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 $\Lambda$ and coupling constants $J = \{J_{\{x,y\}} : x \neq y \in \Lambda\}$, define the Heisenberg Hamiltonian

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

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

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

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 $\Lambda_1$ and $\Lambda_2$ 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 $S = |S_A - S_B|,$

$$E(\Lambda, J, S + 1) > E(\Lambda, J, S) \quad \text{for all} \quad S \geq S,$$  \hspace{1cm} (3)

$$E(\Lambda, J, S) > E(\Lambda, J, S) \quad \text{for all} \quad S < S.$$ \hspace{1cm} (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 $0 = S_B < S_A = S$.

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 $E(\Lambda, J, S) > E(\Lambda, J, S)$ whenever $S < S$. 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

$$E(\Lambda, S) < E(\Lambda, S') \quad \text{whenever} \quad S > S'.$$ \hspace{1cm} (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

\[
\begin{cases}
J_{\{x,y\}} = 0 & \text{for } |x - y| > 1, \\
J_{\{x,x+1\}} < 0 & \text{for } x = 1, \ldots, L - 1.
\end{cases}
\]  (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,

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

\[
h^q_{(x,x+1)} = S_x^3 S_{x+1}^3 + \left(q + q^{-1}\right)^{-1}(S^+_x S^-_{x+1} + S^-_x S^+_x) + \frac{1}{2} \sqrt{1 - q^2} \left(S_x^3 - S_{x+1}^3\right).
\]  (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 $H_{L+1} \succeq H_L$ under the embedding $\text{End}(\mathcal{H}_L) \subset \text{End}(\mathcal{H}_{L+1})$. Defining $\mathcal{E}(L,n)$ to be the infsup 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

$$
\begin{align*}
\text{for } |x-y| > 1.
\end{align*}
$$

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 $\alpha$, Temperley and Lieb defined a highest-weight vector of $SU_q(2)$,

$$\psi^q_{\alpha} = \prod_{(x, y) \in \alpha} (S_y^{-} - qS_x^{-}) |\uparrow\rangle.$$ (9)

They proved $\{\psi^q_{\alpha} : \alpha \text{ an } n\text{-bracket}\}$ 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 $\psi_\alpha$, 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 $\alpha$, and any $(x, x+1) \subset [1, L]$ there is a bracket $\beta$ 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 $\alpha$, $c = 0$;
- If $(x, x+1)$ is a pairing of $\alpha$, 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.

\begin{align}
    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{align}

Then

$$\inf \text{spec } B \leq \inf \text{spec } A.$$  

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.
References


