

Ferromagnetic Ordering of Energy Levels^{1,2}

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We study a natural conjecture regarding ferromagnetic ordering of energy levels in the Heisenberg model which complements the Lieb–Mattis Theorem of 1962 for antiferromagnets: for ferromagnetic Heisenberg models the lowest energies in each subspace of fixed total spin are strictly ordered according to the total spin, with the lowest, i.e., the ground state, belonging to the maximal total spin subspace. Our main result is a proof of this conjecture for the spin-1/2 Heisenberg XXX and XXZ ferromagnets in one dimension. Our proof has two main ingredients. The first is an extension of a result of Koma and Nachtergaele which shows that monotonicity as a function of the total spin follows from the monotonicity of the ground state energy in each total spin subspace as a function of the length of the chain. For the second part of the proof we use the Temperley–Lieb algebra to calculate, in a suitable basis, the matrix elements of the Hamiltonian restricted to each subspace of the highest weight vectors with a given total spin. We then show that the positivity properties of these matrix elements imply the necessary monotonicity in the volume. Our method also shows that the first excited state of the XXX ferromagnet on any finite tree has one less than maximal total spin.

KEY WORDS: Heisenberg ferromagnet; XXZ model; ordering of energy levels; Temperley–Lieb algebra.

1. INTRODUCTION

Given any finite set A , and a set of coupling constants

$$J = \{J_{\{x, y\}} : \{x, y\} \subset A, x \neq y\}$$

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² Dedicated to Elliott Lieb on the occasion of his 70th birthday.

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one defines a Heisenberg model by specifying a Hamiltonian of the following form:

$$H_{A,J} = \sum_{\substack{\{x,y\} \subset A \\ x \neq y}} J_{\{x,y\}} \mathbf{S}_x \cdot \mathbf{S}_y. \quad (1.1)$$

Here $\mathbf{S}_x = (S_x^1, S_x^2, S_x^3)$ is the defining spin vector for an irreducible representation of $SU(2)$ at the site $x \in A$. In general, the magnitude of the spin at site x is $s_x \in \frac{1}{2} \mathbb{N}$.

The Hamiltonian is clearly invariant with respect to the action of $SU(2)$ on $\mathcal{H}(A) = \bigotimes_{x \in A} \mathbb{C}^{2s_x+1}$. Therefore the vectors of a given total spin (a vector has total spin S if it is an eigenvector of the Casimir operator $\sum_{x,y \in A} \mathbf{S}_x \cdot \mathbf{S}_y$ with eigenvalue $S(S+1)$) form an invariant subspace for H_A . We define $E(A, J, S)$ to be the lowest energy among all eigenvectors with total spin S .

We say (A, J) is reducible if there is a proper subset A_1 such that $J_{\{x,y\}} = 0$ whenever $x \in A_1$ and $y \in A \setminus A_1$, or vice versa. Otherwise, we call the model *irreducible*. It is irreducible models which interest us.

If there are two subsets A, B such that $A = A \sqcup B$ and

$$\begin{cases} J_{\{x,y\}} \geq 0 & \text{if } x \in A, y \in B \text{ or } x \in B, y \in A, \\ J_{\{x,y\}} \leq 0 & \text{if } x, y \in A \text{ or } x, y \in B, \end{cases}$$

we call the model (A, B) -bipartite. Such models form a special class. It makes sense to then define $S_A = \sum_{x \in A} s_x$ and $S_B = \sum_{x \in B} s_x$.

The Lieb–Mattis Theorem says the following.

Theorem 1.1 (Ordering of Energy Levels, ref. 14). Suppose the Heisenberg Hamiltonian $H_{A,J}$ is irreducible and (A, B) -bipartite. Define $\mathcal{S} = |S_A - S_B|$. Then

$$E(A, S+1) > E(A, S) \quad \text{for all } S \geq \mathcal{S}, \quad (1.2)$$

$$E(A, S) > E(A, \mathcal{S}) \quad \text{for } S < \mathcal{S}. \quad (1.3)$$

The Lieb–Mattis theorem is simple and elegant, and we repeat the basic argument, here. The main tool is the Perron–Frobenius theorem. We quote the Perron–Frobenius theorem from ref. 22 where a proof can be found (pp. 130–132).

Theorem 1.2 (Perron–Frobenius). If $A = (a_{ij})$ is a square matrix of size $n > 1$ with non-negative entries and such that for some $k \geq 1$, A^k has strictly positive entries, then

1. $\rho(A) = \max_{\lambda \in \text{spec}(A)} |\lambda|$ is an eigenvalue of A .
2. $\rho(A)$ is simple (in the strong sense that it is a simple root of $\det(A - \lambda) = 0$).
3. For any other eigenvalue λ , $|\lambda| < \rho(A)$.
4. The eigenvector v associated to $\rho(A)$ has only strictly positive components.
5. No other eigenvector has only non-negative components.

Proof of Theorem 1.1. (This is only a sketch. See ref. 14 for details.) Let $\{|\sigma\rangle: \sigma = (\sigma_x)_{x \in A}, \sigma_x \in [-s_x, s_x]\}$ be the standard Ising basis of $\mathcal{H}(A)$. Define $\phi(\sigma) = e^{i(\pi/2) \sum_{x \in A} \sigma_x} |\sigma\rangle$. In this basis, $H_{A,J}$ has all real, non-positive off-diagonal entries. Moreover, since it is assumed to be irreducible, this means that restricted to each total S^3 -eigenspace, the matrix representation is irreducible. Hence, in each S^3 -eigenspace, the minimum energy vector is unique. Let $S(A, J, M)$ be the total spin of the minimum energy vector for $H_{A,J}$ in the S^3 -eigenspace with eigenvalue M (henceforth called the M -subspace).

Note that the set of all J such that $H_{A,J}$ is (A, B) -bipartite forms a convex region of $\mathbb{R}^{|A|(|A|-1)/2}$. Hence, it is connected. Clearly, $S(A, J, M)$ is a continuous, integer-valued function on this region for each M ; therefore, it is constant. One particular model which is solvable is

$$J_{\{x,y\}} = \begin{cases} -1 & x \in A, y \in B \quad \text{or} \quad y \in A, x \in B; \\ 0 & x, y \in A \quad \quad \quad \text{or} \quad x, y \in B. \end{cases}$$

For this model, it is easily seen that

$$S(J, M) = \begin{cases} |M| & |M| > \mathcal{S}, \\ \mathcal{S} & |M| \leq \mathcal{S}. \end{cases}$$

This, along with the constancy of $S(A, J, M)$ for J in the convex set, implies the result.

There are three natural categories for (A, B) -bipartite Hamiltonians,

- antiferromagnetic if $\mathcal{S} = 0$;
- ferrimagnetic if $0 < \mathcal{S} < \max(S_A, S_B)$;
- ferromagnetic if $\mathcal{S} = \max(S_A, S_B) > 0$.

Note that for antiferromagnets, the Lieb–Mattis theorem implies

$$E(A, J, S) < E(A, J, S') \quad \text{whenever} \quad S < S'. \tag{1.4}$$

The Lieb–Mattis theorem also implies “ferromagnetic ordering of the ground state.” I.e., for ferromagnetic Hamiltonians, the ground state has maximum possible spin. A natural guess is that for any irreducible, ferromagnetic model,

$$E(A, J, S) > E(A, J, S') \quad \text{whenever } S < S'. \quad (1.5)$$

We call this “ferromagnetic ordering of energy levels.”

Conjecture 1.3. For any irreducible, ferromagnetic Heisenberg model there is ferromagnetic ordering of energy levels. I.e., (1.5) is verified.

In the case of antiferromagnets, the Lieb–Mattis theorem proves full ordering precisely because the dispersion relation for the ground state energy in each M subspace, versus M , is not flat; it is increasing in $|M|$. This is crucial because the Perron–Frobenius theorem only gives direct information about the ground state in each irreducible sector, and for irreducible Heisenberg models, the M -subspaces are the irreducible sectors. The fact that, for the ferromagnet, the dispersion relation is flat proves ferromagnetic ordering of the ground state, but no more. It is not obvious how to prove Conjecture 1.3, in general, though we believe it is true.

We mention a somewhat related difficulty for the ferromagnetic Heisenberg model: the fact that it is not reflection positive.⁽²³⁾ Reflection positivity is a particular property which is valid for the Heisenberg antiferromagnet, and in fact the proof of the Lieb–Mattis theorem for the antiferromagnet can be considered as an early forerunner of reflection positivity. By using reflection positivity, Dyson, Lieb, and Simon were able to prove that the antiferromagnet has a phase transition, at (small) positive temperatures, in dimensions $d \geq 3$.⁽⁴⁾⁵ Jordão–Neves and Fernando Perez first used reflection positivity to prove a phase transition for the Heisenberg antiferromagnet in two dimensions for $s_x \geq 3/2$.⁽²¹⁾ The analogous result for $d = 2$ and $s_x \geq 1$ as well as $d \geq 3$ and $s_x \geq 1/2$ was subsequently proved by Kennedy, Lieb, and Shastry.⁽⁸⁾ Many interesting results on a variety of topics later followed using reflection positivity.^(9, 13, 15–17) However this technique never succeeded to prove a phase transition, at positive temperatures, for the ferromagnetic Heisenberg model, despite the fact that it is completely trivial to prove a phase transition for the ground states. This is simply because the ferromagnetic Heisenberg model is *not* reflection

⁵ The originators of the reflection positivity approach to proving continuous symmetry breaking were.⁽⁵⁾

positive.⁶ Because of this connection, the question of proving ferromagnetic ordering of energy levels seems even more interesting.

We would like to argue that the quantum Heisenberg ferromagnet is just as interesting as the antiferromagnet. The latter has received much more attention because its ground state is a highly non-trivial object, while the same cannot be said of the rather trivial ground states of the ferromagnet. The situation changes dramatically, however, when one focuses on the excitation spectrum, or even just asks for the lowest energy states in invariant subspaces. E.g., Dhar and Shastry studied the lowest excited states in the subspaces of fixed momentum.⁽³⁾ In ref. 20 two of us determined the ground states in subspaces of fixed third component of the spin subject to “droplet” boundary conditions. In the present paper we consider ground states in the subspaces of fixed total spin. In each case, the ferromagnetic model shows interesting structure.

As a step in the direction of ferromagnetic ordering, Koma and Nachtergaele⁽¹⁰⁾ proved, for the case of the spin-1/2 ferromagnetic Heisenberg spin chain of length L , that the lowest excitation above the ground state is a 1-spin deviate vector, i.e., with total spin $S = L/2 - 1$. Thus, for any $S < L/2 - 1$, $E([1, L], S) > E([1, L], L/2 - 1)$. More generally, we will call an n -spin deviate any vector with total spin equal to $L/2 - n$. Their proof involves a very simple argument just using addition of angular momentum for the Lie group $SU(2)$. Moreover, it generalizes to the $SU_q(2)$ symmetric XXZ model with Ising-like anisotropy. Their basic theorem implies that, for any L_0 and n_0 , the minimum energy of all m -spin-deviates is less than the minimum energy of all n -spin-deviates, for $m \leq n \leq n_0$ and chains of length $L \leq L_0$, as long as the minimum energy of any n -spin-deviate, with $n \leq n_0$, is nonincreasing in L for $L \leq L_0$. Hence, they were able to calculate the exact spectral gap above the ground states of the ferromagnetic XXZ model for $s = 1/2$ and $d = 1$, because they could completely diagonalize the Hamiltonian restricted to 0- and 1-spin-deviates.

In the present paper, we will reconsider their basic theorem, and show how it can be generalized to provide information on the ordering of energy levels of $s = 1/2$ ferromagnets. In particular, we use the theorem to prove complete ferromagnetic ordering of energy levels for the XXZ and XXX models for which Koma and Nachtergaele calculated the spectral gap. The Koma–Nachtergaele theorem is only one piece of the puzzle however. The other piece is an inequality for the lowest eigenvalues of (not

⁶ For more about this important problem, see the IAMP website <http://www.math.princeton.edu/~aizenman/OpenProblems.iamp/>.

necessarily symmetric) matrices with non-positive off-diagonal matrix elements. See Lemma 7.3.

Loosely stated, the lemma says that if B is an $n \times n$ matrix with non-positive off-diagonal entries, and A is a $m \times m$ submatrix obtained from B by restricting the range of the indices to m , then the smallest eigenvalue of B is less or equal to the smallest eigenvalue of A .

We apply this lemma to the matrices of the one-dimensional XXX and XXZ models with respect to the generalized Hulthén basis introduced by Temperley and Lieb.⁽²⁴⁾ Indeed, the nearest-neighbor interactions of the XXZ ferromagnet are generators of the Temperley–Lieb algebra, which is of key importance.

Theorem 1.4. Ferromagnetic ordering of energy levels holds for the spin 1/2 ferromagnetic XXZ chain, of arbitrary length, $L \geq 2$, and anisotropy, $\Delta \geq 1$.

Although the result may seem rather special to the case of the Bethe–Ansatz solvable XXZ model, it is not really the case. In particular, we also use the same argument to prove that for the XXX model on any finite tree, the first excitation is a 1-spin deviate, thus generalizing Koma and Nachtergaele’s original spectral gap result to finite trees. This result shows the applicability of these arguments to non-integrable spin systems, and may also be of interest to probabilists since it proves that for any tree, the spectral gap of the symmetric, simple exclusion process equals the spectral gap of the random walk.

We believe that our theorems for these particular examples give credible evidence to Conjecture 1.3.

2. DEFINITION OF THE XXZ MODEL WITH KINK BOUNDARY FIELDS

Our main results regard the spin-1/2 XXZ model for anisotropies $\Delta \in [1, \infty]$. This is a nearest-neighbor Hamiltonian,

$$H_{[1, L]} = \sum_{x=1}^{L-1} h_{x, x+1} \quad (2.1)$$

with nearest-neighbor interaction

$$h_{x, x+1} = j^2 - S_x^3 S_{x+1}^3 - \Delta^{-1} (S_x^1 S_{x+1}^1 + S_x^2 S_{x+1}^2) + j \sqrt{1 - \Delta^{-2}} (S_x^3 - S_{x+1}^3). \quad (2.2)$$

Here, $j = 1/2$. In this definition, Δ is the anisotropy. $\Delta = 1$ gives the isotropic Heisenberg model. $\Delta = \infty$ is the Ising model with kink boundary conditions. There is the usual definition of the spin-1/2 matrices

$$S^1 = \begin{bmatrix} 0 & 1/2 \\ 1/2 & 0 \end{bmatrix}, \quad S^2 = \begin{bmatrix} 0 & -i/2 \\ i/2 & 0 \end{bmatrix}, \quad S^3 = \begin{bmatrix} 1/2 & 0 \\ 0 & -1/2 \end{bmatrix},$$

and a subscript refers to the site, or tensor factor, where the spin matrix acts.

The extra boundary field $\frac{1}{2}\sqrt{1-\Delta^{-2}}(S_x^3 - S_{x+1}^3)$ is chosen to allow a quantum group symmetry, but has some additional nice features even when $j > 1/2$, namely that one can determine all the finite volume ground states in any dimension.^(1,6) In addition, all the infinite volume ground states for the ferromagnetic XXZ (and XXX) interaction in one dimension were determined in ref. 11. This last result is interesting for, among other things, it gives a strong a posteriori justification of the chosen boundary fields (or their spin-flipped/reflected images) on a thermodynamic basis (in addition to its obvious algebraic attraction), as follows: The infinite volume ground states are defined independently of the boundary fields in the Hamiltonian. For this model there is a special property that, restricting any pure, infinite volume ground state to the subalgebra of finite volume observables $\mathcal{B}(\mathcal{H}([1, L])) \subset \mathcal{A}_0$, where \mathcal{A}_0 is the quasilocal algebra⁷ one obtains a density matrix whose range is either in the ground state space of $H_{[1, L]}$, or else is in the ground state space of the spin-flipped/reflected image of $H_{[1, L]}$.

The ground state space of $H_{[1, L]}$ is defined as the $E = 0$ eigenspace, and it is easy to see that $H_{[1, L]} \geq 0$.

3. QUANTUM GROUP SYMMETRY

As mentioned before this Hamiltonian is quantum group symmetric, where the quantum group is $SU_q(2) = \mathcal{U}_q(\mathfrak{sl}(2))$, a deformation of the (universal enveloping algebra for the Lie algebra of the) Lie group $SU(2)$. The q refers in this case to a real deformation parameter, specifically

⁷The algebra of quasilocal observables is $\mathcal{A}_0 = \overline{\bigcup_{A \subset \mathbb{Z}} \mathcal{B}(\mathcal{H}(A))}$ in which the union is restricted to finite subsets $A \subset \mathbb{Z}$, and the closure is in operator norm. A ground state is a state—normalized, positive functional—on this algebra which satisfies local stability. I.e., ω is a ground state iff for any local observable X , one has $\omega(X^*[H, X]) \geq 0$, which expresses the fact that the perturbed state $\omega(X^* \cdots X) / \omega(X^*X)$ has higher energy than ω .

$q \in [0, 1]$ is the solution of $\Delta = (q + q^{-1})/2$. Because q is real, the representation theory of $SU_q(2)$ for $0 < q < 1$ is so similar to that of $SU(2)$ that the reader will hardly notice a difference. The most important difference is that in place of the usual generators $S_{[1, L]}^3$, $S_{[1, L]}^+$, and $S_{[1, L]}^-$ of the representation of $SU(2)$ on $\mathcal{H}([1, L])$, one has three matrices $S_{q, [1, L]}^+$, $S_{q, [1, L]}^-$, and $S_{q, [1, L]}^3$

$$S_{q, [1, L]}^3 = \sum_{x=1}^L S_x^3, \quad (3.1)$$

$$S_{q, [1, L]}^+ = \sum_{x=1}^L q^{-2\sum_{y=1}^{x-1} S_y^3} S_x^+, \quad (3.2)$$

$$S_{q, [1, L]}^- = \sum_{x=1}^L q^{2\sum_{y=x+1}^L S_y^3} S_x^-. \quad (3.3)$$

Of course, $S_{q, [1, L]}^3$ is the same as $S_{[1, L]}^3$. All three of these operators commute with $H_{[1, L]}$.

The Clebsch–Gordan series for $SU_q(2)$ is the same as that for $SU(2)$. In particular there is a unique (up to isomorphisms) irreducible representation of dimension d for $d = 1, 2, 3, \dots$. As usual, let $j = \frac{1}{2}(d-1)$ be called the spin. Then, as for $SU(2)$, the number of irreducible spin $j = L/2 - n$ representation of $SU_q(2)$ in $\mathcal{H}([1, L])$ is the same as the number of noncrossing pairings of $2n$ of the L linearly ordered vertices $\{1, \dots, L\}$ such that no pairing spans an unpaired vertex.⁽²⁴⁾ Perhaps more importantly, if $W^{(j)}$ and $W^{(j')}$ are two irreducible representation of spin j and j' in $\mathcal{H}([1, L])$ and $\mathcal{H}([L+1, L+L'])$, then $W^{(j)} \otimes W^{(j')}$ decomposes into irreducible representations in $\mathcal{H}([1, L+L'])$ according to $W^{(j+j')} \oplus W^{(j+j'-1)} \oplus \dots \oplus W^{|j'-j|}$.

4. REDUCTION TO MONOTONICITY IN THE VOLUME

For each $L \geq 2$, $n = 0, 1, \dots, \lfloor L/2 \rfloor$, let $\mathcal{H}([1, L], n)$ be the sum of all irreducible, spin- $\lfloor L/2 - n \rfloor$ representations of $SU_q(2)$ in $\mathcal{H}([1, L])$. Here $\lfloor x \rfloor$ is the greatest integer n , such that $n \leq x$. These subspaces are invariant under the action of the Hamiltonian $H_{[1, L]}$ due to its quantum group symmetry. For the same set of n , define

$$\mathcal{E}(L, n) = \min\{\langle \psi | H_{[1, L]} \psi \rangle : \psi \in \mathcal{H}([1, L], n), \|\psi\| = 1\}.$$

One can observe the following simple fact, which applies to Hamiltonians more general than Heisenberg or XXZ models.

Lemma 4.1. Let $H_{[1, L]}$ and $H_{[1, L+1]}$ be self-adjoint operators on $\mathcal{H}([1, L]) = (\mathbb{C}^2)^{\otimes [1, L]}$ and $\mathcal{H}([1, L+1]) = (\mathbb{C}^2)^{\otimes [1, L+1]}$, respectively. Suppose both commute with the action of $SU_q(2)$. Also, suppose $H_{[1, L+1]} \geq H_{[1, L]}$, identifying $H_{[1, L]}$ with the operator on $\mathcal{H}([1, L+1])$ obtained by tensoring with the identity on the last factor. Then for any $n < (L+1)/2$,

$$\mathcal{E}(L+1, n) \geq \min\{\mathcal{E}(L, n), \mathcal{E}(L, n-1)\}, \quad (4.1)$$

while $\mathcal{E}(L+1, (L+1)/2) \geq \mathcal{E}(L, (L-1)/2)$.

Proof. By the standard rules of addition of angular momentum, for any $\psi \in \mathcal{H}([1, L+1], n)$, there are four vectors $\psi_1, \psi_2 \in \mathcal{H}([1, L], n)$ and $\psi_3, \psi_4 \in \mathcal{H}([1, L], n-1)$, such that

$$\psi = \psi_1 \otimes | +1/2 \rangle + \psi_2 \otimes | -1/2 \rangle + \psi_3 \otimes | +1/2 \rangle + \psi_4 \otimes | -1/2 \rangle.$$

Note that $\psi_1 \otimes | +1/2 \rangle, \dots, \psi_4 \otimes | -1/2 \rangle$ are orthogonal because they are all eigenvectors for the commuting operators S^3 and $\mathbf{S} \cdot \mathbf{S}$, and for any two vectors, either the eigenvalues of S^3 are different or the eigenvalues of $\mathbf{S} \cdot \mathbf{S}$ are different (or both). Moreover, for that same reason they are also orthogonal with respect to $H_{[1, L]}$. Thus

$$\begin{aligned} \frac{\langle \psi | H_{[1, L+1]} \psi \rangle}{\|\psi\|^2} &\geq \frac{\langle \psi | H_{[1, L]} \psi \rangle}{\|\psi\|^2} \\ &= \sum_{k=1}^4 \frac{\|\psi_k\|^2}{\sum_{l=1}^4 \|\psi_l\|^2} \cdot \frac{\langle \psi_k | H_{[1, L]} \psi_k \rangle}{\|\psi_k\|^2} \\ &\geq \min_{k=1, 2, 3, 4} \frac{\langle \psi_k | H_{[1, L]} \psi_k \rangle}{\|\psi_k\|^2} \\ &\geq \min\{\mathcal{E}(L, n), \mathcal{E}(L, n-1)\}. \quad \blacksquare \end{aligned}$$

The natural generalization to higher spins is immediately obvious. Suppose each factor in $\mathcal{H}([1, L]) = (\mathbb{C}^{2j+1})^{\otimes [1, L]}$ and $\mathcal{H}([1, L+1]) = (\mathbb{C}^{2j+1})^{\otimes [1, L+1]}$ is canonically equipped with a spin- j representation of $SU_q(2)$, and that $H_{[1, L]}$ and $H_{[1, L+1]}$ commute with the actions of $SU_q(2)$ on the products. Defining $\mathcal{H}([1, L], n)$ to be the sum of the spin- $[jL-n]$ representations, we would determine that if $H_{[1, L+1]} \geq H_{[1, L]}$, then

$$\mathcal{E}(L+1, n) \geq \min_{k=0, \dots, 2j+1} \mathcal{E}(L, n-k). \quad (4.2)$$

However, the lemma is most useful as it is stated, for spins-1/2, because of the immediate corollary:

Corollary 4.2. Suppose $H_{[1, L]}$ and $H_{[1, L+1]}$ satisfy the hypotheses of Lemma 4.1, and suppose further that there is a value $n \in \{0, \dots, \lfloor L/2 \rfloor\}$ such that

$$\mathcal{E}(L, n) < \mathcal{E}(L, r) \quad \text{for all } r > n. \quad (4.3)$$

Then, if $\mathcal{E}(L+1, n) < \mathcal{E}(L, n)$, then also

$$\mathcal{E}(L+1, n) < \mathcal{E}(L+1, r) \quad \text{for all } r > n. \quad (4.4)$$

Applying the corollary inductively leads to the following important result.

Proposition 4.3. Suppose that for all $L \in \{2, \dots, L_0\}$, there is defined a self-adjoint operator $H_{[1, L]}$ on $\mathcal{H}([1, L]) = (\mathbb{C}^2)^{\otimes [1, L]}$, commuting with the action of $SU_q(2)$, and such that $H_{[1, L+1]} - H_{[1, L]} \geq 0$ for $L \in \{2, \dots, L_0 - 1\}$. Suppose that, for some $n \in \{0, \dots, \lfloor L_0/2 \rfloor\}$, $\mathcal{E}(L, n)$ is strictly decreasing as a function of L for $L \in \{2n, \dots, L_0\}$. Then

$$\mathcal{E}(L_0, n) < \mathcal{E}(L_0, r) \quad \text{for all } r > n. \quad (4.5)$$

Here is a more explicit statement of Theorem 1.4, expressing ferromagnetic ordering for the spin-1/2 XXZ (and XXX) chains:

Proposition 4.4. For the ferromagnetic, spin-1/2 XXZ chain, with $1 \leq \Delta < \infty$, the sequence $\mathcal{E}(L, n)$ is strictly increasing in n for $n \in \{0, 1, \dots, \lfloor L/2 \rfloor\}$.

The proof of this proposition, and thus of Theorem 1.4, is obtained by combining Proposition 4.3 in this section and Proposition 7.1 in Section 7.

Although the Bethe Ansatz, in principle, should allow one to diagonalize $H_{[1, L]}$ in the sectors $\mathcal{H}([1, L], n)$, it seems nearly impossible to extract the required information on the eigenvalues from such an exact solution even for relatively small n . It turns out that it is useful to reformulate the problem in terms of the following quantities:

$$\tilde{\mathcal{E}}(L, n) = \min_{r \in \{n, \dots, \lfloor L/2 \rfloor\}} \mathcal{E}(L, r),$$

The sequence $(\tilde{\mathcal{E}}(L, n))_{n \geq 0}$ is the lower, nondecreasing hull of the sequence $(\mathcal{E}(L, n))_{n \geq 0}$.

The conclusion of Proposition 4.4 is that $\tilde{\mathcal{E}}(L_0, n) < \tilde{\mathcal{E}}(L_0, n + 1)$. If one relaxes the hypotheses of Proposition 4.4 by allowing non-strict inequalities in place of the strict inequalities, it is clear what the conclusion will be, and this is equivalent to the statement that $\tilde{\mathcal{E}}(L_0, n) = \mathcal{E}(L_0, n)$. We will say that we have proved *ferromagnetic ordering to level n* if we can show that $\tilde{\mathcal{E}}(L, m) = \mathcal{E}(L, m)$ for $m = 1, \dots, n$, and *strict ferromagnetic ordering to level n* if

$$\tilde{\mathcal{E}}(L, 1) < \tilde{\mathcal{E}}(L, 2) < \dots < \tilde{\mathcal{E}}(L, n) < \tilde{\mathcal{E}}(L, n + 1).$$

The property that the ground state subspace has maximal spin is equivalent to “ferromagnetic ordering to level 0;” the existence of a non-vanishing spectral gap above the ground state is equivalent to “strict ferromagnetic ordering to level 0;” the proof that the first excitation lives in the sector $\mathcal{H}([1, L], 1)$ implies “ferromagnetic ordering to level 1;” and the subsequent proof that the first excitation is minimally degenerate, i.e., that the entire eigenspace is a spin $L/2 - 1$ irreducible representation, is proof or “strict ferromagnetic ordering to level 1.” Those four results are contained in refs. 10 and 14.

5. THE SPECTRAL GAP FOR THE XXX AND XXZ SPIN CHAIN

In this section we will show how Proposition 4.3 can be used to obtain the spectral gap of the XXZ model on a chain.

Theorem 5.1 (Koma and Nachtergaele 1997). For the spin-1/2 XXZ spin chain with $SU_q(2)$ symmetry, the spectral gap equals

$$\gamma_L = 1 - \Delta^{-1} \cos(\pi/L). \tag{5.1}$$

Proof. By Proposition 4.3, it suffices to prove that

$$\tilde{\mathcal{E}}(L, 1) = 1 - \Delta^{-1} \cos(\pi/L),$$

because this sequence is decreasing in L . We observe that the quantity $1 - \Delta^{-1} \cos(\pi/L)$ is actually the minimum eigenvalue for the matrix $1 - \Delta^{-1}A$ acting on $\ell^2(\{1, \dots, L - 1\})$, where A is the adjacency matrix of $\{1, \dots, L - 1\}$. Namely,

$$A(x, y) = \frac{1}{2}(\delta_{y, x+1} + \delta_{y, x-1}). \tag{5.2}$$

This is a clue to the calculation.

Note that by the quantum group symmetry one can calculate $\mathcal{E}_{L,1}$ by calculating the spectral gap in the $M = L/2 - 1$ subspace. In this subspace, we can write

$$|x\rangle = S_x^- |\uparrow\rangle, \quad (5.3)$$

where $|\uparrow\rangle$ is the all-upspin state. Then we observe

$$H_{[1,L]} |x\rangle = \frac{1}{1+q^2} \sum_{y=1}^L [\delta_{y,x-1} (|x\rangle - q |y\rangle) + \delta_{x,y-1} (q^2 |x\rangle - q |y\rangle)]. \quad (5.4)$$

The ground state is proportional to

$$\Psi_0 = \sum_{x=1}^L q^x |x\rangle. \quad (5.5)$$

Let us define the *Hulthén bracket basis* for the orthogonal complement of the ground state:

$$|\phi_x\rangle = |x\rangle - q |x-1\rangle \quad (5.6)$$

for $x = 2, \dots, L$. Then observe that

$$H_{[1,L]} |x\rangle = \frac{1}{1+q^2} \sum_{y=1}^L [\delta_{y,x-1} |\phi_x\rangle - q \delta_{x,y-1} |\phi_y\rangle]. \quad (5.7)$$

Hence, if $x \in \{2, \dots, L\}$,

$$\begin{aligned} & H_{[1,L]} |\phi_x\rangle \\ &= \frac{1}{1+q^2} \sum_{y=1}^L [\delta_{y,x-1} |\phi_x\rangle - q \delta_{x,y-1} |\phi_y\rangle - q \delta_{y,x-2} |\phi_{x-1}\rangle + q^2 \delta_{x-1,y-1} |\phi_y\rangle] \\ &= |\phi_x\rangle - \frac{q}{1+q^2} \sum_{y=1}^L [\delta_{x,y-1} |\phi_y\rangle + \delta_{y,x-2} |\phi_{x-1}\rangle]. \end{aligned} \quad (5.8)$$

Hence in this basis, the representation is precisely $1 - A^{-1}A$, as defined above. So we are done. ■

We conclude this section with a few remarks. First of all, the Hulthén basis has been discovered and rediscovered many times. Although here we have used just the simplest version, with just one Hulthén bracket, one can also obtain a *non-orthogonal* basis for the highest weight vectors of total spin j subspace using these brackets, which we will use in Section 7. To the best of our knowledge, the first to prove that the Hulthén basis is actually linearly independent were Temperley and Lieb.⁽²⁴⁾ We also refer the reader

to their paper for more details about the basis. In more recent literature, one often finds the term ‘‘Hulthén bracket’’ replaced by ‘‘valence bond,’’ in analogy with chemistry.

A second remark is in order. The calculation of the spectral gap worked so simply because the representation of the Hamiltonian in the one-bracket Hulthén basis is actually symmetric. Since the basis is not orthogonal, there is no reason to expect that to be the case in general. Indeed, if one considers the two-bracket Hulthén basis then the matrix representation is not orthogonal. As we will show, this is not a serious obstacle as long as the off-diagonal matrix elements are non-negative.

6. THE SPECTRAL GAP OF THE XXX MODEL ON A TREE

Let us consider a sequence of trees $\{T_L\}_{L=2}^\infty$ such that $|T_L| = L$ and T_L is the induced subgraph on some L vertices of T_{L+1} . We consider the usual XXX ferromagnet

$$H_{T_L} = \sum_{\{x,y\} \subset T_L, x \sim y} [\frac{1}{4} - \mathbf{S}_x \cdot \mathbf{S}_y]. \tag{6.1}$$

We can then prove the following theorem.

Theorem 6.1. One has $\mathcal{E}(L, 1) < \mathcal{E}(L, n)$ for any $n > 1$.

Proof. To begin the proof, note that Proposition 4.3 applies to the set of graphs $\{T_L\}_{L=2}^\infty$ with no changes, because the Hamiltonian $H_{T_L} \leq H_{T_{L+1}}$, and this is all that is necessary. Hence one may determine that $\mathcal{E}(L, 1) < \mathcal{E}(L, n)$ for any $n > 1$ if one can prove that $\mathcal{E}(L, 1)$ is strictly decreasing in L .

Defining $|x\rangle = S_x^- |\uparrow\rangle$, as before, we again have for any $x \in T_L$

$$H_{T_L} |x\rangle = \frac{1}{2} \sum_y [\delta_{y,x-1} (|x\rangle - |y\rangle) + \delta_{x,y-1} (|x\rangle - |y\rangle)] \tag{6.2}$$

but with the proper definition of ‘‘ $x-1$ ’’ and ‘‘ $y-1$.’’ Indeed, let us choose a point $O \in T_2$, to call this the root. Then for any T_L , and any $x \in T_L$ there is a unique non-backtracking path from O to x , because T_L is a tree. The definition of $x-1$ is that $x-1$ is the immediate predecessor of x on this path. Note that it is possible that $x-1 = y-1$ for some distinct points x and y in T_L , indeed this will be the case unless the tree is unary (has no splittings, i.e., is a chain). Also note that x and y are connected by an edge in T_L iff $x = y-1$ or $y = x-1$, and this is the reason that (6.2) is correct.

We define the obvious analogue of the one-bracket Hulthén states as

$$|\phi_x\rangle = |x\rangle - |x-1\rangle, \quad (6.3)$$

much as before. Then, again

$$H_{T_L}|x\rangle = \frac{1}{2} \sum_{y \in T_L} [\delta_{y,x-1} |\phi_x\rangle - \delta_{x,y-1} |\phi_y\rangle], \quad (6.4)$$

and

$$\begin{aligned} H_{T_L}|\phi_x\rangle &= \frac{1}{2} \sum_{y \in T_L} [\delta_{y,x-1} |\phi_x\rangle - \delta_{x,y-1} |\phi_y\rangle - \delta_{y,x-2} |\phi_{x-1}\rangle + \delta_{x-1,y-1} |\phi_y\rangle] \\ &= |\phi_x\rangle - \frac{1}{2} \sum_{y \in T_L} [\delta_{x,y-1} |\phi_y\rangle + \delta_{y,x-2} |\phi_{x-1}\rangle + \delta_{x-1,y-1}(1 - \delta_{x,y}) |\phi_y\rangle]. \end{aligned} \quad (6.5)$$

We claim that the matrix A_L defined such that

$$A_L|\phi_x\rangle = \frac{1}{2} \sum_{y \in T_L} [\delta_{x,y-1} |\phi_y\rangle + \delta_{y,x-2} |\phi_{x-1}\rangle + \delta_{x-1,y-1}(1 - \delta_{x,y}) |\phi_y\rangle], \quad (6.6)$$

is actually the adjacency matrix for the line graph of T_L , which we denote \mathcal{T}_L .

Here \mathcal{T}_L is the graph constructed from T_L by taking as a vertex set for \mathcal{T}_L the set of all edges $\{x, x-1\}$ in T_L . Then two distinct vertices are connected in \mathcal{T}_L if the edges are incident to the same vertex for some vertex in T_L . This happens for edges $\{x, x-1\}$, $\{y, y-1\}$ iff $x = y-1$, $y = x-1$ or $x-1 = y-1$. Of course if $y = x-1$ then $y-1 = x-2$ is in T_L and then $|\phi_{x-1}\rangle = |\phi_y\rangle$. Then one does indeed see that

$$A_L|\phi_x\rangle = \frac{1}{2} \sum_{y \in T_L \setminus \{0\}} \chi(\{x, x-1\} \sim \{y, y-1\}) |\phi_y\rangle, \quad (6.7)$$

which is the adjacency matrix (with our $1/2$ normalization). One particular implication is that the matrix representation for H_{T_L} in the one-bracket Hulthén basis is symmetric.

An important point is that \mathcal{T}_L is the induced subgraph of \mathcal{T}_{L+1} , induced by the edges which lie in T_L . Since the matrix $1 - A_L$ has non-positive off-diagonal matrix elements, and since A_L is a submatrix of A_{L+1} , we can apply Lemma 7.3, which is proved in Section 7. Therefore, this proves the ground state energy (and in this case actually also the sum of any first k eigenvalues) is nonincreasing with L . Since T_L is connected, it is easy to see,

by the Perron–Frobenius Theorem, that actually the ground state energy is strictly decreasing. ■

There is a fruitful connection between Markov processes and quantum spin systems. The study of the low-lying spectrum for quantum spin systems relates directly to estimating mixing times for simple exclusion processes, a subject of continued interest (see, e.g., refs. 18 and the references in that paper). In the Markov process language, this theorem implies that the spectral gap of the symmetric simple exclusion process equals the spectral gap of the random walk on any finite tree. This connections between Markov processes and certain quantum spin models such as the XXX and XXZ, as well as closely related models, such as simple exclusion processes, has been fruitfully exploited in the past. E.g., in ref. 2, Caputo and Martinelli proved good lower bounds for the gap of the spin- S XXZ chain by mapping the problem to an asymmetric simple exclusion process and applying probabilistic techniques to the latter. An example where a similar relation was used in the other direction is the work of Gwa and Spohn.⁽⁷⁾ They determine the scaling exponent for the stationary correlation function of the noisy Burgers equation in terms of spectral information of an XXX chain obtained through the Bethe Ansatz.

7. MONOTONICITY OF THE ENERGY

The goal of this section is to prove the following proposition for the XXZ spin chain.

Proposition 7.1.

$$\mathcal{E}(L+1, n) < \mathcal{E}(L, n), \quad \text{for all } L \geq 2, \quad n \geq 0. \quad (7.1)$$

In combination with Proposition 4.3, this result provides the proof for Theorem 1.4.

The proof of this proposition relies on two lemmas, Lemmas 7.2 and 7.3, which we state and prove at the end of this section. These lemmas are applied to the matrices of the spin-1/2 ferromagnetic Heisenberg Hamiltonian restricted to the invariant subspaces of all highest weight vectors of a given total spin.

Proof of Proposition 7.1. $\mathcal{E}_{L+1, n}$ is the minimal energy in the subspace with total spin $L/2 - n$. Clearly, we can restrict the minimization of the energy further to highest weight vectors in this subspace of fixed total spin, i.e., the eigenvectors of S^3 in $\mathcal{H}([1, L], n)$ with eigenvalue $L/2 - n$. A convenient basis for this intersection was introduced by Temperley and

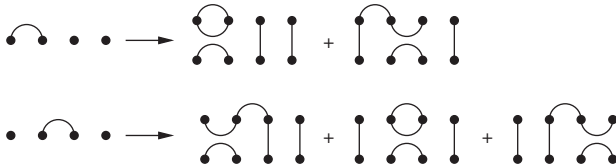


Fig. 1. Example of the action of the Hamiltonian of the spin-1/2 XXX or XXZ chain on a generalized Hulthén bracket, for $L = 4$, $n = 1$.

Lieb.⁽²⁴⁾ They called the element of this basis *generalized Hulthén brackets* and proved that they are linearly independent.

We now apply Lemma 7.3 with $A = A_{L,n}$ and $B = A_{L+1,n}$, which satisfy the conditions due to Lemma 7.2. The strict inequality is obtained by the comments following Lemma 7.3.

Lemma 7.2. The square matrices $A_{L,n}$ have the following properties (i) all of their off-diagonal matrix elements are non-positive, (ii) for all n , and L , $A_{L,n}$ is “embedded” in $A_{L+1,n}$, in the sense that there is a subset of the index set of $A_{L+1,n}$, such that $A_{L,n}$ is the restriction of $A_{L+1,n}$ to that subset.

Proof. Each basis element is labeled by a configuration of n arcs, each of which pairs two sites, say $i, j \in \{1, 2, \dots, L\}$, $i < j$ together, and the configuration has the properties that arcs are non-crossing and do not span unpaired sites. See Figs. 1–3, for a few examples. We will denote such an arc by (ij) , and denote configurations of arcs by α, β, \dots , and the set of all such configurations for given L and n by $\mathcal{B}_{L,n}$.

The highest weight vector $\phi_\alpha \in \mathcal{H}_L$, corresponding to the configuration of arcs α , are obtained as tensor product of the following factors: a factor $|+\rangle$ for each unpaired site, and a factor $q^{-1/2} |+\rangle_i |-\rangle_j - q^{1/2} |-\rangle_i |+\rangle_j$ for each arc (ij) .

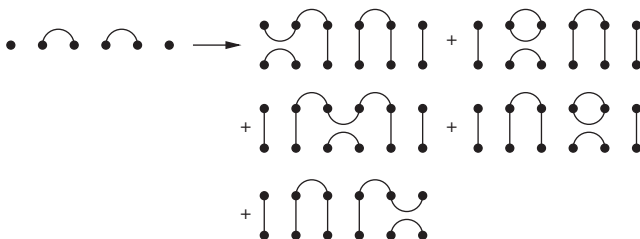


Fig. 2. Example of the action of the Hamiltonian of the spin-1/2 XXX or XXZ chain on a generalized Hulthén bracket, for $L = 6$, $n = 2$.

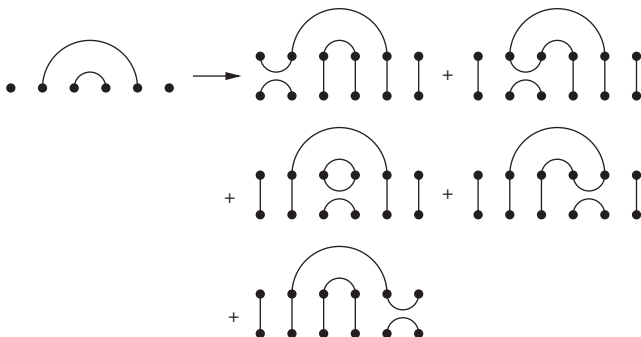


Fig. 3. Example of the action of the Hamiltonian of the spin-1/2 XXX or XXZ chain on a generalized Hulthén bracket, for $L = 6, n = 2$.

Let $A_{L,n}$ denote the matrix of the Hamiltonian (2.1) with respect to this basis. As the basis is not orthogonal we should, in general, not expect $A_{L,n}$ to be symmetric.

The matrix elements of $A_{L,n}$ can be most easily computed by also using a graphical representation of the Hamiltonian, i.e., by writing it in terms of the generators of the Temperley–Lieb algebra $U_{i,i+1}, 1 \leq i \leq L-1$, namely

$$U_{i,i+1} = -(q + q^{-1}) h_{i,i+1}.$$

Let $\phi_\alpha, \alpha \in \mathcal{B}_{L,n}$, be a basis vector. As $H_{[1,L]} = -(q + q^{-1}) \sum_{i=1}^{L-1} U_{i,i+1}$, we just have to calculate $U_{i,i+1} \phi_\alpha$. It turns out that for all i and α there exist β and a real constant c such that $U_{i,i+1} \phi_\alpha = c \phi_\beta$. The configuration β and the constant c are determined by a simple graphical procedure illustrated in Figs. 1–3.

We observe the following general rules: (i) if i and $i+1$ are both unpaired arcs in α , we have $U_{i,i+1} \phi_\alpha = 0$, (ii) if the composition of α and $U_{i,i+1}$ is isotopic to β , with $\beta \neq \alpha$, then the $U_{i,i+1} \phi_\alpha = \phi_\beta$, i.e., $c = 1$, (iii) if $\alpha = \beta, c = -(q + q^{-1})$. This only happens when the “cup” of $U_{i,i+1}$ is paired with an arc in α , i.e., α must contain the arc $(i, i+i)$.

With these observations the proof of the lemma is easily completed. ■

One can easily use the same observations to explicitly calculate any desired matrix element, but the properties given in the above lemma are sufficient for our purposes here.

The next lemma will allow us to compare the smallest eigenvalues of $A_{L,n}$ and $A_{L+1,n}$. For this it is important that the larger matrix, i.e., $B = A_{L+1,n}$, may have positive matrix elements on the diagonal and that there is only the condition that the first k of those are bounded by the corresponding diagonal elements of A . No assumption about the remaining $l - k$ diagonal elements is made.

Lemma 7.3. Let $A = (a_{ij})$ and $B = (b_{ij})$ be two square matrices with real entries of size k and l , respectively, with $l \geq k$, and such that

$$\begin{aligned} a_{ij} \leq 0, \quad b_{ij} \leq 0, \quad \text{for all } i \neq j, \\ b_{ij} \leq a_{ij}, \quad \text{for } 1 \leq i, j \leq k. \end{aligned}$$

Then

$$\inf \text{spec } B \leq \inf \text{spec } A. \quad (7.2)$$

Proof. The main idea for the proof of this lemma is taken from Lemma 3.6 in ref. 19. Let $C = \max\{a_{ii}, b_{jj} \mid 1 \leq i \leq k, 1 \leq j \leq l\}$. Then, the matrices $\tilde{A} = C\mathbb{1} - A$, and $\tilde{B} = C\mathbb{1} - B$, have all non-negative entries, denoted by \tilde{a}_{ij} , and \tilde{b}_{ij} , respectively, and $\tilde{b}_{ij} \geq \tilde{a}_{ij}$, for $1 \leq i, j \leq k$.

By the Perron–Frobenius Theorem, for any square matrix D with non-negative entries, and with spectral radius $\rho(D)$, we have that there is only one eigenvalue with absolute value equal to $\rho(D)$, namely $\rho(D)$ itself. Let $\lambda_0(M)$ denote the smallest eigenvalue of any square matrix M . Then, by the previous consideration, $\lambda_0(A) = C - \rho(\tilde{A})$ and $\lambda_0(B) = C - \rho(\tilde{B})$. Hence, to prove the lemma, we need to show $\rho(\tilde{A}) \leq \rho(\tilde{B})$.

For any $m \times m$ matrix D with non-negative entries, we also have that for any $v \in \mathbb{C}^m$, $\|Dv\| \leq \|D|v|\|$, where $|v|$ is the vector with components given by the absolute values of the components of v . Hence,

$$\|D\| = \sup_{0 \neq v \in \mathbb{C}^m} \frac{\|Dv\|}{\|v\|} = \sup_{0 \neq v \in (\mathbb{R}^+)^m} \frac{\|Dv\|}{\|v\|}.$$

For any $r \geq 1$,

$$\|\tilde{B}^r\| = \sup_{0 \neq v \in (\mathbb{R}^+)^l} \frac{\|\tilde{B}^r v\|}{\|v\|} \geq \sup_{0 \neq w \in (\mathbb{R}^+)^k} \frac{\|\tilde{B}^r \tilde{w}\|}{\|\tilde{w}\|},$$

where, for any $w \in \mathbb{C}^k$, we let $\tilde{w} \in \mathbb{C}^l$ denote the vector with the first k components given by those of w , and the remaining $l - k$ components equal to zero. Clearly, $\|\tilde{w}\| = \|w\|$.

Now, consider $\hat{B} = \tilde{B}_1 \oplus \tilde{B}_2$, where \tilde{B}_1 is the $k \times k$ matrix with entries \tilde{b}_{ij} , $1 \leq i, j \leq k$, and \tilde{B}_2 is the diagonal $(l - k) \times (l - k)$ matrix with diagonal entries \tilde{b}_{ii} , $k + 1 \leq i \leq l$. Then $\tilde{B} \geq \hat{B}$, elementwise, and hence $\tilde{B}^r \geq \hat{B}^r = \tilde{B}_1^r \oplus \tilde{B}_2^r$. Moreover, $\tilde{B}_1 \geq \tilde{A}$ by the assumptions of the lemma. Therefore, we have

$$\|\tilde{B}^r\| \geq \sup_{0 \neq w \in (\mathbb{R}^+)^k} \frac{\|\tilde{A}^r w\|}{\|w\|} = \|\tilde{A}^r\|. \quad (7.3)$$

By taking r th roots and $\lim \sup$'s, from the inequality (7.3) we obtain $\rho(\tilde{A}) \leq \rho(\tilde{B})$. ■

Sufficient conditions under which the inequality in (7.2) is strict are easy to find. E.g., when the matrices are irreducible (in the Perron–Frobenius sense), it is sufficient that one of the off-diagonal matrix elements b_{ij} of B , with at least one of the indices i or $j > k$. This is the situation in our application with $A = A_{L,n}$ and $B = A_{L+1,n}$. Another sufficient condition that guarantees strict inequality in the irreducible case, is that $b_{ij} < a_{ij}$, for at least one pair of $i \neq j$, $1 \leq i, j \leq k$.

8. CONCLUSION

In this paper we have formulated a natural conjecture for ferromagnetic Heisenberg models, Conjecture 1.3. We proved this conjecture for the spin-1/2 XXX chain with open boundary conditions, as well as the analogous results for the $SU_q(2)$ -symmetric spin-1/2 XXZ chain. The techniques developed allow trivial extension to nearest-neighbor spin chains whose coupling constants $J_{\{x, x+1\}}$ are not all constant, but are all negative.

To demonstrate the generality of the underlying techniques, we have also proved that the first excited eigenvector for the XXX model on a tree is always a 1-spin-deviate.

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