) has that property.

The preferred configurations of four spins with antiferromagnetic crossed bonds in a classical Ising system are very similar to the configurations of the four hydrogen atoms that surround each oxygen atom in ice: There are always two hydrogen atoms close and two further away from each oxygen atom, and there are always two spins "up" and two "down", i.e. $M = 0$, in the Ising system. Equation (11) is a (generalized) quantum mechanical version of this – that is why we use the term "ice rule". This phrase is also used in the context of *ferromagnetic* pyrochlore with Ising anisotropy ("spin ice") [8] and we hope that does not cause confusion.

8 Discussion

We would like to discuss similarities between our method and previous work, in particular the approach of [3] for the bipartite antiferromagnet: There, the spin Hamiltonian splits into two parts $H = H_0 + H_1$. The expectation value of H_0 with respect to a state $\psi = \sum f_\alpha \phi_\alpha$, expanded in an appropriate basis $\{\phi_\alpha\}$, depends only on $|f_\alpha|$, and the expectation of H_1 does not increase under the transformation $f_\alpha \to |f_\alpha|$. The variational principle then implies that there must be a ground state with only non-negative coefficients $|f_\alpha|$. The present setup is very similar, except that we use coefficient matrices $(c_{\alpha\beta})$ to expand states, since we work on a tensor product of Hilbert spaces. In our case the expectation value of $H_0 = H_L + H_R$ depends only on c via the positive matrices c_L and c_R, and the expectation value of H_C increases if we "replace" c by these positive matrices. The similarity is even more apparent if h has real matrix elements: In that case we may assume that c is diagonalisable and its eigenvalues play the role of the coefficients f_α. The spin of a positive ground state is established in all cases from the overlap with a state of known spin that is also positive. In a system with sufficient symmetry we can, however, also use the "ice rule" to prove that *all* ground states have total spin zero [7]. (E.g., in a system with constant coefficients j_i and enough translational invariance, so that every spin can be considered to be involved in a crossing bond and thus in an ice rule, we would conclude that all ground states have $S^{(3)}_{\mathrm{tot}} = 0$ and, assuming rotational invariance in spin space, $S_{\mathrm{tot}} = 0$.) It is not clear, if M-subspace methods can be used in the present setting to get information about excited states. An important point in the our work is that we consider not only antiferromagnetic bonds between single sites but also bonds between sets of sites. This frees us from the requirement of bipartiteness and even allows some ferromagnetic crossing bonds, for example in $(s_1 - s_2)(s_{1'} - s_{2'})$. There is no doubt that the scheme can be further generalized, e.g., to other groups or more abstract "crossing bonds". In the present form the most interesting applications are in the field of frustrated spin systems [7].

We did not address the question of the degeneracy of ground states. Classically a characteristic feature of frustrated systems is their large ground state degeneracy. For frustrated quantum spin systems this is an important open problem.

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References

[1] W. Marshall, *Antiferromagnetism*, Proc. Roy. Soc. (London) **A232**, 48 (1955).

[2] E. H. Lieb, T. Schultz, D. Mattis, *Two Soluble Models of an Antiferromagnetic Chain*, Ann. Phys. **16**, 407 (1961).

[3] E. H. Lieb, D. Mattis, *Ordering Energy Levels of Interacting Spin Systems*, J. Math. Phys. **3**, 749 (1962).

[4] E. H. Lieb, *Two Theorems on the Hubbard Model*, Phys. Rev. Lett. **62**, 1201 (1989).

[5] F. J. Dyson, E. H. Lieb, B. Simon, *Phase Transitions in Quantum Spin Systems with Isotropic and Nonisotropic Interactions*, J. Stat. Phys. **18**, 335 (1978).

[6] T. Kennedy, E. H. Lieb, B. S. Shastry, *Existence of Néel Order in Some Spin-1/2 Heisenberg Antiferromagnets*, J. Stat. Phys. **53**, 1019 (1988).

[7] E. H. Lieb, P. Schupp, *Ground state properties of a fully frustrated quantum spin system*, math-ph/9908019, mp_arc 99-304; Phys. Rev. Lett. (1999, in print).

[8] M. J. Harris, S. T. Bramwell, D. F. McMorrow, T. Zeiske, K. W. Godrey, *Geometrical Frustration in the Ferromagnetic Pyrochlore* $Ho_2Ti_2O_7$, Phys. Rev. Lett. **79**, 2554 (1997).