The spectral gap of the ferromagnetic XXZ chain

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Abstract

We prove that the spectral gap of the spin-1/2 ferromagnetic XXZ chain with Hamiltonian

\[ H = -\sum_x S_x^{(1)} S_{x+1}^{(1)} + S_x^{(2)} S_{x+1}^{(2)} + \Delta S_x^{(3)} S_{x+1}^{(3)}, \]

is given by \( \Delta - 1 \) for all \( \Delta \geq 1 \). This is the gap in the spectrum of the infinite chain in any of its ground states, the translation invariant ones as well as the kink ground states, which contain an interface between an up and a down region. In particular, this shows that the lowest magnon energy is not affected by the presence of a domain wall. This surprising fact is a consequence of the \( SU_q(2) \) quantum group symmetry of the model.

Keywords: quantum spin chains, Heisenberg model, ferromagnetic XXZ chain, kink ground states, spectral gap, quantum group symmetry

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Gap of the XXZ chain

1 Introduction

The main purpose of this paper is to determine in a completely rigorous setting the exact value of the spectral gap of the spin-1/2 ferromagnetic XXZ Heisenberg chain in the thermodynamic limit. By the spectral gap we mean the gap above the ground state in the spectrum of the GNS Hamiltonian in one of the ground state representations of the model. The ferromagnetic XXZ chain has translation invariant ground states as well as ground states that contain a domain wall (the so-called kink ground states). It is surprising that the gap does not depend on the reference ground state, i.e., the presence of a domain wall does not affect the energy of the lowest excited state. In general the gap in a kink ground state cannot exceed the gap in the homogeneous ground states (see Section 4.2). That the two gaps coincide for the $S=1/2$ XXZ chain is a consequence of the $SU_q(2)$ quantum group symmetry of the model. The homogeneous and kink ground states considered in this paper are all the infinite volume ground states of the XXZ chain [1].

Our main result is given in Theorem 1 at the end of this introduction. The expression for the spectral gap given there coincides with the Bethe Ansatz result (see e.g. 2, 3, 4). It should be noted that treatments based on the Bethe Ansatz suffer from the fact that the completeness of the eigenstates obtained by this method is still an unproven assumption [5]. Our proof does not use the Bethe Ansatz and is free from any unproven assumptions.

The following finite volume Hamiltonians that include special boundary terms, will be useful:

\[
H_{L}^{XXZ} = A(\Delta) \left( S_{L}^{(3)} - S_{1}^{(3)} \right) - \sum_{x=1}^{L-1} \left[ \Delta^{-1} \left( S_{x}^{(1)} S_{x+1}^{(1)} + S_{x}^{(2)} S_{x+1}^{(2)} \right) + S_{x}^{(3)} S_{x+1}^{(3)} \right]
\]

(1.1)

with the anisotropic coupling $\Delta \geq 1$, where $S_{x}^{(\alpha)}$ ($\alpha = 1, 2, 3$) are the usual $2 \times 2$ spin matrices (with eigenvalues $\pm 1/2$) acting on the site $x$, and $A(\Delta) = \pm \frac{1}{2} \sqrt{1 - 1/\Delta^2}$. For arbitrary finite volumes $\Lambda$ we denote the corresponding Hamiltonians by $H_{\Lambda}^{XXZ}$. The two Hamiltonians corresponding to the positive and negative choice of $A(\Delta)$ are obvi-
ous unitarily equivalent by left-right symmetry. Unless explicitly mentioned we will always refer to the Hamiltonian with the positive choice for \( A(\Delta) \). The boundary conditions and normalization of (1.1) are natural for the following reasons. First of all they make the ground state degeneracy equal to \( L + 1 \) for all \( \Delta \geq 1 \). This property can be explained in terms of a quantum group symmetry that the Hamiltonian, with these particular boundary terms included, possesses \([6]\). The normalization is such that one can consider the limit \( \Delta \to \infty \) without difficulty. In this limit the model becomes the ferromagnetic Ising chain with a boundary term that allows for ground states with a kink, i.e., for any site \( x \) in the finite chain the configuration with all spins to the left of \( x \) up (\( \uparrow \)) and all spins to the right of \( x \) down (\( \downarrow \)), is a ground state. Obviously there are \( L - 1 \) of such kink states. Together with the two translation invariant configurations this yields \( L + 1 \) ground states. As we will see in Section 4 the boundary terms also make the computation of the GNS Hamiltonians of the infinite chain immediate.

In the isotropic limit (\( \Delta = 1 \)) the \( L + 1 \)-fold degeneracy is the dimension of the spin \( L/2 \) representation of SU(2). Note that the boundary terms vanish for \( \Delta = 1 \). In the thermodynamic limit (\( L \to \infty \)) all translation invariant ground states are states of perfectly aligned spins. No non-translation invariant ground states are known.

If \( \Delta > 1 \), there are four different classes of ground states of the model on the infinite chain, which could be called \( \text{up, down, kink, and antikink} \). They consist, respectively, of the state with all spins \( \uparrow \); the state with all spins \( \downarrow \), an infinite number of states in which the spins are \( \uparrow \) at \( -\infty \) and \( \downarrow \) at \( +\infty \), and an infinite number of states in which the spins are \( \downarrow \) at \( -\infty \) and \( \uparrow \) at \( +\infty \). The infinite degeneracy of the ground state in the latter two sectors corresponds to the possible choices for the location of the kink or antikink. The kinks are strictly speaking located at a single bond only in the Ising limit (\( \Delta \to \infty \)). For \( 1 < \Delta < \infty \) the ground states are not described by a single configuration because of the quantum fluctuations, but the kinks, respectively antikinks, are quasi-localized for all \( 1 < \Delta < \infty \). All these properties
The kink states themselves were also written down independently by Alcaraz, Salinas and Wreszinski in [8], who moreover discovered that the exact expressions of ground states containing a domain wall generalize directly to higher spin and higher dimensions. The detailed properties, including the excitation spectrum, of the interface ground states in two and higher dimensions is the subject of a separate paper [9].

It is remarkable that the turning over from up to down in a kink ground state is exponentially localized in this one-dimensional system. One likes to think of the XXZ ferromagnet as the Ising model with quantum fluctuations. In low dimensions, phase boundaries, or domain walls, are unstable against thermal fluctuations. In the XXZ chain (as well as in its higher-dimensional cousins), quantum fluctuations do not destroy domain walls as long as \( \Delta > 1 \). This can be intuitively understood as a consequence of the competition between the \(-S_x^{(1)} S_{x+1}^{(1)} - S_x^{(2)} S_{x+1}^{(2)} \) and the \(-S_x^{(3)} S_{x+1}^{(3)} \) terms in the Hamiltonian. The first term favors configurations with opposite spins at \( x \) and \( x + 1 \). The second term is attractive and favors parallel spins at neighboring sites. First, consider the isotropic chain (\( \Delta = 1 \)). There, all ground states have the full permutation symmetry of the lattice (the set of all states of highest possible spin, \( S_{\text{tot}} = L/2 \), coincides with the set of states that are invariant under arbitrary permutations of the lattice sites). So, the ground state at a fixed value of the third component of the spin is uniquely characterized by the fact that the positions of the down spins are all equally probable (and all configurations occur with the same phase). This means that the two terms in the Hamiltonian exactly balance each other resulting in ground states that are indifferent for the down spins to be neighbors or not. It is therefore not so surprising that increasing the relative weight of the \(-S_x^{(3)} S_{x+1}^{(3)} \) term in the Hamiltonian by any non-vanishing amount, results in an effective attraction between like spins, leading to phase separation in the ground state.
The gap in the thermodynamic limit is a well-defined notion only with respect to one of the aforementioned four superselection sectors: up, down, kink, and antikink. Each of these sectors corresponds to a different representation of the observable algebra of the system. In these representations the Heisenberg dynamics of the model is generated by a densely defined self-adjoint, non-negative definite operator $H$. Theorem 1 below refers to the gap above zero in the spectrum of this operator. Physically it is the gap usually referred to as the “bulk gap”, i.e., the gap in the Hilbert space of states that are quasi-local perturbations of an infinite volume ground state. In particular, edge excitations are not taken into account.

**Theorem 1** For all $\Delta \geq 1$, and in each of the sectors described above as up, down, kink, and antikink, the infinite volume gap $\gamma$ is given by

$$\gamma = 1 - \Delta^{-1}$$

(1.2)

### 2 The ground states of the XXZ chain

Only those aspects of the ground states of the XXZ chain that have direct relevance to our proof and understanding of the spectral gap of the model will be presented here. A more detailed analysis can be found in [7], and various aspect of the ground states have been discussed in the literature (see e.g. [8] and the references therein).

For the study of the finite chains we use the special boundary conditions introduced in (1.1). Up to a constant the Hamiltonian can be written as follows:

$$H^{(q)}_L = H^{XXZ}_L + (L - 1)/4 = \sum_{x=1}^{L-1} h^{q}_{x,x+1}$$

(2.1)

where $h^{q}_{x,x+1}$ is the orthogonal projection on the vector

$$\xi_q = \frac{1}{1 + q^2} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

(2.2)
Here the parameter \( q \) is given by \( \Delta = (q + q^{-1}) \) with the range \( 0 \leq q \leq 1 \). In terms of the spin matrices \( h_{1,2}^q \) is given by

\[
 h_{1,2}^q = -\Delta^{-1}(S_1^{(1)}S_2^{(1)} + S_1^{(2)}S_2^{(2)}) - S_1^{(3)}S_2^{(3)} + \frac{1}{4} + A(\Delta)(S_2^{(3)} - S_1^{(3)})
\]

with \( A \) defined following (1.1). From the definition of \( \xi_q \) it is obvious that \( h_{x,x+1}^q |\uparrow \cdots \uparrow \rangle = 0 \) for all \( x = 1, \ldots, L - 1 \). As \( H_{L}^{(q)} \) is the sum of the \( h_{x,x+1}^q \), which are positive, this implies that the ground state energy of \( H_{L}^{(q)} \) is zero and that \( |\uparrow \cdots \uparrow \rangle \) is a ground state. For all \( 0 \leq q \leq 1 \), the ground state space (\( \equiv \ker H_{L}^{(q)} \)) is \( L + 1 \)-dimensional. We will often omit the superscripts \( q \) to simplify notations.

For all \( \Delta \geq 1 \) the uniform states \( |\uparrow \cdots \uparrow \rangle \) and \( |\downarrow \cdots \downarrow \rangle \) are ground states of the XXZ chain. If \( \Delta = 1 \) the \( L + 1 \)-dimensional ground state space is the spin \( L/2 \) representation of \( \text{SU}(2) \). For all \( \Delta > 1 \) and \( A = \frac{1}{2}\sqrt{1 - 1/\Delta^2} \), the non-uniform ground states can be thought of as kink states, which are roughly described as the Ising kinks plus quantum fluctuations. For \( A = -\frac{1}{2}\sqrt{1 - 1/\Delta^2} \) the kinks have to be replaced by antikinks, i.e., the roles of \( \uparrow \) and \( \downarrow \) spins have to be interchanged (or, equivalently, one can interchange left and right). We refer to [7, 8, 9] for more details and explicit expressions.

In the thermodynamic limit the boundary terms disappear to infinity and the left-right symmetry of the model, broken by the particular boundary terms we have introduced, must be restored. It is therefore obvious that both the kink and antikink states appear as infinite volume ground states of the model.

For our purposes the most convenient way to describe the space of ground states of a chain of length \( L \) is to introduce deformed raising and lowering operators which, together with the third component of the spin, generate the algebra (quantum group) of \( \text{SU}_q(2) \). The representation of \( \text{SU}_q(2) \) on the finite chain is not left-right symmetric, and is different for the boundary terms that produce kink and antikink ground states. In fact, the two mutually non-commuting representations of \( \text{SU}_q(2) \) together generate the infinite-dimensional quantum affine symmetry algebra \( \hat{sl}_q(2) \) that lies at the basis of the integrability of the model (see e.g.
A rigorous formulation of this infinite dimensional symmetry of the XXZ chain, has not yet been obtained (see [12] for a discussion of some of the problems). We will not use it here.

Here, we restrict the discussion of the quantum group symmetry of the XXZ model to the bare minimum (see, e.g., [13] for the representation theory of $SU_q(2)$). One can think of the quantum group symmetry as a systematic way to construct operators that commute with the Hamiltonians $H^{(q)}_L$. The parallelism with the usual arguments in the “theory of angular momentum” in quantum mechanics (representations of $SU(2)$) is so perfect that the reader will hardly notice the difference.

For $0 < q < 1$ define the $2 \times 2$ matrix $t$ by $t = q^{-2S}$, and define as usual $S^{\pm} = S^{(1)} \pm iS^{(2)}$. It is trivial to check that $S^{\pm}$ and $t$ satisfy the following commutation relations

$$tS^{\pm} = q^{\mp 2S}t,$$

$$[S^{+}, S^{-}] = \frac{t - t^{-1}}{q - q^{-1}} = 2S$$

They are just the $SU(2)$ commutation relations in disguise. The remarkable fact is that there is a simple definition of the tensor product (coproduct of the quantum group) of any two representations of the commutation relations (2.4), yielding a new representation. The representation on a chain of $L$ spins is given by

$$S^{(3)}_{[1,L]} = \sum_{x=1}^{L} I_1 \otimes \cdots \otimes S_x^{(3)} \otimes I_{x+1} \otimes \cdots \otimes I_L$$

$$S^+_{[1,L]} = \sum_{x=1}^{L} t_1 \otimes \cdots \otimes t_{x-1} \otimes S_x^+ \otimes I_{x+1} \otimes \cdots \otimes I_L$$

$$S^-_{[1,L]} = \sum_{x=1}^{L} I_1 \otimes \cdots \otimes S_x^- \otimes t_{x+1}^{-1} \otimes \cdots \otimes t_L^{-1}$$

where we used an index to identify the sites on which the tensor factors act. Note that, for $L \geq 2$, the operators $S^{\pm}_{[1,L]}$ depend on $q$ through $t$. One can easily check that the “spin” operators as defined in (2.5-a)–(2.5-c) commute with the interaction terms $h^q_{x,x+1}$ and hence with the Hamiltonian $H^{(q)}_L$ itself. Therefore, all states of the form $(S^-_{[1,L]})^k |\uparrow \cdots \uparrow\rangle$ are
ground states. This way we obtain \( L + 1 \) ground states. That there are no other ground states follows from the ground state equations \( h_{x,x+1}^q \psi = 0 \), for \( 1 \leq x \leq L - 1 \), and for an arbitrary \( \psi = \sum_{\{\sigma_x\}} \psi(\{\sigma_x\}) |\{\sigma_x\}\rangle \). This set of equations is equivalent to the equations 
\[
\psi(\cdots \downarrow \upa \cdots) = q \psi(\cdots \upa \cdots),
\]
where the \( \upa \) and \( \downarrow \) spins are at the sites \( \{x, x+1\} \). It is then obvious that there is only one solution in each sector of fixed number of \( \downarrow \) spins.

3 The gap for finite chains

In the proof of Theorem \( \square \) we will need the exact spectral gap for finite chains with the boundary conditions of (1.1). As will become clear in Section \( \square \), this choice of boundary conditions is the optimal one and essentially the only choice that when taking the thermodynamic limit will yield a lower bound that is, in fact, the exact gap in the thermodynamic limit.

Denote by \( \gamma_L \) the spectral gap of \( H_L^q \), which, as the ground state energy vanishes, is equal to the energy of first excited state and let \( \varepsilon_L \) be the first excited state in the sector with exactly one down spin. The aim of this section is to prove the following proposition.

**Proposition 2** For the \( SU_q(2) \) invariant spin-1/2 ferromagnetic XXZ chain with Hamiltonian (1.1), \( L \geq 2 \), and \( \Delta \geq 1 \) one has

\[
\gamma_L = \varepsilon_L = 1 - \Delta^{-1} \cos(\pi/L)
\]  

and in particular

\[
\gamma_L \geq 1 - \Delta^{-1}.
\]

The proof of this proposition combines two rather elementary facts:

1) There is a first excited state of the chain of \( L \) sites with total spin equal to \( (L/2) - 1 \), i.e., the maximal possible value of the total spin minus one (see Lemma \( \square \)).

2) In the sector of total spin \( (L/2) - 1 \), \( H_L^{(q)} \) can easily be diagonalized (see Lemma \( \square \)).
The remainder of this section is devoted to proving two lemmas that together establish 1) and 2) and hence prove (3.1).

Consider an arbitrary spin chain of \(L\) sites and with Hilbert space \(\mathcal{H}_L = \bigotimes_{x=1}^{L} (\mathbb{C}^d)_x\), and with local Hamiltonians of the following form:

\[
H_L = \sum_{x=1}^{L-1} h_{x,x+1}
\]  

(3.3)

where \(h_{x,x+1}\) acts non-trivially only at the nearest neighbor pair \(\{x, x+1\}\) and \(h_{x,x+1} \geq 0\). Assume that \(\ker H_L \neq \{0\}\). It is obvious that \(\ker H_L = \bigcap_{x=1}^{L-1} \ker h_{x,x+1}\). For an arbitrary subset \(\Lambda\) let \(G_\Lambda\) be the orthogonal projection onto

\[
\ker \sum_{x,\{x,x+1\} \subseteq \Lambda} h_{x,x+1}
\]  

(3.4)

For intervals \([a, b]\), \(1 \leq a < b \leq L\), \(G_{[a,b]}\) is the orthogonal projection onto the zero eigenvectors of \(\sum_{x=a}^{b-1} h_{x,x+1}\), and \(G_{\{x\}} = \mathbb{1}\) for all \(x\). It then follows that

\[
G_{\Lambda_2} G_{\Lambda_1} = G_{\Lambda_1} G_{\Lambda_2} = G_{\Lambda_2} \quad \text{if } \Lambda_1 \subseteq \Lambda_2  \\
G_{\Lambda_1} G_{\Lambda_2} = G_{\Lambda_2} G_{\Lambda_1} \quad \text{if } \Lambda_1 \cap \Lambda_2 = \emptyset
\]  

(3.5-a, 3.5-b)

We will often write \(G_n\) instead of \(G_{[1,n]}\). Define operators \(E_n, 1 \leq n \leq L\), on \(\mathcal{H}_L\) by

\[
E_n = \begin{cases} 
\mathbb{1} - G_{[1,2]} & \text{if } n = 1 \\
G_{[1,n]} - G_{[1,n+1]} & \text{if } 2 \leq n \leq L - 1 \\
G_{[1,L]} & \text{if } n = L
\end{cases}
\]  

(3.6)

One can then easily verify, using the properties \((3.5-a)-(3.5-b)\), that \(\{E_n \mid 1 \leq n \leq L\}\) is a family of mutually orthogonal projections summing up to \(\mathbb{1}\).

Next, we add the assumption that the interaction terms are \(SU(2)\) or \(SU_q(2)\) invariant, and that the space of all ground states for a finite chain is the irreducible representation of maximal spin. Of course, \(SU(2)\) is a special case of \(SU_q(2)\) (\(q = 1\)). We treat the cases of \(SU_q(2)\) and \(SU(2)\) in exactly the same way and will therefore not distinguish between
them. E.g., we will label the irreducible representations by their dimension $2s + 1$ using a half-integer $s$ that we will call “spin” both in the group and the quantum group case. There is still no need to restrict ourselves to spin-1/2 chains. So, let $H_n$ be a Hamiltonian for a spin-$s$ chain of $n$ sites, with arbitrary $s = 1/2, 1, 3/2, \ldots$. Define $\varepsilon_n^{(J)}$ by

$$
\varepsilon_n^{(J)} = \min_{0 \neq \psi \perp \ker H_n, \psi \in H_{S^{(3)}_{[1,n]}}} \frac{\langle \psi | H_n \psi \rangle}{\|\psi\|^2} \quad (3.7)
$$

where $H_{S^{(3)}_{[1,n]}}$ is the subspace of $H_{[1,n]}$ where $S^{(3)}_{[1,n]} \geq ns - J$, i.e., the subspace spanned by the eigenvectors of $S^{(3)}_{[1,n]}$ with eigenvalues $= ns, ns - 1, \ldots, ns - J$.

**Lemma 3** Consider an $SU_q(2)$ invariant spin-$s$ ferromagnetic chain of $L$ sites with a nearest neighbor Hamiltonian $H_L = \sum_{x=1}^{L-1} h_{x,x+1}$, and for which the space of all ground states of a finite chain of $n$ sites is the irreducible representation of maximal spin ($= ns$), for $2 \leq n \leq L$. Let $\gamma_n$ denote the spectral gap of $H_n$ and let $\varepsilon_n^{(J)}$ be defined by (3.7). If

$$
\varepsilon_n^{(2s)} \geq \varepsilon_{n+1}^{(2s)} \quad (3.8)
$$

for all $n, 2 \leq n \leq L - 1$, then

$$
\gamma_L = \varepsilon_L^{(2s)} \quad (3.9)
$$

**proof:** We will first show that for all $n, 2 \leq n \leq L - 1$ at least one of the following must be true: i) $\gamma_{n+1} = \varepsilon_{n+1}^{(2s)}$, or ii) $\gamma_{n+1} \geq \gamma_n$.

Let $\varphi_{n+1}$ be an eigenvector of $H_{n+1}$ with eigenvalue $\gamma_{n+1}$. We can assume that $\varphi_{n+1}$ is also an eigenvector of the Casimir operator (i.e., $S^2_{[1,n+1]}$, in the $SU(2)$ case). This means that $\varphi_{n+1}$ belongs to an irreducible representation. We distinguish two cases: a) $E_n \varphi_{n+1} \neq 0$, and b) $E_n \varphi_{n+1} = 0$. Here $E_n$ is the projection defined in (3.7). We show that a) implies i) and b) implies ii), and therefore, i) or ii) (or both) must hold.

**case a):** If $E_n \varphi_{n+1} \neq 0$ there is a $\psi$ in the range of the projection $E_n$ such that $\langle \psi | \varphi_{n+1} \rangle \neq 0$. $E_n \psi = \psi$ is equivalent to $G_n \psi = \psi$ and $G_{n+1} \psi = 0$. $G_{[1,n]} \psi = \psi$ implies that $\psi \in \psi \perp \ker H_n$. Hence, $\varphi_{n+1}$ is an eigenvector of $H_n$ with eigenvalue $\gamma_{n+1} = \varepsilon_{n+1}^{(2s)}$. Therefore, i) holds.

**case b):** $E_n \varphi_{n+1} = 0$. Since $\gamma_{n+1} \geq \gamma_n$, we have $\gamma_{n+1} \geq \gamma_n$. Therefore, ii) holds.
$D^{(n_s)}_{[1,n]} \otimes D^{(s)}_{[n+1]} \subset \mathcal{H}_{n+1}$, where $D^{(J)}_\Lambda$ denotes a spin $J$ representation of $SU_q(2)$ acting on $\mathcal{H}_\Lambda$. As $D^{(n_s)} \otimes D^{(s)} \cong D^{((n-1)s)} \oplus \cdots \oplus D^{((n+1)s)}$, $G_{[1,n+1]} \psi = 0$ implies that $\psi \in \bigoplus_{J=1}^{2s} D^{((n+1)s-J)}$. Because, by assumption, $\varphi_{n+1}$ belongs to an irreducible representation, the fact that it is not orthogonal to $\psi$, implies that $\varphi_{n+1}$ belongs to an irreducible representation $D^{(J)}$ with $J \in \{(n+1)s - 1, (n+1)s - 2, \ldots, (n-1)s\}$. From the definition of $\varepsilon^{(2s)}_{n+1}$ in (3.7) it is then obvious that $\gamma_{n+1} = \varepsilon^{(2s)}_{n+1}$.

**case b):** If $E_n \varphi_{n+1} = 0$ we have also $G_n \varphi_{n+1} = 0$ because by assumption $G_{n+1} \varphi_{n+1} = 0$. But then

$$\gamma_{n+1} = \frac{\langle \varphi_{n+1} | H_{n+1} \varphi_{n+1} \rangle}{\| \varphi_{n+1} \|^2} \geq \frac{\langle \varphi_{n+1} | (I - G_n) H_n (I - G_n) \varphi_{n+1} \rangle}{\| (I - G_n) \varphi_{n+1} \|^2} \geq \gamma_n$$

(3.10)

Here, both $G_n$ and $H_n$ are considered as operators on $\mathcal{H}_{n+1}$, and we used the obvious bound $(I - G_n) H_n (I - G_n) \geq \gamma_n (I - G_n)$.

The proof of the lemma can now be completed by contraposition. $\gamma_2 = \varepsilon^{(2s)}_2$ is obvious. Let $m > 2$ be the smallest integer for which $\gamma_m \neq \varepsilon^{(2s)}_m$. As $\gamma_n \leq \varepsilon^{(2s)}_n$, for all $n$, this means $\gamma_m < \varepsilon^{(2s)}_m$. Therefore, i) from above cannot hold with $n + 1 = m$, and hence ii) must hold, i.e., $\gamma_m \geq \gamma_{m-1}$. We assumed that $m$ was the smallest integer such that $\gamma_m \neq \varepsilon^{(2s)}_m$, hence $\gamma_{m-1} = \varepsilon^{(2s)}_{m-1}$. We conclude that $\varepsilon^{(2s)}_m > \gamma_m \geq \gamma_{m-1} = \varepsilon^{(2s)}_{m-1}$, which is in contradiction with the assumption (3.8). Therefore, no $m \geq 2$ such that $\gamma_m \neq \varepsilon^{(2s)}_m$ exists and the lemma is proved. 

We now return to the spin-1/2 XXZ Heisenberg chain for the computation of $\varepsilon^{(1)}_n$.

**Lemma 4** For the $SU_q(2)$ invariant spin-1/2 ferromagnetic XXZ chain with $\Delta \geq 1$, $\varepsilon^{(1)}_n$ defined in (3.7) is given by

$$\varepsilon^{(1)}_n = 1 - \Delta^{-1} \cos(\pi/n)$$

(3.11)

In particular one has $\varepsilon^{(1)}_{n+1} < \varepsilon^{(1)}_n$. 


**proof:** We calculate the eigenvalues \( E \) of the Hamiltonian \( H_L^{(q)} \) of (2.1) in the one down spin sector by using a transfer matrix method. An arbitrary vector \( \psi \) in that subspace can be written as

\[
\psi = \sum_{x=1}^{L} a_x D_x, \tag{3.12}
\]

where \( D_x \) denotes the basis vector with all spins up except at the site \( x \) where the spin is down. For \( \psi \) to be an eigenvector the coefficients \( a_x \) must satisfy

\[
\langle D_y | H_L^{(q)} | \psi \rangle = E a_y \text{ where } E \text{ is the eigenvalue, which amounts to}
\]

\[
a_{y+1} = 2\Delta (1 - E) a_y - a_{y-1} \quad \text{for} \quad 2 \leq y \leq L - 1, \tag{3.13}
\]

\[
a_2 = 2\Delta [1/2 + A(\Delta) - E] a_1, \quad a_{L-1} = 2\Delta [1/2 - A(\Delta) - E] a_L. \tag{3.14}
\]

The equations (3.13) can be rewritten as

\[
\begin{pmatrix} a_{y+1} \\ a_y \end{pmatrix} = T \begin{pmatrix} a_y \\ a_{y-1} \end{pmatrix}, \quad \text{with} \quad T = \begin{pmatrix} 2\Delta (1 - E) & -1 \\ 1 & 0 \end{pmatrix}. \tag{3.15}
\]

By using (3.15) repeatedly, we get

\[
\begin{pmatrix} a_L \\ a_{L-1} \end{pmatrix} = T^{L-2} \begin{pmatrix} a_2 \\ a_1 \end{pmatrix}. \tag{3.16}
\]

Combining this with (3.14), we have

\[
a_L \begin{pmatrix} 1 \\ 2\Delta [1/2 - A(\Delta) - E] \end{pmatrix} = a_1 T^{L-2} \begin{pmatrix} 2\Delta [1/2 + A(\Delta) - E] \\ 1 \end{pmatrix}. \tag{3.17}
\]

This equation can be solved in terms of the eigenvalues and -vectors of the transfer matrix \( T \). The eigenvalues \( \lambda \) of \( T \) are given by the roots of the equation

\[
\lambda^2 - 2\Delta (1 - E) \lambda + 1 = 0, \tag{3.18}
\]

given by

\[
\lambda_{\pm} = \Delta (1 - E) \pm \sqrt{\Delta^2 (1 - E)^2 - 1}. \tag{3.19}
\]
Consider first the case $\Delta(1 - \mathcal{E}) \neq \pm 1$. Then the eigenvectors are determined by

$$u_\pm = \begin{pmatrix} \lambda_\pm \\ 1 \end{pmatrix}. \quad (3.20)$$

In terms of $u_\pm$, the vector with $A(\Delta) = \sqrt{1 - \Delta^2}/2$ in (3.17) can be rewritten as

$$\begin{pmatrix} 2\Delta[1/2 + A(\Delta) - \mathcal{E}] \\ 1 \end{pmatrix} = \begin{pmatrix} \Delta + \sqrt{\Delta^2 - 1 - 2\mathcal{E}} \\ 1 \end{pmatrix} = \alpha_+ u_+ + \alpha_- u_- \quad (3.21)$$

with

$$\alpha_\pm = \frac{1}{2} \left[ 1 \pm \frac{1}{\sqrt{\Delta^2(1 - \mathcal{E})^2 - 1}}(\sqrt{\Delta^2 - 1 - \Delta\mathcal{E}}) \right]. \quad (3.22)$$

Similarly the vector in the left-hand side of (3.17) can be rewritten as

$$\begin{pmatrix} 1 \\ \Delta - \sqrt{\Delta^2 - 1 - 2\mathcal{E}} \end{pmatrix} = \beta_+ \begin{pmatrix} 1 \\ \lambda_- \end{pmatrix} + \beta_- \begin{pmatrix} 1 \\ \lambda_+ \end{pmatrix} = \beta_+ \lambda_- u_+ + \beta_- \lambda_+ u_- \quad (3.23)$$

with

$$\beta_\pm = \frac{1}{2} \left[ 1 \pm \frac{1}{\sqrt{\Delta^2(1 - \mathcal{E})^2 - 1}}(\sqrt{\Delta^2 - 1 + \Delta\mathcal{E}}) \right], \quad (3.24)$$

where we have used $\lambda_+\lambda_- = 1$. Substituting (3.21) and (3.23) into (3.17), we have

$$\left( a_L/a_1 \right) \left[ \beta_+ \lambda_- u_+ + \beta_- \lambda_+ u_- \right] = T^{L-2} (\alpha_+ u_+ + \alpha_- u_-) = \alpha_+ \lambda_+^{L-2} u_+ + \alpha_- \lambda_-^{L-2} u_. \quad (3.25)$$

Here we have assumed $a_1 \neq 0$. Actually $a_1 = 0$ implies $\psi = 0$. Since the vectors $u_+$ and $u_-$ are independent of each other, we get

$$(a_L/a_1)\beta_+ = \alpha_+ \lambda_+^{L-1} \quad \text{and} \quad (a_L/a_1)\beta_- = \alpha_- \lambda_-^{L-1}. \quad (3.26)$$

If $\alpha_- = 0$, we get $\mathcal{E} = 0$, $\beta_- = 0$, $\alpha_+ = \beta_+ = 1$ and $\lambda_+ = \Delta + \sqrt{\Delta^2 - 1}$ from (3.22) and (3.24). The eigenvalue $\mathcal{E} = 0$ is the ground state in the one down spin sector.

When $\alpha_+ \neq 0$, $\alpha_+, \beta_\pm$ are all non-vanishing. Therefore, from (3.26), we have

$$\lambda_+^{2L-2} = \frac{\alpha_-}{\alpha_+} \times \frac{\beta_+}{\beta_-}, \quad (3.27)$$
where we have used $\lambda_+\lambda_- = 1$. Note that

$$\frac{\alpha_-}{\alpha_+} = \frac{\Delta - \sqrt{\Delta^2 - 1}}{\lambda_+} \times \frac{\lambda_+ - (\Delta + \sqrt{\Delta^2 - 1})}{\lambda_+ - (\Delta - \sqrt{\Delta^2 - 1})}$$  \hspace{1cm} (3.28)$$

and

$$\frac{\beta_+}{\beta_-} = \frac{\Delta + \sqrt{\Delta^2 - 1}}{\lambda_+} \times \frac{\lambda_+ - (\Delta - \sqrt{\Delta^2 - 1})}{\lambda_+ - (\Delta + \sqrt{\Delta^2 - 1})}$$  \hspace{1cm} (3.29)$$

from (3.22), (3.24) and (3.19). Combining these with the above (3.27), we have $\lambda_+^L = 1$. This implies that $\lambda_+ = e^{i\pi\ell/L}$, with $\ell$ an integer. From (3.19), we get the energy eigenvalues

$$E_L(\ell) = 1 - \lambda_+ + \lambda_- = 1 - \Delta^{-1}\cos(\pi \ell/L).$$  \hspace{1cm} (3.30)$$

Here $\ell = 1, 2, \ldots, L - 1$ because $\lambda_\pm \neq \pm 1$ which are the degenerate roots of (3.18) when $\Delta(1 - E) = \pm 1$. Since we have found $L$ distinct eigenvalues, we obtained the complete set of eigenvalues. In particular this implies that there are no solutions with $\Delta(1 - E) = \pm 1$ (except when $\Delta = 1$).

4 The infinite chain

Before we can prove rigorous statements about the spectrum of the infinite chain we need to introduce the mathematical objects that define the infinite system. Although all interesting properties of the infinite chain can be expressed as results for limits of quantities defined for finite chains, the converse is not true. Not all limits of finite chain quantities give interesting or even sensible statements about the infinite chain.

Let the symbols $\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow$ denote the four superselection sectors of the infinite XXZ chain with $\Delta > 1$, corresponding to up, kinks, antikinks, and down respectively. We can describe the GNS Hilbert spaces $[14]$ of these four superselection sectors as the so-called incomplete tensor products $[15]$ $\mathcal{H}_{\alpha\beta}$, for $\alpha$ and $\beta = \uparrow$ or $\downarrow$, defined by

$$\mathcal{H}_{\alpha\beta} = \bigcup_{\Lambda} \left( \bigotimes_{x \in \Lambda} \mathbb{C}^2 \otimes \bigotimes_{y \in \Lambda^c} \Omega_{\alpha\beta}(y) \right)$$  \hspace{1cm} (4.1)$$
where

\[ \Omega_{\alpha\beta}(y) = \begin{cases} |\alpha\rangle & \text{if } y \leq 0 \\ |\beta\rangle & \text{if } y > 0 \end{cases} \quad (4.2) \]

We also define the vectors \( \Omega_{\alpha\beta} \) as the infinite product vectors

\[ \Omega_{\alpha\beta} = \bigotimes_{y \in \mathbb{Z}} \Omega_{\alpha\beta}(y) \in \mathcal{H}_{\alpha\beta} \quad (4.3) \]

Let \( A_\Lambda \) denote the local observables acting non-trivially only on the sites in the finite set \( \Lambda \). Local observables \( X \in A_\Lambda \) act on \( \mathcal{H}_{\alpha\beta} \) in the obvious way, e.g., the spin matrices at the site \( x \) act on the \( x^{th} \) factor of the tensor product (4.1). From the definitions above it is clear that vectors \( \psi \) of the form

\[ \psi = X\Omega_{\alpha\beta}, \quad X \in \bigcup_\Lambda A_\Lambda \quad (4.4) \]

form a dense subspace of \( \mathcal{H}_{\alpha\beta} \). Note that if \( \alpha \neq \beta \), \( \Omega_{\alpha\beta} \) is not the GNS vector representing one of the kink (or antikink) ground states. Let \( \Omega_{\alpha\beta}^{\text{GNS}} \) denote the GNS vector in the \( \alpha\beta \) sector, or one of the GNS vectors in the case of kinks or antikinks. That \( \Omega_{\alpha\beta}^{\text{GNS}} \in \mathcal{H}_{\alpha\beta} \) follows from the explicit expansion [7]

\[ \Omega_{\alpha\beta}^{\text{GNS}} = Z(q)^{-1} \sum_{k=0}^{\infty} \sum_{x_1 < x_2 < \cdots < x_k \leq 0 < y_1 < \cdots < y_k} q^{\sum_{j=1}^{k} (y_j - x_j)} \prod_{j=1}^{k} \sigma_{x_j}^{(1)} \sigma_{y_j}^{(1)} \Omega_{\alpha\beta} \]

where \( \sigma^{(1)} = 2S^{(1)} \), and \( Z(q) \) is the normalization factor given by

\[ Z(q)^2 = \sum_{k=0}^{\infty} \sum_{x_1 < x_2 < \cdots < x_k \leq 0 < y_1 < \cdots < y_k} q^{2 \sum_{j=1}^{k} (y_j - x_j)} < +\infty \]

The Hamiltonian is represented on \( \mathcal{H}_{\alpha\beta} \) as the generator \( H_{\alpha\beta} \) of the Heisenberg dynamics of observables acting on \( \mathcal{H}_{\alpha\beta} \). The dense subspace of the vectors \( \psi \) defined in (4.4) is in the domain of \( H_{\alpha\beta} \), and the selfadjoint operator \( H_{\alpha\beta} \) is uniquely determined by the requirement

\[ H_{\alpha\beta}X\Omega_{\alpha\beta}^{\text{GNS}} = \lim_{\Lambda \to \mathbb{Z}} [H_{\alpha\beta}^{\text{XXZ}}, X]\Omega_{\alpha\beta}^{\text{GNS}} \quad (4.5) \]

We remark that \( H_{\alpha\beta} \) does not depend on boundary terms such as \( A(S_a^{(3)} - S_b^{(3)}) \) added to the XXZ Hamiltonian for finite chains. It is well-known [14] that \( H_{\alpha\beta} \) is a positive operator
in any ground state representation and in the present case this could not be more clear. An explicit formula for $H_{\alpha\beta}$ is

$$H_{\alpha\beta} X_{\Omega\alpha\beta} = \sum_{\{x,x+1\} \cap (\Lambda \cup \{0\}) \neq \emptyset} h_{x,x+1}^{\alpha\beta} X_{\Omega\alpha\beta}$$

(4.6)

for arbitrary $X \in \mathcal{A}_\Lambda$, and where $h_{x,x+1}^{\alpha\beta}$ can be taken to be $h_{x,x+1}^q$ if $\alpha\beta = \uparrow\uparrow$, $\downarrow\downarrow$, or $\uparrow\downarrow$. If $\alpha\beta = \downarrow\uparrow$ the sign of the boundary term has to be reversed.

The spectral gap $\gamma_{\alpha\beta}$ is then just the gap above 0 in the spectrum of $H_{\alpha\beta}$, i.e.,

$$\gamma_{\alpha\beta} = \inf_{\psi \neq 0, \ker H_{\alpha\beta}} \frac{\langle \psi | H_{\alpha\beta} \psi \rangle}{\langle \psi | \psi \rangle}$$

(4.7)

There is no a priori reason why the spectrum, of $H_{\alpha\beta}$ should be independent of the reference ground state. We already know that the multiplicity of the lowest eigenvalue is different: it is 1 for $H_{\uparrow\uparrow}$ and $H_{\downarrow\downarrow}$ and infinite for $H_{\uparrow\downarrow}$ and $H_{\downarrow\uparrow}$. Therefore, a priori, we should not expect $\gamma_{\alpha\beta}$ to be independent of $\alpha\beta$. One can easily convince oneself, however, that $\gamma_{\alpha\beta} = \gamma_{\beta\alpha}$ and that $\gamma_{\uparrow\uparrow} = \gamma_{\downarrow\downarrow}$. From a simple argument given in Section 4.2 it follows that $\gamma_{\alpha\beta} \leq \gamma_{\uparrow\uparrow}$. The upper and lower bounds that we derive here are independent of $\alpha\beta$, and they are equal, thus proving Theorem 1.

4.1 Proof that $1 - \Delta^{-1}$ is a lower bound

In order to prove that $1 - \Delta^{-1}$ is a lower bound of the gap we simply have to show that the lower bound (3.2) on the finite volume gap obtained in Section 3 remains valid in the thermodynamic limit, irrespective of the particular zero energy ground state that we are considering. It is important that the finite volume gap estimates were obtained for the “correct” boundary conditions of (1.1). More explicitly we show that for any choice of $\alpha\beta$ and all local observables $X$ the following inequality holds:

$$\langle \Omega_{\alpha\beta} | X^* H_{\alpha\beta}^3 X_{\Omega\alpha\beta} \rangle \geq (1 - \Delta^{-1}) \langle \Omega_{\alpha\beta} | X^* H_{\alpha\beta}^2 X_{\Omega\alpha\beta} \rangle$$

(4.8)
Gap of the XXZ chain

This proves that $1 - \Delta^{-1}$ is a lower bound for the gap because the vectors of the form (4.4) are a core for all powers of $H_{\alpha\beta}$.

The inequality (4.8) follows from Proposition 2 when one observes that for $X \in \mathcal{A}_{\Lambda}$

$$\langle \Omega_{\alpha\beta} | X H_{\alpha\beta}^3 X \Omega_{\alpha\beta} \rangle = \langle \Omega_{\alpha\beta} | (H_{\Lambda \pm 3}^{(q)})^3 X \Omega_{\alpha\beta} \rangle$$

(4.9)

Obviously, $X^*(H_{\Lambda \pm 3}^{(q)})^3 X \in \mathcal{A}_{\Lambda \pm 3}$. Therefore the expectation value in the right side of (4.9) can be computed in the density matrix $\rho_{\Lambda \pm 3}$ which describes the state $\Omega_{\alpha\beta}$ in the finite volume $\Lambda \pm 3$. The same is true for the right side of (4.8). We conclude that it is sufficient to ascertain that

$$\text{Tr} \rho_{\Lambda \pm 3} X^*(H_{\Lambda \pm 3}^{(q)})^3 X \geq (1 - \Delta^{-1}) \text{Tr} \rho_{\Lambda \pm 3} X^*(H_{\Lambda \pm 3}^{(q)})^2 X$$

(4.10)

which immediately follows from the finite volume result of Proposition 2.

4.2 Proof that $1 - \Delta^{-1}$ is an upper bound

First we argue that it suffices to prove the upper bound for $H_{\uparrow\uparrow}$. It is obvious that the gap of $H_{\downarrow\downarrow}$ will satisfy the same bound. For the gap of the model in the kink and antikink sectors we have an inequality which can be derived as follows. The translation invariant ground states can be obtained as weak limits of the kink or antikink states by letting the position of the kink (or antikink) tend to $\pm \infty$. We then have

$$\inf_{\Lambda, X \in \mathcal{A}_{\Lambda}} \frac{\langle \Omega_{\alpha\beta} | X^*(H_{\Lambda \pm 3}^{(q)})^3 X \Omega_{\alpha\beta} \rangle}{\langle \Omega_{\alpha\beta} | X^*(H_{\Lambda \pm 3}^{(q)})^2 X \Omega_{\alpha\beta} \rangle}$$

(4.11)

$$\leq \inf_{\Lambda, X \in \mathcal{A}_{\Lambda}} \lim_{n \to \pm \infty} \frac{\langle \Omega_{\alpha\beta} | \tau_n(X^*(H_{\Lambda \pm 3}^{(q)})^3 X) \Omega_{\alpha\beta} \rangle}{\langle \Omega_{\alpha\beta} | \tau_n(X^*(H_{\Lambda \pm 3}^{(q)})^2 X) \Omega_{\alpha\beta} \rangle} = \inf_{\Lambda, X \in \mathcal{A}_{\Lambda}} \frac{\langle \Omega_{\uparrow\uparrow} | X^*(H_{\Lambda \pm 3}^{(q)})^3 X \Omega_{\uparrow\uparrow} \rangle}{\langle \Omega_{\uparrow\uparrow} | X^*(H_{\Lambda \pm 3}^{(q)})^2 X \Omega_{\uparrow\uparrow} \rangle}$$

(4.12)

where $\tau_n$ denotes the translation over $n$ lattice units in the chain. It follows that $\gamma_{\alpha\beta} \leq \gamma_{\uparrow\uparrow}$.

For the proof of the upper bound on $\gamma_{\uparrow\uparrow}$ we use the variational principle (4.7) and observe that the spaces $\ker H_{\Lambda}^{(q)} \subset \mathcal{H}_{\alpha\beta}$ are decreasing in $\Lambda$. Therefore, in order to assure that $\psi \perp \ker H_{\alpha\beta}$, it suffices to check that $\psi \perp \ker H_{\Lambda}^{(q)}$ for some suitable $\Lambda$. 
Fix an interval \([1, n]\) and introduce the usual spin wave operators \(X_k\), \(k = 2\pi m/n, m = 0, 1, \ldots, n - 1\), given by

\[
X_k = \frac{1}{\sqrt{n}} \sum_{x=1}^{n} e^{ikx} S_x^{-}
\]  
(4.13)

The normalization and the allowed values for \(k\) are chosen such that

\[
\langle \Omega_{1\uparrow} | X_l^* X_k \Omega_{1\uparrow} \rangle = \delta_{k,l}
\]  
(4.14)

The vectors \(\psi\) we need for the upper bound are linear combinations of two spin waves, i.e. \(\psi = (c_1 X_{k_1} + c_2 X_{k_2}) \Omega_{1\uparrow}\). Due to (4.14) we have \(\|\psi\|^2 = |c_1|^2 + |c_2|^2\). For any pair of distinct \(k_1, k_2\), the coefficients \(c_1, c_2\) can be chosen such that \(G_{[1,n]} \psi = 0\), i.e. \(\psi \perp \ker H_{[1,n]}^{(q)}\).

This follows from the fact that \(\ker H_{[1,n]}^{(q)}\) contains exactly one vector for each eigenvalue of \(S_{[1,n]}^{(3)}\). All vectors \(X_k \Omega_{1\uparrow}\) have \(S_{[1,n]}^{(3)} = (n - 2)/2\). It follows that any two-dimensional space of vectors \(\psi\) with fixed, distinct \(k_1, k_2\) and arbitrary \(c_1, c_2\) must contain a ray \(\perp \ker H_{[1,n]}^{(q)}\).

Hence the upper bound can be proved by showing that

\[
\inf_{n,k_1,k_2,c_1,c_2} \sup_{\psi} \frac{\langle \psi | H_{1\uparrow} \psi \rangle}{\langle \psi | \psi \rangle} = 1 - \Delta^{-1}
\]  
(4.15)

which we do next. From the definition (4.13) of the \(X_k\) it is clear that the only matrix elements of \(H_{1\uparrow}\) we need are the \(T_{x,y}, 1 \leq x, y \leq n\), defined by

\[
T_{x,y} = \langle \Omega_{1\uparrow} | S_x^+ H_{[0,n+1]}^{(q)} S_y^- \Omega_{1\uparrow} \rangle = \frac{1}{2\Delta} \{2\Delta \delta_{x,y} - \delta_{x,y-1} - \delta_{x,y+1}\}
\]  
(4.16)

It is then easily seen that the \(\sup_{c_1,c_2}\) in the left side of (4.15) yields the norm of the \(2 \times 2\) matrix \(M(n,k_1,k_2)\) with matrix elements \(M(n,k_1,k_2)_{i,j} = M_n(k_i,k_j)\) where \(M_n(k,l)\), for \(k, l\) of the form \(2\pi m/n\), is the function

\[
M_n(k,l) = \frac{1}{n} \sum_{x,y=1}^{n} e^{-ikx} T_{x,y} e^{ily} = \delta_{k,l}(1 - \Delta^{-1} \cos k) + (e^{il} + e^{-ik})/(2\Delta n)
\]  
(4.17)

It is now obvious that \(\inf_{n,k_1,k_2} \|M(n,k_1,k_2)\| = 1 - \Delta^{-1}\).

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