Ferromagnetic Ordering of Energy Levels for XXZ Spin Chains

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The Lieb-Mattis theorem on ordering of energy levels

Definitions:

Given a finite set Λ and coupling constants $J = \{J_{\{x,y\}} : x \neq y \in \Lambda\}$, define the *Heisenberg Hamiltonian*

$$H_{\Lambda,J} = \sum_{x \neq y \in \Lambda} J_{\{x,y\}} S_x \cdot S_y \tag{1}$$

At each site $x \in \Lambda$, there is supposed to be a spin-s_x representation of SU(2), for $s_x \in \frac{1}{2}\mathbb{N}$.

If there are two subsets A, B with $\Lambda = A \sqcup B$ and

$$\begin{cases} J_{\{x,y\}} \leq 0 & \text{if } x \in A, y \in B\,, \\ J_{\{x,y\}} \geq 0 & \text{if } x, y \in A \text{ or } x, y \in B\,, \end{cases} \tag{2}$$

call the model (A, B)-*bipartite*. Then, define $S_A = \sum_{x \in A} s_x$ and $S_B = \sum_{x \in B} s_x$.

The model is called *reducible* if two sets Λ_1 and Λ_2 exist, such that $\Lambda = \Lambda_1 \sqcup \Lambda_2$ and $J_{\{x,y\}} = 0$ for all $x \in \Lambda_1$, $y \in \Lambda_2$. Otherwise the model is *irreducible*.

Finally, define $E(\Lambda, J, S)$ as the infspec of $H_{\Lambda,J}$, restricted to the subspace of vectors with total spin equal to S.

Theorem 1. (Ordering of energy levels [5]) *Suppose the Heisenberg Hamiltonian $H_{\Lambda,J}$ is irreducible and (A,B)-bipartite. Then, defining $\mathcal{S} = |S_A - S_B|$,*

$$E(\Lambda, J, S+1) > E(\Lambda, J, S) \quad \textit{for all} \quad S \geq \mathcal{S}\,, \tag{3}$$
$$E(\Lambda, J, S) > E(\Lambda, J, \mathcal{S}) \quad \textit{for all} \quad S < \mathcal{S}\,. \tag{4}$$

There are three natural categories of (A,B)-bipartite models:

- *antiferromagnetic* if $0 < S_A = S_B$;
- *ferrimagnetic* if $0 < S_B < S_A$;
- and *ferromagnetic* if $0 = S_B < S_A = \mathcal{S}$.

The Lieb-Mattis theorem implies that for antiferromagnetic models, $E(\Lambda, J, S) < E(\Lambda, J, S')$ whenever $S < S'$.

It also implies that for ferromagnetic models $E(\Lambda, J, S) > E(\Lambda, J, \mathcal{S})$ whenever $S < \mathcal{S}$. We call this "ferromagnetic ordering of the ground state".

It is natural to guess:

Conjecture 2. (Ferromagnetic ordering of energy levels) *Suppose the Heisenberg Hamiltonian $H_{\Lambda,J}$ is irreducible and ferromagnetic. Then*

$$E(\Lambda, S) < E(\Lambda, S') \quad \textit{whenever} \quad S > S'\,. \tag{5}$$

Main Result

Our main result is a proof of Conjecture 2 for spin chains with all $s_x = 1/2$.

Theorem 3. *Suppose* $\Lambda = [1, L]$ *for* $L \geq 2$ *and that* J *satisfies*

$$\begin{cases} J_{\{x,y\}} = 0 & \textit{for} \quad |x-y| > 1\,, \\ J_{\{x,x+1\}} < 0 & \textit{for} \quad x = 1, \dots, L-1\,. \end{cases} \tag{6}$$

Then $E([1, L], J, S) < E([1, L], J, S')$ *for* $S > S'$. *Also, for* $0 < q < 1$, *define the* $SU_q(2)$*-symmetric XXZ model with Ising-type anisotropy,*

$$H^q_{[1,L],J} = \sum_{x=1}^{L-1} J_{(x,x+1)} h^q_{(x,x+1)}\,, \tag{7}$$

$$h^q_{(x,x+1)} = S^3_x S^3_{x+1} + (q+q^{-1})^{-1}(S^+_x S^-_{x+1} + S^-_x S^+_{x+1}) + \frac{1}{2}\sqrt{1-q^2}(S^3_x - S^3_{x+1})\,. \tag{8}$$

Define $E^q([1, L], J, S)$ *as the infspec of* $H^q_{[1,L],J}$ *restricted to vectors with total* $SU_q(2)$*-spin equal to* S. *Then* $E^q([1, L], J, S) < E^q([1, L], J, S')$ *for* $S > S'$.

Outline of Proof : Koma and Nachtergaele's Lemma

The proof proceeds by several lemmas, none of which is entirely new.

The first is a result due to Koma and Nachtergaele, which we paraphrase as follows:

Lemma 4. (Addition of angular momentum [3]) *Suppose, for $L = 2, 3, \ldots,$ H_L is a $SU_q(2)$-symmetric Hamiltonian on $\mathcal{H}_L = (\mathbb{C}^2)^{\otimes[1,L]}$, and that $H_{L+1} \geq H_L$ under the embedding $\mathrm{End}(\mathcal{H}_L) \subset \mathrm{End}(\mathcal{H}_{L+1})$. Defining $\mathcal{E}(L,n)$ to be the infspec of H_L restricted to $S = L/2 - n$, if*
- $\mathcal{E}(L,n) < \mathcal{E}(L,m)$ *for* $m > n$,
- *and* $\mathcal{E}(L+1,n) \leq \mathcal{E}(L,n)$,

then
- $\mathcal{E}(L+1,n) < \mathcal{E}(L+1,m)$ *for* $m \geq n$.

The reader can guess the proof, from the two facts:

1. The variational energy of any vector with respect to H_{L+1} is bounded below by its energy with respect to H_L.

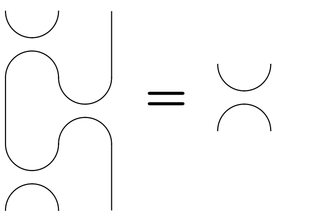
2. Any vector with total spin S, when tensored with a spin 1/2 vector, decomposes into two vectors, with spins $S \pm 1/2$.

Using this lemma inductively, one can prove Theorem 3 by proving that $\mathcal{E}(L,n)$ is decreasing with L.

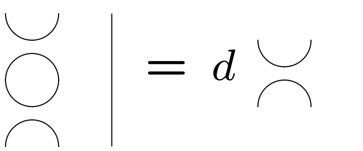
The Temperley-Lieb algebra

In [7], Temperley and Lieb defined an algebra (implicitly) which is useful in graph theory for several purposes*.

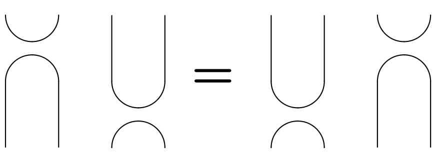
The generators are $U^q_{x,x+1} = -(q+q^{-1})h^q_{x,x+1}$, $x = 1, \ldots, L-1$. The relations (which one can easily check) are represented graphically



$$U_{x,x+1}\,U_{x+1,x+2}\,U_{x,x+1} \;=\; U_{x,x+1},$$



$$U_{x,x+1}\,U_{x,x+1} \;=\; -(q+q^{-1})\,U_{x,x+1},$$



$$U_{x,x+1}\,U_{y,y+1} \;=\; U_{y,y+1}\,U_{x,x+1}, \quad \text{for } |x-y| > 1.$$

Here, $d = -(q+q^{-1})$.

This is particularly useful when combined with the *generalized Hulthén brackets* which Temperley and Lieb also defined in [7].

*The roots of which are Lieb's work on the 6-vertex model, which is closely related to the XXZ model [4].

Generalized Hulthén brackets

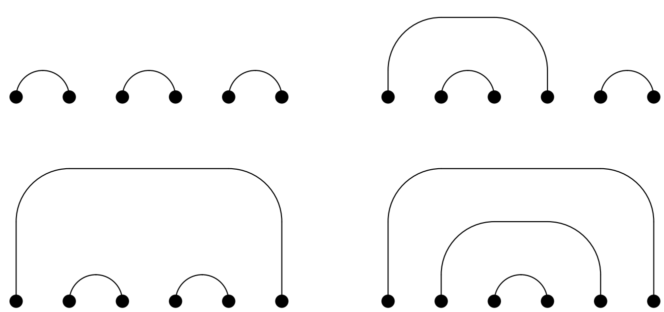
Call an n-*bracket* a set $\alpha = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ s.t.
• $1 \leq x_i < y_i \leq L$ for all i.
• Pairings are *noncrossed*, where *crossed* means $x_i < x_j < y_i < y < j$.
• No pairing spans an unpaired site.

For each bracket α, Temperley and Lieb defined a highest-weight vector of $\mathrm{SU}_q(2)$,

$$\psi_\alpha^q = \prod_{(x,y)\in\alpha} (S_y^- - qS_x^-) \, |\!\uparrow\rangle \ . \qquad (9)$$

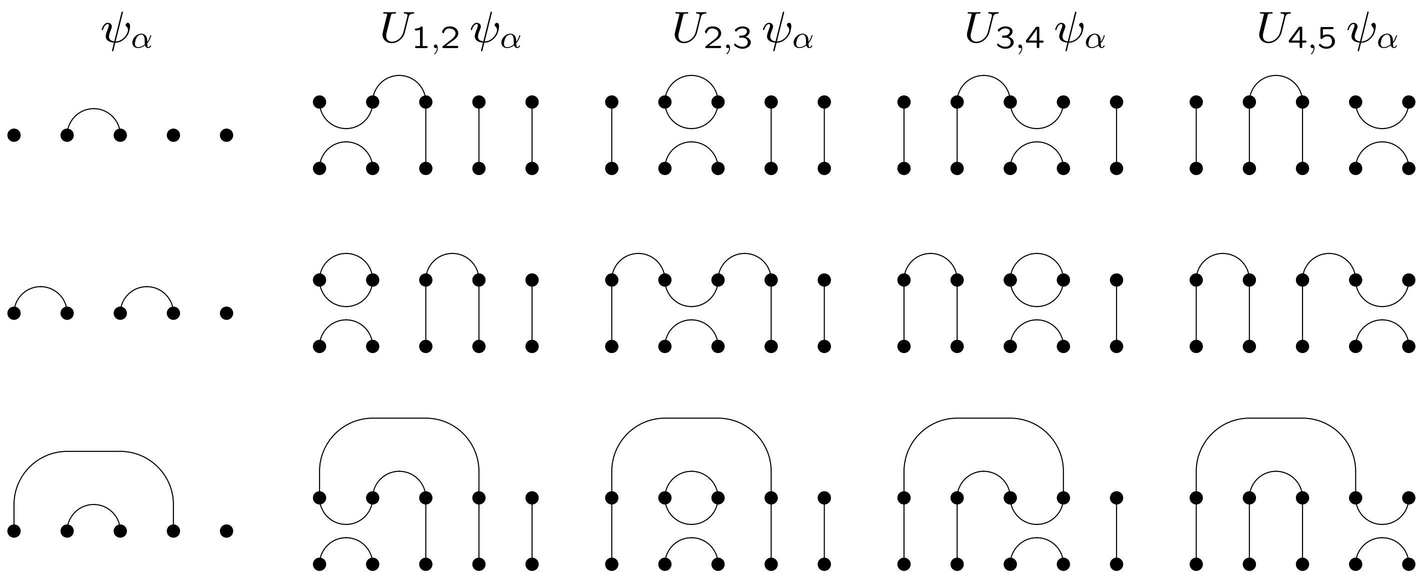
They proved $\{\psi_\alpha^q : \alpha \text{ an } n\text{-bracket}\}$ is a (nonorthogonal) basis for the highest-weight vectors with spin $L/2 - n$.

They can be represented graphically. E.g., for $L = 6$ and $n = 3$,



There is a simple graphical way of calculating $U_{i,i+1}\psi_\alpha$. Namely, compose the graph for $U_{i,i+1}$ with that of ψ_α, and isotope relative to the bottom line. Any free circle becomes a numerical factor equal to $d = -(q + q^{-1})$. If there is a free semicircle, then the result is 0.

Some examples are shown below:



From the graphical representation one deduces:

Lemma 5. (Positivity properties) *For any admissible bracket* α*, and any* $(x, x+1) \subset [1, L]$ *there is a bracket* β *and a number* c*, such that* $U_{x,x+1}\psi_\alpha = c\,\psi_\beta$*, and*

- *If neither* x *nor* $x+1$ *is in any pairing of* α*,* $c = 0$*;*
- *If* $(x, x+1)$ *is a pairing of* α*, then* $c = -(q + q^{-1})$*, and* $\beta = \alpha$*;*
- *Otherwise,* $c = 1$ *and* $\beta \neq \alpha$ *is obtained by isotoping the graph as described above.*

Perron-Frobenius Theorem

We wish to prove that $\mathcal{E}(L,n)$ is decreasing with L for every n. A natural approach is to use the variational principle. Unfortunately, since the Hulthén bracket basis is not orthogonal, the matrix for $H_{[1,L],J}$, is generally not symmetric; so the usual variational principle doesn't apply.

However, due to the positivity properties of the last lemma, we can apply a different variational principle, which was previously used in [6].

Lemma 6. (Positive variational principle) *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 s.t.*

$$a_{ij} \leq 0, b_{ij} \leq 0, \text{ for all } i \neq j, \tag{10}$$

$$b_{ij} \leq a_{ij}, \text{ for } 1 \leq i,j \leq k\,. \tag{11}$$

Then

$$\inf \operatorname{spec} B \leq \inf \operatorname{spec} A\,. \tag{12}$$

To prove that $\mathcal{E}(L,n)$ is decreasing is the same as proving that the ground state of $H_{[1,L],J}$ restricted to h.w. vectors of spin $L/2-n$ is no less than the ground state of $H_{[1,L+1],J}$ restricted to h.w. vectors of spin $(L+1)/2-n$.

In the Hulthén basis, both matrices have nonpositive off-diagonal entries and any diagonal components common to both matrices have the same entries. So the negative of these matrices satisfy the hypotheses of the lemma.

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