The Spectral Gap for the

Ferromagnetic Spin-J XXZ Chain

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Abstract

We investigate the spectrum above the kink ground states of the spin J ferromagnetic XXZ chain with Ising anisotropy Δ. Our main theorem is that there is a non-vanishing gap above all ground states of this model for all values of J. Using a variety of methods, we obtain additional information about the magnitude of this gap, about its behavior for large Δ, about its overall behavior as a function of Δ and its dependence on the ground state, about the scaling of the gap and the structure of the low-lying spectrum for large J, and about the existence of isolated eigenvalues in the excitation spectrum.

By combining information obtained by perturbation theory, numerical, and asymptotic analysis we arrive at a number of interesting conjectures. The proof of the main theorem, as well as some of the numerical results, rely on a comparison result with a Solid-on-Solid (SOS) approximation. This SOS model itself raises interesting questions in combinatorics, and we believe it will prove useful in the study of interfaces in the XXZ model in higher dimensions.

1   Introduction

The subject of our paper is the ferromagnetic XXZ model. The XXZ model is one of the best studied quantum spin systems, benefiting from both algebraic and analytic techniques. But, while the mathematical techniques that have been applied to the XXZ model are impressive (c.f. in [14]), many of the most basic physical questions remain open [22]. We address an unresolved issue of the one-dimensional XXZ model, which is the following. It is known, by rigorous methods [16], that there is a spectral gap above the infinite volume ground state for spin 1/2, but the proof relies on an algebraic tool which is not present for higher spins. How does one prove the existence of a spectral gap in the more general setting? We answer the question in the present paper. Our methods are somewhat more general than those of [16] since we do not rely on the quantum group symmetry. On the other hand, it is essential for our proof that we know the spectral gap exists for the spin 1/2 XXZ model. Still, we believe our techniques may be applied to other spin models, as well as shedding light on this corner of the general knowledge of the XXZ model.

The XXZ spin chain is a generalization of the Heisenberg model where one allows anisotropic spin couplings. The Hamiltonian for the spin J model is

$$H_\Lambda^{(J)} = - \sum_{\langle \alpha, \beta \rangle \in \Lambda} \left(S_\alpha^1 S_\beta^1 + S_\alpha^2 S_\beta^2 + \Delta S_\alpha^3 S_\beta^3 \right), \tag{1.1}$$

where $S_\alpha^{1,2,3}$ are the spin J matrices acting on the site α, tensored with the identity operator acting on the other sites. $\langle \alpha, \beta \rangle$ denotes a pair of nearest neighbors. The local Hilbert space is $\mathcal{H}_\alpha \cong \mathbb{C}^{2J+1}$, and H_Λ is a Hermitian operator on $\mathcal{H}_\Lambda = \bigotimes_{\alpha \in \Lambda} \mathcal{H}_\alpha$. For now we think of Λ as a finite subset of $\mathbb{Z}$, though we are also interested in the case that $\Lambda = \mathbb{N}$ or $\mathbb{Z}$. The main parameter of the model is the anisotropy $\Delta \in \mathbb{R}$. By choosing $\Delta = \pm 1$ we can obtain the isotropic ferromagnet or antiferromagnet. Alternatively, by taking $\Delta \to \pm\infty$ we recover the spin J Ising ferromagnet and antiferromagnet. In this paper we restrict $\Delta > 1$, which corresponds to a ferromagnet with the strongest coupling along the S^3-axis. We note that $H_\Lambda(\Delta)$ and $-H_\Lambda(-\Delta)$ are unitarily equivalent. It is useful to introduce two other forms of Δ: $q = \Delta - \sqrt{\Delta^2 - 1}$ and $\eta = -\log q$. Observe that $\Delta = \frac{1}{2}(q + q^{-1}) = \cosh(\eta)$.

The parameter q is the one which labels the quantum group $SU_q(2)$ when J = 1/2. As Δ increases from 1 to ∞, q decreases from 1 to 0, and η increases from 0 to ∞.

For $\Delta > 1$, it is widely known that there are two infinite volume ground states which correspond to all spins up, $|+J\rangle$ and all spins down, $|-J\rangle$. It is considerably less well known that there are in fact many more infinite volume ground states. These extra ground states come in two families: the kink states and the antikink states. The kink states are an infinite family of ground states all with the same GNS space, which break discrete translation symmetry as well as the continuous U(1) symmetry associated to the XXZ model. They have the property of being asymptotically all down spins at $-\infty$ and all up spins at $+\infty$. They clearly also break left-right symmetry: their reflected counterparts are the antikink states. Our main results concern the spectral gap above these kink ground states. The kink states are physically interesting for several reasons: They exhibit domain walls, an important feature of real ferromagnets (see [25] for an application of the XXZ model to spin droplets in one dimension); For J > 1 the kink ground states of the XXZ model are more stable than the Ising ground states, which is a new result and subject of the present paper. Also, the XXZ spin chain plays an important role in explaining the phenomenon of negative resistance jumps and hysteresis in recent magnetoresistance experiments [18, 29].

Although our main subject is the XXZ model for J > 1/2, let us briefly recall some important facts about the spin 1/2 model. What is probably most well known is that the spin 1/2 model is Bethe ansatz solvable. This is not applicable to our case however, and we will not use the Bethe ansatz in any way. A second interesting feature of the spin 1/2 XXZ model is that it possesses a quantum group symmetry. Specifically, in [26] it was shown that adding a boundary field

$$B = J\sqrt{\Delta^2 - 1}(S_1^3 - S_L^3) \qquad (1.2)$$

makes the Hamiltonian commute with $SU_q(2)$ on $\mathcal{H}_\Lambda$. (Actually there are two representation of $SU_q(2)$ corresponding to the two opposite linear orderings of its tensor factors; $H_\Lambda + B_\Lambda$ commutes with one representation and $H_\Lambda - B_\Lambda$ commutes with the other. We will only consider $H_\Lambda + B_\Lambda$.) For $0 < q < 1$ the representation theory of $SU_q(2)$ is equivalent to that of $SU(2)$ (c.f. [15]), and it plays the same role in the analysis of the XXZ model that $SU(2)$ plays in the analysis of the isotropic model. For example, the ground state space corresponds to the highest-dimensional irreducible representation of $SU_q(2)$. In [16], Koma and Nachtergaele used the quantum group symmetry to calculate the spectral gap for the XXZ model by proving that the lowest excitations of the XXZ model form a next-highest dimensional irreducible representation of $SU_q(2)$. There are still open conjectures relating to the representations of $SU_q(2)$ and the XXZ model such as: Prove the lowest (highest) energy of $H_\Lambda + B_\Lambda$ restricted to the spin s representations in $\mathcal{H}_\Lambda$ is lower than the lowest (highest) energy of the spin $s - 1$ representations. This is almost certainly true, and would generalize the Lieb and Mattis result [20], but remains open.

We now turn our attention to the spin > 1/2 models. The first important fact is that the ground states have been explicitly calculated for all finite volumes, in all dimensions, all choices of spin, and even allowing different values of anisotropy along bonds in the different coordinate directions [1]. In [12] the ground states were

independently dicovered for J = 1/2 and one dimension, and these ground states were generalized to infinite volume ground states. They have the property of being frustration free, which means that they not only minimize the expectation of the infinite volume Hamiltonian, they minimize every nearest neighbor interaction, too. Gottstein and Werner found all the frustration free ground states, and conjectured that there were no other ground states. In [21], their conjecture was proved correct, and the analogous statement for J > 1/2 was proved in [17]. Thus, one has a complete list of ground states for the one dimensional XXZ model with any choice of J. Unfortunately, the results on infinite volume ground states are valid only in one dimension. Finding the complete set of ground states in dimensions two and higher is an important open problem.

In this paper we prove that there is a nonvanishing spectral gap above the infinite volume ground states for every J, thus extending the results of [16]. We mention that the existence of a spectral gap is generally believed to follow from the fact that the quantum interface of the kink ground states is exponentially localized. Our results verify the conventional wisdom, and our proof does rely on the exponentially localized interface. However there are other important elements to our proof: most notably, a rigorous comparison of the spin J chain with a spin 1/2 ladder with 2J legs. The spin J XXZ chain is a quantum many body Hamiltonian. The Hilbert space for the L-site spin chain is $(2J+1)^L$, its dimension grows exponentially with L. The dimension of the spin ladder is even larger, at 2^{2JL}. But an important bound, Lemma 4.1, allows us to restrict attention to an $(L+1)^{2J}$ dimensional subspace. This allows the proof of the existence of the spectral gap, and also allows more efficient numerical methods for studying the XXZ model. The reduced system resembles a quantum solid on solid model for the spin ladder. We view the present problem as a warm up for the QSOS method, which we believe will play an important role in proving stability of the 111 interface for the XXZ model. We also expect the spin ladder technique will be useful in proving the existence of a spectral gap for other spin chains where a gap is known in J = 1/2 but not for J > 1/2. In this paper, in addition to giving a rigorous proof of the existence of a gap, we present a new type of numerical method for studying the XXZ model. We also present an asymptotic model for the low lying spectrum of the XXZ model as J → ∞, in terms of a free Bose gas. The asymptotics explain new qualitative features of the XXZ model for J > 1/2, and is in excellent agreement with numerical data for J sufficiently high.

The remainder of the paper is organized as follows. In Section 2 we present our main theorem, as well as a number of conjectures which are supported by numerical evidence and asymptotic analysis. In Section 3 we introduce some background material which is useful for our proof. In Section 4 we derive the spin chain / spin ladder reduction. In Section 5 we finish the proof of the main theorem. In Section 6 we combine the lower bounds for the spectral gap with numerical methods to obtain data for the spectral gap. In Section 7 we derive a boson model for the XXZ spin system which explains the asymptotic behavior of the gap as J → ∞. This boson model is similar to [13, 9, 10], but without the need for a large external field (other than the boundary field which vanishes in the thermodynamic limit).

2   Main Result and Conjectures

(The notation $[a, b]$ will always refer to the discrete interval $\{a, a + 1, \ldots, b\}$. It is not necessary that a and b are integers as long as the difference $b - a$ is.)

The Hamiltonian we will use is the following spin J XXZ Hamiltonian:

$$H_\Lambda^J = \sum_{\{\alpha, \alpha+1\} \subset \Lambda} h^J(\alpha, \alpha + 1)$$

$$h^J(\alpha, \alpha + 1) = \left(J^2 - S_\alpha^3 S_{\alpha+1}^3 - \Delta^{-1}(S_\alpha^1 S_{\alpha+1}^1 + S_\alpha^2 S_{\alpha+1}^2) \right. \tag{2.3}$$
$$\left. + J\sqrt{1 - \Delta^{-2}}(S_\alpha^3 - S_{\alpha+1}^3) \right).$$

In comparison to the Hamiltonian (1.1), we have just added the boundary fields (1.2), scaled by Δ^{-1} and added a constant. One can easily check that the interaction $h^J(\alpha, \alpha + 1)$ is nonnegative. For finite volume Λ, it is an easy but important observation that the Hamiltonian commutes with $S_\Lambda^3 = \sum_{\alpha \in \Lambda} S_\alpha^3$. We use this symmetry to block diagonalize H_Λ^J. In particular, we let $\mathcal{H}(\Lambda, J)$ be the spin J Hilbert space, and we define $\mathcal{H}(\Lambda, J, M)$ to be the eigenspace of S_Λ^3 with eigenvalue $M \in \{-J|\Lambda|, \ldots, J|\Lambda|\}$. We call these subspaces "sectors". They are invariant subspaces for H_Λ^J.

For finite volumes Λ, the ground states of H_Λ^J may be expressed in closed form, as was pointed out in [1]. We will give a formula for these ground states in the next section. For now we merely mention the fact that for each sector there is a unique ground state $\Psi_0(\Lambda, J, M)$, and it has the property that its energy is zero. We define the ground state space $\mathcal{G}(\Lambda, J, M)$ to be the one-dimensional span of $\Psi_0(\Lambda, J, M)$, then the spectral gap is given by

$$\gamma(\Lambda, J, M) = \inf_{\substack{\psi \in \mathcal{H}(\Lambda, J, M) \\ \psi \perp \mathcal{G}(\Lambda, J, M)}} \langle H_\Lambda^J \rangle_\psi \tag{2.4}$$

where $\langle \cdots \rangle_\psi = \langle \psi | \cdots \psi \rangle / \langle \psi | \psi \rangle$.

One passes to the thermodynamic limit, by considering the infinite volume Hamiltonian as the generator of the Heisenberg dynamics on the algebra of quasilocal observables $\mathcal{A}_0$. The definition of a ground state is a state on $\mathcal{A}_0$ such that for any local observable $X \in \mathcal{A}_\Lambda$, $|\Lambda| < \infty$, ω satisfies

$$\omega(X^* \delta(X)) \geq 0 \tag{2.5}$$

where $\delta(X) = \lim_{\Lambda \nearrow \mathbb{Z}} [H_\Lambda^J, X]$. As in the case of finite volumes, there is a collection of ground states whose GNS representation is explicit. These ground states were discovered in [12], and they were proven to be the complete list in [17]. The infinite volume ground states are the following: a translation invariant up spin state determined by the equation $\omega^\uparrow(S_\alpha^3) = +J$ for all α; a translation invariant down spin state $\omega^\downarrow$; an infinite number of kink states which we label $\omega_M^{\downarrow\uparrow}$; and an infinite number of antikink states, $\omega_M^{\uparrow\downarrow}$. The kink states have the property that, if T is

the translation to the left one unit (so $T^{-1}S_\alpha^3 T = S_{\alpha+1}^3$), then for any quasilocal observable X

$$\lim_{n \to \infty} \omega_M^{\downarrow\uparrow}(T^{-n}XT^n) = \omega^\uparrow(X) \,,$$
$$\lim_{n \to \infty} \omega_M^{\downarrow\uparrow}(T^n XT^{-n}) = \omega^\downarrow(X) \,. \tag{2.6}$$

The label M is any integer and is determined as follows. All the kink states are also local perturbations of one another, which we will see in the next section when we write the explicit GNS representation. So there is only one GNS Hilbert space for all the kink states, and only one GNS Hilbert space for all the antikink states.

For any ground state ω, the infinite volume Hamiltonian can be represented as the generator of the Heisenberg dynamics for the algebra of observables on $\mathcal{H}_{\text{GNS}}$, the GNS Hilbert space of ω. This means that there is a densely defined, self adjoint operator H_{GNS} with the property that for any $X \in \mathcal{A}_0$,

$$H_{\text{GNS}}\pi(X)\Omega_{\text{GNS}} = \pi(\delta(X))\Omega_{\text{GNS}} \,,$$

where Ω_{GNS} is the representation of the ground state as a vector, π is the representation of the quasilocal observable algebra on the observable algebra of $\mathcal{H}_{\text{GNS}}$, and $\delta(X) = \lim_{\Lambda \nearrow \mathbb{Z}}[H_\Lambda^J, X]$ is the derivation defining the Heisenberg dynamics. The bottom of the spectrum of H_{GNS} is 0. The spectral gap above ω is defined to be the gap (if one exists) above 0 in the spectrum of H_{GNS}. Note that there is one spectral gap for each of the four classes of ground states: all up, all down, kinks, and antikinks.

We can now state the main result of [16]:

Theorem 2.1. *[16] For the $SU_q(2)$ invariant spin-1/2 ferromagnetic XXZ chain with the length $L \geq 2$ and $\Delta \geq 1$, the spectral gap is*

$$\gamma([1,L], 1/2, M) = 1 - \Delta^{-1}\cos(\pi/L) \,,$$

in any sector $\mathcal{H}([1,L], 1/2, M)$, $-L/2 < M < L/2$. Above any of the infinite-volume ground states (all up, all down, kink or antikink) the spectral gap is

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

$\blacksquare$

The previous theorem is the starting point of our own analysis. Our main result is an analogous theorem, extending the existence of the spectral gap to all J instead of just J = 1/2.

Theorem 2.2. *For any $J \in \frac{1}{2}\mathbb{N}$, and any $\Delta > 1$, the gap above the translation invariant ground states is*

$$\gamma_{up} = \gamma_{down} = 2J(1 - \Delta^{-1}) \,.$$

The gap above the kink states satisfies the bounds

$$0 < \gamma_{kink} \leq \gamma_{up} \,.$$

Specifically the spectral gap above the kink ground state is nonvanishing.

Remark In the theorem, the formula for γ_{up} is well-known, The inequality $\gamma_{\text{kink}} \leq \gamma_{\text{up}}$ is also well-known and easy to deduces. We include proofs of these facts for the convenience of the reader. Our main result, which is new, is that γ_{kin} is strictly positive.

We can say something more specific about the low excitation spectrum by considering an extra symmetry of the Hamiltonian. Since H_Λ^J commutes with S_Λ^3 for each finite volume Λ, we would like to define an infinite volume analogue of S_Λ^3. For the GNS space above the kink ground states the correct definition is the following renormalized version

$$\widetilde{S}^3 = \sum_{\alpha \in \mathbb{Z}} (S_\alpha^3 - \text{sign}(\alpha - 1/2)J) \,,$$

which is a densely defined self adjoint operator on the $\mathcal{H}_{\text{GNS}}$. The ground state space of H_{GNS} is spanned by the orthogonal family of vectors $\{\Psi_0(\mathbb{Z}, J, M) : M \in \mathbb{Z}\}$ which are determined up to scalar multiplication by the properties that

$$H_{\text{GNS}}\Psi_0(\mathbb{Z}, J, M) = 0 \,, \quad \widetilde{S}_{\mathbb{Z}}^3 \Psi_0(\mathbb{Z}, J, M) = M\Psi_0(\mathbb{Z}, J, M) \,.$$

We define a version of the spectral gap for Hamiltonian restricted to the sectors of $\widetilde{S}^3$ in the following way. Let $\gamma(\mathbb{Z}, J, M)$ be the largest number such that for any local observable $X \in \mathcal{A}_\Lambda$ commuting with S_Λ^3 we have

$$\langle \Psi_0(\mathbb{Z}, J, M) | \pi(X)^* H_{\text{GNS}}^3 \pi(X) \Psi_0(\mathbb{Z}, J, M) \rangle$$
$$\geq \gamma(\mathbb{Z}, J, M) \langle \Psi_0(\mathbb{Z}, J, M) | \pi(X)^* H_{\text{GNS}}^2 \pi(X) \Psi_0(\mathbb{Z}, J, M) \rangle \,.$$

An arbitrary local observable does not commute with S_Λ^3. However, one may define X_M for $-J|\Lambda| \leq M \leq J|\Lambda|$ so that each X_M commutes with S_Λ^3 and $\pi(X)\Psi_0(\mathbb{Z}, J, M) = \sum_{M'} \pi(X_{M'})\Psi_0(\mathbb{Z}, J, M + M')$. This is just due to the fact that the GNS representation $(\mathcal{H}_{\text{GNS}}, \pi, \Psi_0(\mathbb{Z}, J, M))$ is cyclic for any choice of M. From this we see that

$$\gamma_{\text{kink}} = \inf_{M \in \mathbb{Z}} \gamma(\mathbb{Z}, J, M) \,.$$

Let T be translation to the left, as before. We have $T^{-1}\widetilde{S}^3 T = 2J + \widetilde{S}^3$, which implies

$$T\Psi_0(\mathbb{Z}, J, M) = \Psi_0(\mathbb{Z}, J, M + 2J) \,,$$

since T clearly commutes with the Hamiltonian. Hence,

$$\gamma(\mathbb{Z}, J, M) = \gamma(\mathbb{Z}, J, M + 2J) \,.$$

Another symmetry of the Hamiltonian is obtained by taking a left-right reflection of the lattice about the origin, and simultaneously flipping the spin at every site. This is a unitary transformation of $\mathcal{H}_{\text{GNS}}$ to itself. Calling this symmetry $\mathcal{R}$ we have $\mathcal{R}\widetilde{S}^3\mathcal{R} = -\widetilde{S}^3$. So

$$\gamma(\mathbb{Z}, J, M) = \gamma(\mathbb{Z}, J, -M) \,.$$

To prove that the gap above the infinite volume kink states is nonzero, it suffices to check that

$$\gamma(\mathbb{Z}, J, M) > 0$$

for $M = 0, 1, \ldots, \lceil J \rceil$, where $\lceil J \rceil$ is the least integer greater than J. This fact does not actually simplify the proof, but the symmetries above are an important part of our proof.

In Figure 1 we show the spectrum for some small spin chains, as calculated by Lanczos iteration. Even though the lengths are finite, one sees that the gap is an even function of M, and is nearly periodic of period 2J. As one takes $L \to \infty$, the gap for any finite region of M values is periodic and even.

Our main theorem proves existence of a spectral gap, but it is obviously just as interesting to know what the gap is. Unfortunately, the most information we can gain from our proof is that the spectral gap can be well approximated by calculating the gap in a finite volume, L, with an error which decreases like q^L. This still leaves the problem of calculating the gap in a finite volume $L \propto 1/\eta$. We do not have any rigorous bounds for the spectral gap valid for all $q \in (0, 1)$. However we have studied the problem in three ways: numerically, by perturbation series, and asymptotically; and we propose the following conjectures based on our findings.

2.1   Numerical results

We performed two types of numerical methods. The first, and more efficient method is based on the spin ladder reduction from our proof. In Theorem 4.1 below, we obtain a rigorous lower bound for $\gamma([1, L], J, M)$ as

$$\gamma([1, L], J, M) \geq 2J(1 - \Delta^{-1})(1 - \delta([1, L], J, M))$$

where $1 - \delta([1, L], J, M)$ is the spectral gap for a reduced model resembling a quantum solid-on-solid model for the spin ladder. What is important about the bound is that the reduced model has dimension $(L + 1)^{2J}$ as opposed to the original system with dimension $(2J + 1)^L$. We then numerically diagonalized the reduced system to find the spectral gap for some values of J and L. The second numerical method was simply to numerically diagonalize the original Hamiltonian for some small values of L and J. We did this primarily to check the qualitative results of the lower bound. In Figure 2 we show the results of the lower bound calculation, and in Figure 3 the result of the Lanczos iteration. What emerges qualitatively is that for $J > 1$ there is a local maximum for the spectral gap with $1 < \Delta < \infty$. This is other than expected based on the spin $1/2$ results. Based on our numerical evidence we make the following conjecture.

Conjecture 2.3. *We have defined $\gamma(\mathbb{Z}, J, M)$ above for fixed Δ. Let us rewrite this as $\gamma(\mathbb{Z}, J, M, \Delta^{-1})$ to take account of the anisotropy $0 \leq \Delta^{-1} \leq 1$. We conjecture that*

$$\min_M \gamma(\mathbb{Z}, J, M, \Delta^{-1}) = \gamma(\mathbb{Z}, J, 0, \Delta^{-1}),$$

and that for each J there exists a Δ_J^{-1} such that

$$\gamma(\mathbb{Z}, J, 0, \Delta^{-1}) \leq \gamma(\mathbb{Z}, J, 0, \Delta_J^{-1})$$

whenever $0 \leq \Delta^{-1} \leq 1$, equality holding only if $\Delta^{-1} = \Delta_J^{-1}$. For $J = 1/2$, the conjecture is a known fact following from Proposition 2.1, and one sees $\Delta_{1/2}^{-1} = 0$. We conjecture that $\Delta_1^{-1} = 0$ as well, but that, for $J \geq 3/2$, $0 < \Delta_J^{-1} < 1$.

2.2   Ising Perturbation

If we write the Hamiltonian as an expansion in Δ^{-1}, we can make a perturbation expansion off of the Ising model. The Ising model spectrum is well known, but some interesting facts arise. One fact which is useful is that the Hamiltonian obtained by changing Δ^{-1} to $-\Delta^{-1}$ is unitarily equivalent to the original: just rotate every other site by π about S^3. This means that $\Delta^{-1} = 0$ is either a local minimum or a local maximum of $\gamma(\mathbb{Z}, J, M, \Delta^{-1})$. For $J = 1/2$, the first excitation above a kink ground state in the Ising limit is infinitely degenerate. This is why the slope of $\gamma(\mathbb{Z}, 1/2, M, \Delta^{-1}) = 1 - \Delta^{-1}$ is not zero at $\Delta^{-1} = 0$. Similarly for $J = 1$ and M odd. However, for all other choices of J and M, the first excitations are at most finitely degenerate, and for $J > 1$ and $M = 0$ the first excitations are nondegenerate. This means that the first derivative of $\gamma(\mathbb{Z}, J, M, \Delta^{-1})$ vanishes for all other values of J and M. For $J = 1$, $M = 0$ the second derivative is negative, while for $J > 1$ and $M = 0$ the second derivative is always positive, indicating that the Ising limit does not maximize the spectral gap, but minimizes it locally. This argument, which will be expanded in Section 6, illuminates part of Conjecture 2.3. The nondegeneracy of the first excitations suggests a second gap. Based in part on this evidence, we make the following conjecture:

Conjecture 2.4. *1) For $1 < \Delta < \infty$, $J \geq 3/2$ and any $M \in \mathbb{Z}$, the lowest excited state is an isolated eigenvalue, i.e. there is a nonvanishing gap to the rest of the spectrum.*
2) For $J = 1$ and M any odd integer, the lowest excited state is the bottom of a branch of continuous spectrum. For $J = 1$ and M even, the lowest excited state is again an isolated eigenvalue.

2.3   Asymptotics

From the numerics it became clear that for $M = 0$ and Δ fixed, the gap $\gamma(\mathbb{Z}, J, 0, \Delta^{-1})$ scales like J. Also, a careful analysis of the exact formula for the ground states of [1], which will be presented in the next section, shows that for large J, the wave vector has Gaussian fluctuation on the order of $J^{1/2}$. These two facts together suggest a scaling analysis of the bottom of the spectrum of H_Λ^J in the limit $J \to \infty$. Consistent with the Gaussian form for the ground states, our asymptotic analysis leads to a free Boson gas model for the bottom of the spectrum, at least to first order in $J^{-1/2}$. We derive a boson model for the XXZ spin system analogous to [13]. (See also [9, 10] for a better introduction to spin waves. Unfortunately our treatment is not as well developed.) This is not the same analysis as was done in [19], nor in any other coherent states approach. We analyze the eigenstates whose energy scales like J, whereas coherent states give rigorous bounds on the bulk spectrum which

scales like J^2. The higher energy states are much greater in number, so typically they control the thermodynamic behavior. However, the low energy states may be more important for dynamical properties (cf [9]), since that part of the spectrum is separated by spectral gaps. Also note, the asymptotic model is that of a free Bose gas, with a nontrivial dispersion relation for the energy of each oscillator. In fact, the energy is such that excitations which give least energy are exponentially localized about the interface. We believe that this makes it plausible to prove the Boson gas estimate is correct with small errors for large but fixed $J < \infty$, because even as one takes $L \to \infty$, the low excitations are "essentially finite" and we can more or less prove the large J asymptotics for the finite system. Of course J would have to depend on the number of excitations that you wanted to estimate by the Bose gas picture; as the number of excitations goes to ∞ so must J. Our boson model has a quadratic coupling, but a Bogoliubov transformation diagonalizes it. The spectrum of the coupling matrix, then gives the value for the limiting curve of the spectral gap, and other information about the low spectrum. Based on our analysis we make the following conjecture:

Conjecture 2.5. [1] *There is a function* $\gamma_\infty : (1, \infty) \times \mathbb{R} \to \mathbb{R}$ *with the property that*

$$\lim_{J \to \infty} J^{-1} \gamma(\mathbb{Z}, J, \mu J, \Delta) = \gamma_\infty(\mu, \Delta).$$

This function satisfies

$$\gamma_\infty(\mu + 2, \Delta) = \gamma_\infty(\mu, \Delta) \qquad and \qquad \gamma_\infty(-\mu, \Delta) = \gamma_\infty(\mu, \Delta).$$

Moreover $\gamma_\infty(\mu, \Delta)$ *is equal to the spectral gap of a bi-infinite Jacobi operator A (really $A(\Delta, \mu)$) defined on $l^2(\mathbb{Z})$*

$$Ae_n = [2e_n - \operatorname{sech}(\eta)e_{n-1} - \operatorname{sech}(\eta)e_{n+1}]$$
$$- \frac{4\sinh^2(\eta)}{\cosh(2\eta(n-r)) + \cosh(2\eta)} e_n. \qquad (2.7)$$

Above, $r = r(\mu, \Delta)$ *is a phase defined implicitly by the equation*

$$\mu = \lim_{n \to \infty} \sum_{-n+1}^{n} \tanh(\eta(n-r)).$$

Remark 1. The implicit formula for $\gamma_\infty(\mu, \Delta)$ has a specific consequence that

$$\lim_{J \to \infty} \Delta_J^{-1} = 0.49585399 \pm 10^{-8},$$

which is obtained by numerical diagonalization of large Jacobi matrices.

Remark 2. Equation (2.7) has a simple physical interpretation. The bracketed term on the RHS is the usual matrix for a one-magnon spin wave, which by itself

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[1]**Note Added in Proof:** Since the submission of this paper to the arXiv, Caputo and Martinelli have obrtained further results which prove part of Conjecture 2.5. In [7] they obtain a lower bound for the gap of the form $J \times$ constant.

would give the energy $2(1 - \text{sech}\eta)$ for the spectral gap, just as in the translation invariant ground states. The second term on the RHS of (2.7) represents the attractive potential due to the domain wall with center r.

In Figure 4 we show the function $\gamma_\infty(r, \Delta^{-1})$ as obtained by numerically diagonalizing the Jacobi operator for 50 sites. Note that the number of sites reflects the extreme simplicity of the Bose model over the true XXZ model; we could not numerically diagonalize a spin chain of 50 sites even for spin 1/2.

3 Ground states of the XXZ model

In this section we give formulas for the ground states of the finite volume XXZ model as in [1]. We show how the ground states of the spin J chain can be derived by looking at the ground states of a spin 1/2 ladder with 2J legs, which is essential for our proof. We also recall the explicit GNS representation of the infinite volume ground states in a Guichardet Hilbert space (also called incomplete tensor product) [12, 17]. This concrete representation is convenient, especially for proving that certain sequences of finite volume ground states have unique limits.

We begin by rewriting (2.3) for spin 1/2. It is easy to check that for the two site interaction $h^{1/2}(1, 2)$, the three vectors

$$|+\frac{1}{2}, +\frac{1}{2}\rangle, \quad |-\frac{1}{2}, -\frac{1}{2}\rangle, \quad |-\frac{1}{2}, +\frac{1}{2}\rangle + q|+\frac{1}{2}, -\frac{1}{2}\rangle$$

are ground states, while $|+1/2, -1/2\rangle - q|-1/2, +1/2\rangle$ is a state with energy one. In other words, we may view $h^{1/2}(1, 2)$ as $\mathbb{1} - U(\tau(1, 2))$, where $\tau(1, 2) \in \mathfrak{S}_2$ is the transposition, and U is the (non-unitary) action of $\mathfrak{S}_2$ defined by

$$U(\tau(1, 2))\phi(m_1, m_2) = \phi(m_2, m_1),$$

where the $\phi(m_1, m_2)$ are the (non-normalized) basis vectors

$$\phi(\frac{1}{2}, \frac{1}{2}) = |\frac{1}{2}, \frac{1}{2}\rangle, \qquad \phi(\frac{1}{2}, -\frac{1}{2}) = q^{-1/2}|\frac{1}{2}, -\frac{1}{2}\rangle,$$

$$\phi(-\frac{1}{2}, -\frac{1}{2}) = |-\frac{1}{2}, -\frac{1}{2}\rangle, \quad \phi(-\frac{1}{2}, \frac{1}{2}) = q^{1/2}|-\frac{1}{2}, \frac{1}{2}\rangle.$$

In other words, the ground states of the two site Hamiltonian are the symmetric tensors with respect to the nonunitary action U. We can generalize this result to linear chains of any length, and to many other domains as well. Specifically, what we need to properly define the XXZ Hamiltonian with boundary fields is a collection of sites Λ and a collection of oriented bonds among those sites $\mathcal{B}$, in other words a digraph. Then we define

$$H^J_{\Lambda, \mathcal{B}} = \sum_{(\alpha, \beta) \in \mathcal{B}} h^J(\alpha, \beta).$$

(We write H^J_Λ when $\mathcal{B}$ is obvious.) We define a height function to be any function $l : \Lambda \to \mathbb{Z}$ such that $l(\beta) - l(\alpha) = 1$ for all $(\alpha, \beta) \in \mathcal{B}$. The condition to have such

a height function is that for any closed loop, where a loop is defined as a sequence $\alpha_1, \alpha_2, \ldots, \alpha_n = \alpha_1 \in \Lambda$ such that for each i either $(\alpha_i, \alpha_{i+1}) \in \mathcal{B}$ or $(\alpha_{i+1}, \alpha_i) \in \mathcal{B}$, there are equal numbers of bonds with positive orientation $(\alpha_i, \alpha_{i+1}) \in \mathcal{B}$ as with negative orientation $(\alpha_{i+1}, \alpha_i) \in \mathcal{B}$. The following lemma is an interpretation of a result in [1].

Lemma 3.1. *If $(\Lambda, \mathcal{B})$ is a connected digraph such that a height function l exists, then there is a unique ground state of $H_{\Lambda, \mathcal{B}}^{1/2}$ in each sector $\mathcal{H}(\Lambda, 1/2, M)$ for $M \in [-|\Lambda|/2, |\Lambda|/2]$.*

Proof: The proof is like the analogous statement (without the requirement of a height function) for the isotropic model. Suppose that l exists. Define a (non-normalized) basis of vectors

$$\phi(\{m_\alpha\}) = q^{-\sum_{\alpha \in \Lambda} m_\alpha l(\alpha)} |\{m_\alpha\}\rangle.$$

Then define an action of $\mathfrak{S}_\Lambda$ on $\mathcal{H}(\Lambda, 1/2, M)$ by

$$U(\pi)\phi(\{m_\alpha\}) = \phi(\{m_{\pi^{-1}(\alpha)}\}).$$

As we have already seen, for any $(\alpha, \beta) \in \mathcal{B}$, $h^{1/2}(\alpha, \beta) = \mathbb{1} - U(\tau(\alpha, \beta))$, where $\tau(\alpha, \beta)$ is the transposition. Thus, the unique ground state vectors are those vectors which are symmetric under the action of $U(\mathfrak{S}_\Lambda)$,

$$\Psi_0(\Lambda, 1/2, M) = \sum_{\substack{\{m_\alpha\} \in [-1/2, 1/2]^\Lambda \\ \sum_\alpha m_\alpha = M}} \phi(\{m_\alpha\}),$$

one for each sector.   ∎

We note that one can trivially prove the converse of this lemma, that if there exist ground state vectors in any sector other than $M = \pm|\Lambda|/2$, then there is a height function (as long as $0 < q < 1$). We now mention a second lemma (which is also implicit in [1]) which gives the construction of the spin J ground states by using spin ladders.

Lemma 3.2. *Suppose that $(\Lambda, \mathcal{B})$ satisfies the hypotheses of the last lemma. Then for any spin $J \in \frac{1}{2}\mathbb{N}$, there is a unique ground state of $H_{\Lambda, \mathcal{B}}^J$ in each sector $\mathcal{H}(\Lambda, J, M)$. Moreover, this ground state is associated to the ground state of the spin 1/2 spin ladder*

$$\widetilde{\Lambda} = \{(\alpha, j) : \alpha \in \Lambda, j \in [1, 2J]\},$$
$$\widetilde{\mathcal{B}} = \{((\alpha, j), (\beta, k)) : (\alpha, \beta) \in \mathcal{B}, (j, k) \in [1, 2J]^2\}.$$

Define $Q_\alpha : \mathcal{H}(\{\alpha\} \times [1, 2J], 1/2) \to \mathcal{H}(\{\alpha\}, J)$ to be the projection onto the unique highest spin representation in the decomposition of $\mathcal{H}(\{\alpha\} \times [1, 2J], 1/2)$ into irreducibles, so that $Q_\alpha^* Q_\alpha$ is the projection onto symmetric tensors. Then $Q_\Lambda = \prod_{\alpha \in \Lambda} Q_\alpha$ gives an isomorphism of ground states

$$\Psi_0(\Lambda, J, M) = Q_\Lambda \Psi_0(\widetilde{\Lambda}, 1/2, M), \quad \Psi_0(\widetilde{\Lambda}, 1/2, M) = Q_\Lambda^* \Psi_0(\Lambda, J, M).$$

Proof: Most of the proof is self evident, the point being just to introduce the notation necessary for later work. We note that we can define a height function $\tilde{l}$ by $\tilde{l}(\alpha, j) = l(\alpha)$. Then the ground states of $H_{\tilde{\Lambda}, \tilde{\mathcal{B}}}^{1/2}$ are in the range of $Q_\Lambda^* Q_\Lambda$ because for any permutation π which preserves the rungs of the ladder, i.e. $\pi(\{\alpha\} \times [1, 2J]) = \{\alpha\} \times [1, 2J]$ for all α, $U(\pi)$ coincides with the normal action. So

$$Q_\Lambda^* Q_\Lambda \Psi_0(\tilde{\Lambda}, 1/2, M) = \Psi_0(\tilde{\Lambda}, 1/2, M). \tag{3.1}$$

On the other hand $Q_\Lambda H_{\tilde{\Lambda}}^{1/2} Q_\Lambda^*$ equals H_Λ^J. So $Q_\Lambda \Psi_0(\tilde{\Lambda}, 1/2, M)$ is a ground state of H_Λ^J, in fact all the ground states are obtained like this by an easy Perron-Frobenius argument. Rewriting (3.1) with $\Psi_0(\Lambda, J, M)$ in place of $Q_\Lambda \Psi_0(\tilde{\Lambda}, 1/2, M)$ finishes the proof. ∎

In the particular case of $\Lambda \subset \mathbb{Z}$, one can take $l(\alpha) = \alpha$. Let us for future notational ease define $\mathcal{M}(\Lambda, J, M)$ to be the set of all $\{m_\alpha\} \in [-J, J]^\Lambda$ with the property that $\sum_\alpha m_\alpha = M$. Then the formula one derives for the spin J ground states is

$$\Psi_0(\Lambda, J, M) = \sum_{\{m_\alpha\} \in \mathcal{M}(\Lambda, J, M)} \prod_{\alpha \in \Lambda} \binom{2J}{J + m_\alpha}^{1/2} q^{-\alpha m_\alpha} |\{m_\alpha\}\rangle.$$

We now turn our attention to the infinite volume ground states. We will merely define the ground states, the proof of completeness was done in [17]. Given a countably infinite set of sites Λ_∞, and a finite dimensional Hilbert space $\mathcal{H}_\alpha$ and unit vector Ω_α at each site, one can define the Guichardet Hilbert space

$$\bigotimes_{\alpha \in \Lambda_\infty} (\mathcal{H}_\alpha, \Omega_\alpha) = \mathrm{cl}\left(\bigoplus_{n=1}^\infty \left[(\bigotimes_{j=1}^n \mathcal{H}_{\alpha_j} \otimes \bigotimes_{j=n+1}^\infty \mathbb{C}\Omega_{\alpha_j}) \right. \right.$$
$$\left. \left. \cap (\bigotimes_{j=1}^{n-1} \mathcal{H}_{\alpha_j} \otimes \bigotimes_{j=n}^\infty \mathbb{C}\Omega_{\alpha_j})^\perp \right] \right),$$

where $\alpha_1, \alpha_2, \ldots$ is any enumeration of Λ_∞, and cl means the usual L^2 closure. If Λ is any finite subset of Λ_∞ then we can define the finite dimensional Hilbert space $\mathcal{H}_\Lambda = \bigotimes_{\alpha \in \Lambda} \mathcal{H}_\alpha$, as usual, and an obvious inclusion

$$i_{\Lambda, \Lambda_\infty} : \mathcal{H}_\Lambda \to \bigotimes_{\alpha \in \Lambda_\infty} (\mathcal{H}_\alpha, \Omega_\alpha).$$

This is the proper framework to discuss the one dimensional infinite-volume ground states of the XXZ model, because of the following

Definition 3.3. *For any $J \in \frac{1}{2}\mathbb{N}$ we make the following definitions. Consider $\Lambda_\infty = \mathbb{N}$. For each $\alpha \in \Lambda_\infty$ let $\mathcal{H}_\alpha = \mathbb{C}^{2J+1}$ and $\Omega_\alpha = |J\rangle$. Denote the Guichardet Hilbert space so obtained by*

$$\mathcal{H}(\mathbb{N}, J, up) = \bigotimes_{\alpha \in \mathbb{N}} (\mathcal{H}_\alpha, \Omega_\alpha).$$

Now let $\Lambda_\infty = \mathbb{Z}$ *instead. For each* $\alpha \in \Lambda_\infty$ *let* $\mathcal{H}_\alpha = \mathbb{C}^{2J+1}$ *as before, but let* $\Omega_\alpha = |J\rangle$ *for* $\alpha \geq 1$ *and* $\Omega_\alpha = |-J\rangle$ *for* $\alpha \leq 0$. *Define*

$$\mathcal{H}(\mathbb{Z}, J, kink) = \bigotimes_{\alpha \in \mathbb{Z}} (\mathcal{H}_\alpha, \Omega_\alpha).$$

Then

Lemma 3.4. *(a) If* L_k *is a sequence of integers with* $L_k \to \infty$, *and* $N \in \mathbb{N}$, *then the normalized sequence*

$$\frac{i_{[1,L_k],\mathbb{N}}\Psi_0([1,L_k], J, JL_k - N)}{\|\Psi_0([1,L_k], J, JL_k - N)\|}$$

converges in norm.
(b) If $M_k = L_k J - 2Jr_k + N$ *where* $N \in [0, J-1]$, $r_k \in \mathbb{N}$ *and both* r_k *and* $L_k - r_k$ *tend to* ∞, *then the normalized sequence*

$$\frac{T^{-r_k}i_{[1,L_k],\mathbb{Z}}\Psi_0([1,L_k], J, M_k)}{\|\Psi_0([1,L_k], J, M_k)\|}$$

converges in norm, where T *is the translation one unit to the left.*

Proof: We prove this for spin $1/2$. Then the analogue follows for ground states of $H_\Lambda^{1/2}$, and by the last lemma this proves it for arbitrary spin.

For (a), note that defining

$$\Psi_0'([1,L], 1/2, N) = \sum_{1 \leq \alpha_1 < \cdots < \alpha_N \leq L} q^{\alpha_1 + \cdots + \alpha_N} S_{\alpha_1}^- \cdots S_{\alpha_N}^- \Omega_\mathbb{N},$$

where $\Omega_\mathbb{N}$ is the all up spin vector, we have

$$\frac{i_{[1,L],\mathbb{Z}}\Psi_0([1,L], 1/2, \frac{1}{2}L - N)}{\|\Psi_0([1,L], 1/2, \frac{1}{2}L - N)\|} = \frac{\Psi_0'([1,L], 1/2, N)}{\|\Psi_0'([1,L], 1/2, N)\|}.$$

Then (a) is proved if we prove that the sequence $\Psi_0'([1,L], 1/2, N)$ converges. But this follows by the Monotone Convergence Theorem, thinking of the coefficient of $S_{\alpha_1} \cdots S_{\alpha_N} \Omega_\mathbb{N}$ as a function $f_L(\alpha_1, \ldots, \alpha_N)$. We still need to check that the limit is finite, i.e. that

$$\sum_{1 \leq \alpha_1 < \cdots < \alpha_N} q^{2(\alpha_1 + \cdots + \alpha_N)} < \infty.$$

We can evaluate the series explicitly; it is $q^{N(N+1)}/\prod_{j=1}^N (1 - q^{2j})$.

For (b), we do a similar thing. We define $\Omega_\mathbb{Z}$ to be the vector $\bigotimes_{\alpha \in \mathbb{Z}} \Omega_\alpha$. Since $J = 1/2$, now $M_k = \frac{1}{2}L_k - r_k$ where $r_k, L_k - r_k \to \infty$. Then

$$\frac{T^{-r_k}i_{[1,L_k],\mathbb{Z}}\Psi_0([1,L_k], 1/2, M_k)}{\|\Psi_0([1,L_k], 1/2, M_k)\|} = \frac{\Psi_0'([1-r_k, L_k - r_k], 1/2, 0)}{\|\Psi_0'([1-r_k, L_k - r_k], 1/2, 0)\|}$$

where

$$\Psi_0'([-a,b],1/2,0) = \sum_{n=0}^{\infty} \sum_{-a \le \alpha_1 < \cdots < \alpha_n \le 0 < \beta_1 < \cdots < \beta_n \le b} \prod_{k=1}^{n} q^{\beta_k - \alpha_k} S_{\alpha_k}^+ S_{\beta_k}^- \, \Omega_{\mathbb{Z}}.$$

The lemma will follow by the Dominated Convergence Theorem if we prove that $\Psi_0'(\mathbb{Z}, 1/2, 0)$ is summable. This is equivalent to

$$Z = \sum_{n=0}^{\infty} \sum_{\alpha_1 < \cdots < \alpha_n \le 0 < \beta_1 < \cdots < \beta_n} q^{2[\beta_1 + \cdots + \beta_n - (\alpha_1 + \cdots + \alpha_n)]} < \infty.$$

We can also evaluate this explicitly

$$\begin{aligned} Z &= \sum_{n=0}^{\infty} \frac{q^{n(n+1)}}{\prod_{j=1}^{n}(1 - q^{2j})} \cdot \frac{q^{n(n-1)}}{\prod_{j=1}^{n}(1 - q^{2j})} \\ &= \sum_{n=0}^{\infty} \frac{q^{2n^2}}{\prod_{j=1}^{n}(1 - q^{2j})^2} \\ &= \frac{1}{\prod_{j=1}^{\infty}(1 - q^{2j})} \end{aligned}$$

by Heine's theorem (c.f. [11]). In particular it is finite. ∎

Let

$$\Psi_0(\mathbb{Z}, \mathrm{J}, M) = \lim_{L \to \infty} \frac{\Psi_0([-L+1, L], \mathrm{J}, M)}{\|\Psi_0([-L+1, L], \mathrm{J}, M)\|}.$$

The limit exists by the lemma. We claim that this vector gives an infinite volume ground state. The representation of quasi-local observables on $\mathcal{H}(\mathbb{Z}, \mathrm{J}, \mathrm{kink})$ is clear: the local observables $\mathcal{A}_\Lambda$ are operators of $\mathcal{H}_\Lambda$ which includes by $i_{\Lambda, \mathbb{Z}}$ into $\mathcal{H}(\mathbb{Z}, \mathrm{J}, \mathrm{kink})$. Take the weak-$*$ completion and we are done. The state is then $\omega_{\mathrm{J}, M}^{\mathrm{kink}}(X) = \langle \Psi_0(\mathbb{Z}, \mathrm{J}, M) | X \Psi_0(\mathbb{Z}, \mathrm{J}, M) \rangle$. All one needs to check is that for any local observable X,

$$\lim_{\Lambda \to \infty} \langle \Psi_0(\mathbb{Z}, \mathrm{J}, M) | X^*[H_\Lambda, X] \Psi_0(\mathbb{Z}, \mathrm{J}, M) \rangle \ge 0$$

Suppose $X \in \mathcal{A}_\Lambda$. Define Λ_1 to be the union of Λ with all nearest neighbors. Then for $\Lambda' \supset \Lambda_1$, $[H_{\Lambda'}, X] = [H_{\Lambda_1}, X]$. Using the frustration free property of $\Psi_0([-L, L], \mathrm{J}, M)$, we see that as soon as $\Lambda_2 \subset [-L, L]$, we have

$$\langle \Psi_0([-L+1, L], \mathrm{J}, M) | X^*[H_{\Lambda_2}, X] \Psi_0([-L+1, L], \mathrm{J}, M) \rangle \ge 0.$$

Taking the limit, we see that $\omega_{\mathrm{J}, M}^{\mathrm{kink}}$ is an infinite volume ground state. We define the $\gamma(\mathrm{J}, M)$ to be the gap above zero in the spectrum of the Hamiltonian acting on the GNS space of the ground state $\omega_{\mathrm{J}, M}^{\mathrm{kink}}$.

There are three other classes of ground states. The antikink ground states are the states $\omega_{\mathrm{J}, M}^{\mathrm{anti}} = \omega_{\mathrm{J}, M}^{\mathrm{kink}} \circ \mathcal{F}$ where $\mathcal{F}$ is uniquely determined by the formula $\mathcal{F}(S_k^+) = S_k^-$ for all $k \in \mathbb{Z}$. There are also the all up spin states and all down spin states, which are well known and characterized by $\omega_{\mathrm{J}}^{\mathrm{up, down}}(S_\alpha^3) = \pm \mathrm{J}$ for all α. We mention that the GNS space for them is also a Guichardet Hilbert space where $\Omega_\alpha^{\mathrm{up, down}} = |\pm \mathrm{J}\rangle$ for all α, and $\Omega_{\mathbb{Z}}^{\mathrm{up, down}}$ is the vector representing the ground state. That these are all the ground states is proved by Koma and Nachtergaele [17].

4   Spin ladder reduction

We now elaborate on the spin ladder construction introduced in Lemma 3.2. Let us define $\widetilde{H}_{\widetilde{\Lambda}} = H_{\widetilde{\Lambda},\widetilde{\mathcal{B}}}$ introduced in the lemma. Then, defining $\mathcal{G}(\Lambda, \mathrm{J}, M)$ to be the one dimensional ground state space of H_{Λ}^{J} in the sector $\mathcal{H}(\Lambda, \mathrm{J}, M)$, and $\mathcal{G}(\widetilde{\Lambda}, M)$ to be the one dimensional ground state space of $\mathcal{H}(\widetilde{\Lambda}, M)$, the lemma tells us that

$$Q_{\Lambda}\mathcal{G}(\widetilde{\Lambda}, M) = \mathcal{G}(\Lambda, M)\,, \quad Q_{\Lambda}^{*}\mathcal{G}(\Lambda, M) = \mathcal{G}(\widetilde{\Lambda}, M) = \mathcal{G}(\Lambda, M)\,.$$

The spectral gap in the sector $\mathcal{H}(\Lambda, \mathrm{J}, M)$ is defined

$$\gamma(\Lambda, \mathrm{J}, M) = \inf_{\substack{\psi \in \mathcal{H}(\Lambda,\mathrm{J},M) \\ \psi \perp \mathcal{G}(\Lambda,\mathrm{J},M)}} \frac{\langle \psi | H_{\Lambda}^{\mathrm{J}} \psi \rangle}{\langle \psi | \psi \rangle}\,.$$

In view of the lemma, defining $P_{\Lambda} = Q_{\Lambda}^{*}Q_{\Lambda}$, we can rewrite the spectral gap

$$\gamma(\Lambda, \mathrm{J}, M) = \inf_{\substack{\psi \in \mathcal{H}(\widetilde{\Lambda},M)\backslash \ker P_{\Lambda} \\ \psi \perp \mathcal{G}(\widetilde{\Lambda},M)}} \frac{\langle P_{\Lambda}\psi | \widetilde{H}_{\widetilde{\Lambda}} P_{\Lambda}\psi \rangle}{\langle P_{\Lambda}\psi | P_{\Lambda}\psi \rangle}\,.$$

We now introduce a second Hamiltonian on $\mathcal{H}(\widetilde{\Lambda}, M)$ which is

$$\widetilde{\widetilde{H}}_{\widetilde{\Lambda}} = H_{\widetilde{\Lambda},\widetilde{\widetilde{\mathcal{B}}}}\,,$$

where

$$\widetilde{\widetilde{\mathcal{B}}} = \{((\alpha, j), (\beta, j)) : (\alpha, \beta) \in \mathcal{B}\,, j \in [1, 2\mathrm{J}]\}\,.$$

This is clearly equivalent to 2J disjoint copies of $H_{\Lambda}^{1/2}$. So, if $\Lambda = [1, L]$, Theorem 2.1 guarantees that the spectral gap of $\widetilde{\widetilde{H}}_{\widetilde{\Lambda}}$ is equal to $1 - \Delta^{-1}\cos(\pi/L) > 1 - \Delta^{-1}$. Let us introduce some notation: Let $\mathcal{H}_{0}(\widetilde{\Lambda}, M)$ be the ground state space of $\widetilde{\widetilde{H}}_{\widetilde{\Lambda}}$ in the sector $\mathcal{H}(\widetilde{\Lambda}, M)$, and let $\mathcal{H}_{\mathrm{exc}}(\widetilde{\Lambda}, M)$ be its orthogonal complement in the sector $\mathcal{H}(\widetilde{\Lambda}, M)$. Then

$$\inf_{\psi \in \mathcal{H}_{\mathrm{exc}}(\widetilde{\Lambda},M)} \frac{\langle \psi | \widetilde{\widetilde{H}}_{\widetilde{\Lambda}} \psi \rangle}{\langle \psi | \psi \rangle} \geq 1 - \Delta^{-1}\,. \tag{4.2}$$

Defining $P_{\alpha} = Q_{\alpha}^{*}Q_{\alpha}$ to be symmetrization in the rung $\{\alpha\} \times [1, 2\mathrm{J}]$, we observe that

$$P_{\alpha}\boldsymbol{S}_{(\alpha,j)}P_{\alpha} = \frac{1}{2\mathrm{J}}\sum_{k=1}^{2\mathrm{J}} P_{\alpha}\boldsymbol{S}_{(\alpha,k)}P_{\alpha}\,.$$

From this it follows that

$$P_{\alpha}P_{\beta}h^{1/2}((\alpha, j), (\beta, j))P_{\alpha}P_{\beta} = \frac{1}{(2\mathrm{J})^{2}}\sum_{k,l=1}^{2\mathrm{J}} P_{\alpha}P_{\beta}h^{1/2}((\alpha, k), (\beta, l))P_{\alpha}P_{\beta}\,,$$

and finally that

$$P_\Lambda \widetilde{\widetilde{H}}_{\widetilde{\Lambda}} P_\Lambda = \frac{1}{2J} P_\Lambda \widetilde{H}_{\widetilde{\Lambda}} P_\Lambda \,.$$

Then we can rewrite the spectral gap formula once more

$$\gamma(\Lambda, J, M) = 2J \inf_{\substack{\psi \in \mathcal{H}(\widetilde{\Lambda}, M) \setminus \ker P_\Lambda \\ \psi \perp \mathcal{G}(\widetilde{\Lambda}, M)}} \frac{\langle P_\Lambda \psi | \widetilde{\widetilde{H}}_{\widetilde{\Lambda}} P_\Lambda \psi \rangle}{\langle P_\Lambda \psi | P_\Lambda \psi \rangle} \,. \tag{4.3}$$

This is useful because we have a spectral gap for $\widetilde{\widetilde{H}}_{\widetilde{\Lambda}}$. Also note that it is now trivial that $\mathcal{G}(\widetilde{\Lambda}, M) \subset \mathcal{H}_0(\widetilde{\Lambda}, M)$. We define

$$\mathcal{H}_{0,\perp}(\widetilde{\Lambda}, M) = \mathcal{H}_0(\widetilde{\Lambda}, M) \cap \mathcal{G}(\widetilde{\Lambda}, M)^\perp \,.$$

Then

$$\mathcal{H}(\widetilde{\Lambda}, M) = \mathcal{G}(\widetilde{\Lambda}, M) \oplus \mathcal{H}_{0,\perp}(\widetilde{\Lambda}, M) \oplus \mathcal{H}_{\mathrm{exc}}(\widetilde{\Lambda}, M) \,.$$

We now state the main lemma of this section, which is the key to our theorem

Lemma 4.1. *If* $\psi \in \mathcal{H}(\widetilde{\Lambda}, M)$ *and* $\psi \perp \mathcal{G}(\widetilde{\Lambda}, M)$, *then for some* $\psi' \in \mathcal{H}_{0,\perp}(\widetilde{\Lambda}, M)$ *and* $\psi'' \in \mathcal{H}_{exc}(\widetilde{\Lambda}, M)$, *we have*

$$P_\Lambda \psi = \psi' + \psi'' \,.$$

Moreover,

$$\frac{\langle P_\Lambda \psi | \widetilde{\widetilde{H}}_{\widetilde{\Lambda}} P_\Lambda \psi \rangle}{\langle P_\Lambda \psi | P_\Lambda \psi \rangle} \geq (1 - \Delta^{-1}) \left(1 - \frac{\langle \psi' | P_\Lambda \psi' \rangle}{\langle \psi' | \psi' \rangle} \right)$$

where the ratio is interpreted as zero if $\psi' = 0$. *Hence*

$$\gamma(\Lambda, J, M) \geq 2J(1 - \Delta^{-1}) \left(1 - \sup_{\psi \in \mathcal{H}_{0,\perp}(\widetilde{\Lambda}, M)} \frac{\langle \psi | P_\Lambda \psi \rangle}{\langle \psi | \psi \rangle} \right) \,.$$

Proof: First note that $P_\Lambda \mathcal{G}(\widetilde{\Lambda}, M) = \mathcal{G}(\widetilde{\Lambda}, M)$, so if $\psi \perp \mathcal{G}(\widetilde{\Lambda}, M)$ then $P_\Lambda \psi \perp \mathcal{G}(\widetilde{\Lambda}, M)$, which proves that $P_\Lambda \psi \in \mathcal{H}_{0,\perp}(\widetilde{\Lambda}, M) \oplus \mathcal{H}_{\mathrm{exc}}(\widetilde{\Lambda}, M)$. Now suppose $P_\Lambda \psi = \psi' + \psi''$. Then $\widetilde{\widetilde{H}}_{\widetilde{\Lambda}} \psi' = 0$. Hence, by Theorem 2.1

$$\langle P_\Lambda \psi | \widetilde{\widetilde{H}}_{\widetilde{\Lambda}} P_\Lambda \psi \rangle = \langle \psi'' | \widetilde{\widetilde{H}}_{\widetilde{\Lambda}} \psi'' \rangle \geq (1 - \Delta^{-1}) \langle \psi'' | \psi'' \rangle \,.$$

So

$$\frac{\langle P_\Lambda \psi | \widetilde{\widetilde{H}}_{\widetilde{\Lambda}} P_\Lambda \psi \rangle}{\langle P_\Lambda \psi | P_\Lambda \psi \rangle} \geq (1 - \Delta^{-1}) \left(1 - \frac{\|\psi'\|^2}{\|P_\Lambda \psi\|^2} \right) \,.$$

By Cauchy-Schwarz and the fact that $\langle \psi' | \psi'' \rangle = 0$, we have

$$\langle \psi' | \psi' \rangle = \langle \psi' | P_\Lambda \psi \rangle = \langle P_\Lambda \psi' | P_\Lambda \psi \rangle \leq \|P_\Lambda \psi'\| \cdot \|P_\Lambda \psi\| \,.$$

I.e.

$$\frac{\|\psi'\|}{\|P_\Lambda \psi\|} \leq \frac{\|P_\Lambda \psi'\|}{\|\psi'\|} \,.$$

∎

Thus we may define

$$\delta(\Lambda, \mathrm{J}, M) = \sup_{\psi \in \mathcal{H}_{0,\perp}(\tilde{\Lambda}, M)} \frac{\langle \psi | P_\Lambda \psi \rangle}{\langle \psi | \psi \rangle} \,.$$

The positivity of a gap $\gamma(\Lambda, \mathrm{J}, M)$ is then equivalent to $\delta(\Lambda, \mathrm{J}, M) < 1$. We will numerically estimate $\delta(\Lambda, \mathrm{J}, M)$ in Section 6, directly from its definition. For now, we use the lemma to prove the main theorem.

5   Proof of Theorem 2.2

We begin this section with the trivial part of the theorem, namely the calculation of the spectral gap above the state $\omega_{\mathrm{J}}^\uparrow$ which is the translation invariant all up spin state. This is a well-known result, but we include it for completeness. To prove that there is a spectral gap, we have to prove that there is a number $\gamma_{\mathrm{J}} > 0$ such that for any local observable

$$\omega_{\mathrm{J}}^\uparrow(\delta(X)^* \delta(\delta(X)) - \gamma_{\mathrm{J}} \delta(X^*) \delta(X)) \geq 0 \,,$$

where $\delta(X) = \lim_{\Lambda \nearrow \infty} [H_\Lambda^{\mathrm{J}}, X]$. If $X \in \mathcal{A}_\Lambda$ is local, we can take $\delta(\delta(X)) = [H_{\Lambda+[-2,2]}^{\mathrm{J}}, [H_{\Lambda+[-1,1]}^{\mathrm{J}}, X]]$ and so on. We observe that the boundary terms of H^{J} are equal to zero, i.e.

$$\lim_{L \to \infty} \omega_{\mathrm{J}}^\uparrow(\delta(X)^* (S_{-L}^3 - S_L^3) \delta(X)) = 0 \,.$$

So we may rewrite the Hamiltonian in the GNS space of $\omega_{\mathrm{J}}^\uparrow$

$$H^{\mathrm{J}} = \Delta^{-1} H_{\mathrm{iso}}^{\mathrm{J}} + (1 - \Delta^{-1}) H_{\mathrm{Ising}}^{\mathrm{J}} \,,$$

$$H_{\mathrm{iso}}^{\mathrm{J}} = \sum_{x=-\infty}^{\infty} (\mathrm{J}^2 - \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1}) \,,$$

$$H_{\mathrm{Ising}}^{\mathrm{J}} = \sum_{x=-\infty}^{\infty} (\mathrm{J}^2 - S_x^3 S_{x+1}^3) \,.$$

Clearly $H_{\mathrm{iso}}^{\mathrm{J}} \geq 0$, so γ_{J} is bounded below by the spectral gap of $H_{\mathrm{Ising}}^{\mathrm{J}}$. It is important that $\omega_{\mathrm{J}}^\uparrow$ is a ground state of both $H_{\mathrm{iso}}^{\mathrm{J}}$ and $H_{\mathrm{Ising}}^{\mathrm{J}}$. It is easy to see that the first excitations for $H_{\mathrm{Ising}}^{\mathrm{J}}$ are the one magnon states. The one magnon states are those obtained from $\omega_{\mathrm{J}}^\uparrow$ by conjugating with observables of the form

$$X = \sum_{x \in \mathbb{Z}} \frac{c_x}{\sqrt{2\mathrm{J}}} S_x^-$$

where $\{c_x\}$ is any complex, square-summable sequence. Then one observes that $\omega_{\mathrm{J}}^\uparrow(X) = 0$, $\omega_{\mathrm{J}}^\uparrow(X^* X) = 1$, and $\omega_{\mathrm{J}}^\uparrow(X^* H_{\mathrm{Ising}}^{\mathrm{J}} X) = 2\mathrm{J}$. We claim that it is easy to

see that among all quasilocal perturbations, satisfying the first two equalities, these minimimize the Ising energy. So the spectral gap of $H_{\text{Ising}}^{\text{J}}$ is 2J, and the spectral gap of H^{J} is at least $(1 - \Delta^{-1})2\text{J}$. It is also very well known that the Heisenberg model acts as the discrete Laplacian on the space of one magnon states. We can see this since

$$[H_{\text{isotropic}}^{\text{J}}, X] = \sum_{x \in \mathbb{Z}} \frac{(c_x - c_{x-1})S_{x-1}^3 + (c_x - c_{x+1})S_{x+1}^3}{\sqrt{2\text{J}}} S_x^- ,$$

which implies

$$\omega_{\text{J}}^{\uparrow}(X^* H_{\text{isotropic}}^{\text{J}} X) = \text{J} \sum_{x=-\infty}^{\infty} \overline{c_x}(2c_x - c_{x+1} - c_{x-1}) .$$

We can choose a sequence of one magnon excitations

$$X_L = \frac{1}{\sqrt{L}} \sum_{x=1}^{L} \frac{1}{\sqrt{2\text{J}}} S_x^-$$

such that $\omega_{\text{J}}^{\uparrow}(X_L^* H_{\text{isotropic}}^{\text{J}} X_L) = 2\text{J}/L$. Therefore,

$$2\text{J}(1 - \Delta^{-1}) \leq \gamma_{\text{J}} \leq \omega_{\text{J}}^{\uparrow}(X_L^* H^{\text{J}} X_L) = 2\text{J}(1 - \Delta^{-1}) + 2\text{J}\Delta^{-1}L^{-1} ,$$

for all L, which shows that $\gamma_{\text{J}} = 2\text{J}(1 - \Delta^{-1})$.

The other trivial facts in the theorem are that for the gaps above the kink $\gamma(\text{J}, M) = \gamma(\text{J}, M + 2\text{J})$, which follows by translational symmetry, and $\gamma(\text{J}, M) = \gamma(\text{J}, -M)$, which follows by spin-flip reflection symmetry.

We now begin the proof of the nontrivial parts of the theorem. Fix $\text{J} \in \frac{1}{2}\mathbb{N}$ and Δ^{-1} in the range $0 < \Delta^{-1} < 1$.

Definition 5.1. *We say that a sequence of triples (L_k, M_k, ψ_k) satisfies hypothesis (H1) if for all $k \in \mathbb{N}$ the following holds: $L_k \in \mathbb{N}_{\geq 2}$, $M_k \in [-JL_k, JL_k]$, ψ_k in $\mathcal{H}_{0,\perp}([1, L_k] \times [1, 2J], M_k)$, and $\|\psi_k\|^2 = 1$. We note that the most important part of (H1) is that $\psi_k \in \mathcal{H}_{0,\perp}$. In particular, this means that $P_{[1,L_k]}\psi_k \neq \psi_k$. We say that a sequence of triples (L_k, M_k, ψ_k) satisfies hypothesis (H2) if additionally*

$$\lim_{k \to \infty} \|P_{[1,L_k]}\psi_k\| = 1 .$$

The main component of our proof is the following

Proposition 5.2. *No sequence satisfies both hypotheses (H1) and (H2).*

We observe of both (H1) and (H2) that if any sequence (L_k, M_k, ψ_k) satisfies (H1) or (H2), then every subsequence does as well. Using this fact and the previous proposition, one can deduce that there is a constant $\delta > 0$, depending on Δ^{-1} and J, such that for any sequence (L_k, M_k, ψ_k) satisfying (H1), one has

$$\limsup_{k \to \infty} \|P_{[1,L_k]}\psi_k\| \leq 1 - \delta .$$

Hence by Lemma 4.1 and the discussion following it,

$$\inf_{L \in \mathbb{N}_{\geq 2}} \inf_{-\mathrm{J}L \leq M \leq \mathrm{J}L} \gamma([1,L],\mathrm{J},M) \geq 2\mathrm{J}(1 - \Delta^{-1})\delta\,.$$

All the finite volume spectral gaps have a uniform lower bound. Since the kink ground states are frustration free, this gives the following corollary, which is a reformulation of our main theorem

Corollary 5.3. *For* $0 < \Delta^{-1} < 1$ *and any* $J \in \frac{1}{2}\mathbb{N}$, *there is a nonvanishing spectral gap above all of the infinite volume kink states.*

Proof: (**of Corollary 5.3 given Proposition 5.2**) Let $\omega_{\mathrm{J},M}^{\downarrow\uparrow}$ be the ground state of the kink. To prove that there is a spectral gap, we have to prove that there is a number $\gamma(\mathrm{J},M) > 0$ such that for any local observable

$$\omega_{\mathrm{J},M}^{\downarrow\uparrow}(\delta(X)^*\delta(\delta(X)) - \gamma(\mathrm{J},M)\delta(X^*)\delta(X)) \geq 0\,,$$

where $\delta(X) = \lim_{\Lambda \nearrow \infty}[H_\Lambda, X]$. On the other hand, by Lemma 3.4, for any local observable X

$$\omega_{\mathrm{J},M}^{\downarrow\uparrow}(X) = \lim_{L \to \infty} \frac{\langle \Psi_0(\Lambda_L,\mathrm{J},M)|X\Psi_0(\Lambda_L,\mathrm{J},M)\rangle}{\|\Psi_0(\Lambda_L,\mathrm{J},M)\|^2}\,,$$

where $\Lambda_L = [-L+1,L]$. If X is a local observable with support in Λ then one can take $\delta(\delta(X)) = [H_{\Lambda_L},[H_{\Lambda_L},X]]$, for any $\Lambda_L \supset \Lambda + [-2,2]$. Also for $M' \in [-\mathrm{J}|\Lambda_L|,\mathrm{J}|\Lambda_L|]$,

$$\langle \Psi_0(\Lambda_L,\mathrm{J},M')|(H_{\Lambda_L}X - XH_{\Lambda_L})\Psi_0(\Lambda_L,\mathrm{J},M)\rangle = 0$$

because $\Psi_0(\Lambda_L,\mathrm{J},M')$ and $\Psi_0(\Lambda_L,\mathrm{J},M)$ have the same energy. Hence $\delta(X)\Psi_0(\Lambda_L,\mathrm{J},M)$ is orthogonal to all ground states. Thus, we see that in this case the infinite volume gap corresponds to the naive guess, i.e. the liminf of all finite volume gaps. To be more explicit, let $\gamma(M,\mathrm{J})$ be a positive lower bound on all the finite volume gaps $\gamma([-L+1,L],\mathrm{J},M)$, which exists by Proposition 5.2. Define ω_L and ω_L' to be the states on $\mathcal{A}_{\Lambda_L}$ corresponding to $\Psi_0(\Lambda_L,\mathrm{J},M)$ and $\delta(X)\Psi_0(\Lambda_L,\mathrm{J},M)$, respectively. Then

$$\begin{aligned}
\omega_{\mathrm{J},M}^{\downarrow\uparrow}&(\delta(X)^*\delta(\delta(X)) - \gamma(\mathrm{J},M)\delta(X^*)\delta(X))\\
&= \lim_{L \to \infty} \omega_L(\delta(X)^*\delta(\delta(X)) - \gamma(\mathrm{J},M)\delta(X^*)\delta(X))\\
&= \lim_{L \to \infty} \omega_L'(H_{\Lambda_L} - \gamma(\mathrm{J},M))\omega_L(\delta(X)^*\delta(X))\\
&\geq \lim_{L \to \infty} (\gamma(\Lambda_L,\mathrm{J},M) - \gamma(\mathrm{J},M))\frac{\|\delta(X)\Psi_0(\Lambda_L,\mathrm{J},M)\|^2}{\|\Psi_0(\Lambda_L,\mathrm{J},M)\|^2}\\
&\geq 0\,.
\end{aligned}$$

∎

We will show that (H1) and (H2) are incompatible in a series of lemmas.

Lemma 5.4. *If (L_k, M_k, ψ_k) satisfies (H1) and (H2), then $L_k \to \infty$.*

Proof: (of Lemma 5.4) Suppose not. Then there is some sequence satisfying (H1) and (H2) and such that $L_k = L < \infty$ for all k. But $\mathcal{H}_0([1, L], \mathrm{J}) = \bigoplus_{M=-JL}^{JL} \mathcal{H}_0([1, L], \mathrm{J}, M)$ is a finite dimensional space. The finite matrix obtained by restricting and projecting $P_{[1,L]}$ to this space is Hermitian, and its largest eigenvalue is 1. Moreover, the eigenspace corresponding to 1 is $\mathcal{G}([1, L], \mathrm{J}) = \bigoplus_{M=-JL}^{JL} \mathcal{G}([1, L], \mathrm{J}, M)$. All the vectors ψ_k are orthogonal to $\mathcal{G}([1, L], \mathrm{J})$ by hypothesis (H1). Since finite matrices have discrete spectra, this contradicts hypothesis (H2). ∎

Lemma 5.5. *If (L_k, M_k, ψ_k) satisfies (H1) and (H2) then $JL_k - |M_k| \to \infty$.*

Before giving the proof of this easy lemma, we need to define some new notation.

Definition 5.6. *For $L \in \mathbb{N}$, let $\mathcal{M}(L, J, M)$ be the set of all vectors $\boldsymbol{m} = (m_1, \dots, m_{2J}) \in [-L/2, L/2]^{2J}$ whose sum is M, i.e. $\sum_j m_j = M$. For each $\boldsymbol{m} \in \mathcal{M}(L, J, M)$, define*

$$\Psi_0([1, L] \times [1, 2J], \boldsymbol{m}) = \bigotimes_{j=1}^{2J} \Psi_0([1, L] \times \{j\}, 1/2, m_j).$$

Related to this, let $\mathcal{N}(J, N)$ be the set all vectors $\boldsymbol{n} = (n_1, \dots, n_{2J}) \in \mathbb{N}^{2J}$ satisfying $\sum_j n_j = N$. Let $\boldsymbol{e} = (1, 1, \dots, 1) \in \mathbb{N}^{2J}$. Recall a previous definition

$$\Psi_0'([1, L], 1/2, n) = \sum_{1 \le x_1 < x_2 < \cdots < x_n \le L} q^{x_1 + \cdots + x_n} S_{x_1}^- \cdots S_{x_n}^- \Omega_{\mathbb{N}}.$$

Define

$$\Psi_0'([1, L] \times [1, 2J], \boldsymbol{n}) = \bigotimes_{j=1}^{2J} \Psi_0'([1, L] \times \{j\}, 1/2, n_j)$$

Let $\mathcal{H}(\mathbb{N} \times [1, 2J], up)$ be the Guichardet Hilbert space

$$\bigotimes_{(x,j) \in \mathbb{N}[1, 2J]} (\mathbb{C}_{(x,j)}^2, |+1/2\rangle_{(x,j)}).$$

Define $\mathcal{D}([1, L] \times [1, 2J], N)$ to be the projection on $\mathcal{H}(\mathbb{N} \times [1, 2J], up)$ which projects onto vectors ψ such that

$$\sum_{(x,j) \in [1, L] \times [1, 2J]} (\frac{1}{2} - S_{(x,j)}^3)\psi = N\psi,$$

and $S_{(x,j)}^3 \psi = \frac{1}{2}\psi$ for $(x, j) \in (\mathbb{N} \setminus [1, L]) \times [1, 2J]$. Finally, let

$$\Psi_0'([1, L] \times [1, 2J], N)$$

be the unique normalized ground state of $\widetilde{H}_{[1,L] \times [1, 2J]}$ in the range of $\mathcal{D}([1, L] \times [1, 2J], N)$. Specify the phase to that $\Psi_0'([1, L] \times [1, 2J], N)$ has real coefficients in

the Ising basis. This ground state exists and is unique (and has real coefficients) since $\widetilde{H}_{[1,L]\times[1,2J]}$ acting on the range $\mathcal{D}([1,L]\times[1,2J],N)$ is unitarily equivalent to the finite matrix $\widetilde{H}_{[1,L]\times[1,2J]}$ acting on $\mathcal{H}([1,L]\times[1,2J],M)$. (We apologize for the abuse of notation : the same notation is used for the operator acting on two different, but isomorphic, Hilbert spaces.)

The following are easy and useful observations. The set

$$\{\Psi_0([1,L]\times[1,2J],m) : m \in \mathcal{M}(L,J,M)\}$$

is an orthogonal basis for $\mathcal{H}_0([1,L]\times[1,2J],M)$. The set of indices $\mathcal{N}(J,n)$ is finite, while if one defined the analogue of $\mathcal{M}(L,J,M)$ replacing L by $\mathbb{N}$ it would not be finite. There is a simple translation between the two vectors defined above:

$$\frac{\Psi_0'([1,L]\times[1,2J],n)}{\|\Psi_0'([1,L]\times[1,2J],n)\|} = \frac{i_{[1,L],\mathbb{Z}}\Psi_0([1,L]\times[1,2J],\frac{1}{2}Le-n)}{\|\Psi_0([1,L]\times[1,2J],\frac{1}{2}Le-n)\|}.$$

By Lemma 3.4, the following strong limit exists

$$\Psi_0'(\mathbb{N}\times[1,2J],n) = \lim_{L\to\infty}\Psi_0'([1,L]\times[1,2J],n).$$

One has the following simple formula for the action of $\mathcal{D}([1,L]\times[1,2J],N)$ on $\mathcal{H}_0([1,L']\times[1,2J],M)$:

$$\mathcal{D}([1,L]\times[1,2J],N)\Psi_0'([1,L']\times[1,2J],n) = \Psi_0'([1,L'\wedge L]\times[1,2J],n).$$

By Lemma 3.4, again, the following limit holds for all $n \in \mathcal{N}(J,N)$:

$$\lim_{L\to\infty}\lim_{L'\to\infty}\frac{\|\mathcal{D}([1,L]\times[1,2J],N)\Psi_0'([1,L']\times[1,2J],n)\|}{\|\Psi_0'([1,L']\times[1,2J],n)\|} = 1. \qquad (5.4)$$

By Lemma 3.4, again, the following strong limit exists

$$\Psi_0'(\mathbb{N}\times[1,2J],N) = \lim_{L\to\infty}\Psi_0'([1,L]\times[1,2J],N). \qquad (5.5)$$

We note for the reader that for large enough L

$$\Psi_0'([1,L]\times[1,2J],N) \propto \sum_{n\in\mathcal{N}(J,N)}\Psi_0'([1,L]\times[1,2J],n),$$

and that

$$\Psi_0'(\mathbb{N}\times[1,2J],N) \propto \sum_{n\in\mathcal{N}(J,N)}\Psi_0'(\mathbb{N}\times[1,2J],n).$$

The proportionality constants are necessary because both $\Psi_0'([1,L]\times[1,2J],N)$ and $\Psi_0'(\mathbb{N}\times[1,2J],N)$ are chosen to be normalized.

Proof: **(Lemma 5.5)** We will verify that $JL_k - M_k \to \infty$; the fact that $JL_k + M_k \to \infty$ then follows by spin-flip/reflection symmetry. If it fails for some sequence, then some subsequence, also satisfying (H1) and (H2), has the property that $JL_{l_k} - M_{l_k} = M$ is a finite constant. We assume that this subsequence was taken at the

beginning to avoid double subscripts. Since each $\psi_k \in \mathcal{H}_{0,\perp}([1, L_k] \times [1, 2J], M)$, we can write

$$\psi_k = \sum_{n \in \mathcal{N}([1,L_k],N)} c_k(n) \frac{\Psi_0([1, L_k] \times [1, 2J], \frac{1}{2}L_k e - n)}{\|\Psi_0([1, L_k] \times [1, 2J], \frac{1}{2}L_k e - n)\|} .$$

So

$$\psi'_k := i_{[1,L_k],\mathbb{N}} \psi_k = \sum_{n \in \mathcal{N}([1,L_k],N)} c_k(n) \frac{\Psi'_0([1, L_k] \times [1, 2J], n)}{\|\Psi'_0([1, L_k] \times [1, 2J], n)\|} .$$

We know $L_k \to \infty$ by the last lemma. So $\Psi'_0([1, L_k] \times [1, 2J], n) \to \Psi'_0(\mathbb{N} \times [1, 2J], n)$ as $k \to \infty$ for each n. Furthermore, $\{c_k(n) : n \in \mathcal{N}(J, N)\}$ is a unit vector in the finite-dimensional space $\mathbb{C}^{|\mathcal{N}(J,N)|}$, for each k. So there is a subsequence with $c_{l_k}(n) \to c(n)$ for each n. Again, we assume this subsequence was chosen at the beginning to avoid double subscripts. Thus, ψ'_k converges to the vector

$$\psi = \sum_{n \in \mathcal{N}(J,N)} c(n) \Psi'_0(\mathbb{N} \times [1, 2J], n) .$$

For $L < \infty$ and k large enough, $P_{[1,L]} \geq P_{[1,L_{l_k}]}$. Hence, by (H2)

$$\langle \psi | P_{[1,L]} \psi \rangle = \lim_{k \to \infty} \langle \psi'_k | P_{[1,L]} \psi'_k \rangle \geq \lim_{k \to \infty} \langle \psi'_k | P_{[1,L_k]} \psi'_k \rangle = 1$$

for all L. Also, $\widetilde{\widetilde{H}}_{[1,L_k] \times [1,2J]} \geq \widetilde{\widetilde{H}}_{[1,L] \times [1,2J]}$, so $\widetilde{\widetilde{H}}_{[1,L] \times [1,2J]} \psi = 0$. Recall

$$P_{[1,L]} \widetilde{\widetilde{H}}_{[1,L] \times [1,2J]} P_{[1,L]} = \frac{1}{2J} P_{[1,L]} \widetilde{H}_{[1,L] \times [1,2J]} P_{[1,L]} .$$

So

$$\widetilde{H}_{[1,L] \times [1,2J]} \psi = 0 \tag{5.6}$$

for every finite L.

Notice,

$$\lim_{L \to \infty} \|\mathcal{D}([1, L] \times [1, 2J], N) \psi\| = \lim_{L \to \infty} \lim_{k \to \infty} \|\mathcal{D}([1, L] \times [1, 2J], N) \psi_k\| = 1 \tag{5.7}$$

by (5.4). Together, (5.6) and (5.7) imply that

$$\lim_{L \to \infty} |\langle \psi | \Psi'_0([1, L] \times [1, 2J], N) \rangle| = 1 ,$$

i.e. that $\psi = e^{i\phi} \Psi'_0(\mathbb{N} \times [1, 2J], N)$. Since $\psi'_k \to \psi$,

$$\lim_{k \to \infty} \frac{|\langle \psi'_k | \Psi'_0(\mathbb{N} \times [1, 2J], N) \rangle|}{\|\psi'_k\|} = 1 . \tag{5.8}$$

On the other hand, we know $\langle \psi'_k | \Psi'_0([1, L_k] \times [1, 2J], N) \rangle = 0$, because $\psi_k \perp \mathcal{G}([1, L_k] \times [1, 2J], N)$. So, by (5.5), this implies

$$\lim_{k \to \infty} \frac{|\langle \psi'_k | \Psi'_0(\mathbb{N} \times [1, 2J], N) \rangle|}{\|\psi'_k\|} = 0 . \tag{5.9}$$

Clearly, (5.8) and (5.9) are incompatible and we have a contradiction.   ∎

Proof: (Proposition 5.2)

Let $\mathcal{M}(J, M)$ be the set of all $(m_1, \ldots, m_{2J})$ with $\sum_j m_j = M$. Define for any $m \in \mathbb{Z}$,

$$\Psi_0'([-a,b], 1/2, m) = \sum_n \sum_{-a \leq \alpha_1 < \cdots < \alpha_n \leq 0 < \beta_1 < \cdots < \beta_{m+n} \leq b} q^{\beta_1 + \ldots \beta_{m+n} - \alpha_1 - \cdots - \alpha_n} S_{\alpha_1}^+ \cdots S_{\alpha_n}^+ S_{\beta_1}^- \cdots S_{\beta_{m+n}}^- \Omega_\mathbb{Z}.$$

Let

$$\Psi_0'([-a,b] \times [1, 2J], m) = \bigotimes_{j=1}^{2J} \Psi_0'([-a,b] \times \{j\}, 1/2, m_j).$$

Suppose that (L_k, M_k, ψ_k) is a sequence satisfying (H1) and (H2). By Lemmas 5.4 and 5.5 we may assume that $L_k \to \infty$ and $JL_k - |M_k| \to \infty$. We may choose a subsequence so that $JL_k - M_k = 2Jr_k - N$ for all k, where $r_k \in \mathbb{N}_{\geq 0}$ is arbitrary and $N \in [0, 2J - 1]$ is fixed. Let

$$\psi_k' = T^{-r_k} i_{[1,L_k], \mathbb{Z}} \psi_k.$$

let $\Lambda_k = [1 - r_k, L_k - r_k]$. Then we can write

$$\psi_k' = \sum_{m \in \mathcal{M}(J, N)} C_k(m) \frac{\Psi_0'(\Lambda_k \times [1, 2J], m)}{\|\Psi_0'(\Lambda_k \times [1, 2J], m)\|}.$$

Now, for each k, $\{C_k(m) : m \in \mathcal{M}(J, N)\}$ is a normalized l^2 sequence, instead of a finite dimensional vector. So we only know that a weakly convergent subsequence exists, not a strongly convergent one. We need some kind of tightness result, which is given in the following lemma.

Lemma 5.7. *Let $\mathcal{M}_R(J, N)$ be those $m \in \mathcal{M}(J, N)$ such that all components lie in the range $[-R + 1, R]$. Then we have*

$$\lim_{R \to \infty} \liminf_{k \to \infty} \sum_{m \in \mathcal{M}_R(J,N)} |C_k(m)|^2 = 1.$$

We give the proof of this technical but important lemma at the end of the section. First, we see how Proposition 5.2 follows.

Lemma 5.8. *Define $\mathcal{F}_R$ to be the projection onto those vectors with all down spins at sites (α, j) when $\alpha \leq -R$, all up spins at sites (α, j) with $\alpha \geq R + 1$, and $S_{[-R+1,R] \times [1,2J]}^3$ equal to N. We have*

$$\lim_{R \to \infty} \liminf_{k \to \infty} \|\mathcal{F}_R \psi_k'\| = 1.$$

Proof: By lemma 5.7, for any $\epsilon > 0$, we can choose R large enough that

$$\liminf_{k \to \infty} \sum_{m \in \mathcal{M}_R(J,M)} |C_k(m)|^2 > 1 - \epsilon .$$

By Lemma 3.4, the following strong limit exists

$$\Psi_0'(\mathbb{Z} \times [1, 2J], m) = \lim_{k \to \infty} \Psi_0'(\Lambda_k \times [1, 2J], m) .$$

Furthermore,

$$\lim_{R_1 \to \infty} \frac{\|\mathcal{F}_{R_1} \Psi_0'(\mathbb{Z} \times [1, 2J], m)\|}{\|\Psi_0'(\mathbb{Z} \times [1, 2J], m)\|} = 1 .$$

Thus

$$\liminf_{R_1 \to \infty} \|\mathcal{F}_{R_1} \psi_k'\|^2 > 1 - \epsilon .$$

Since ϵ was arbitrary, we are done. ∎

We know that $\widetilde{\widetilde{H}}_{\widetilde{\Lambda}_k} \psi_k' = 0$ and $\lim_k \|P_{\Lambda_k} \psi_k'\| = 1$. As before, these two facts are sufficient to guarantee that for any finite $\Lambda \subset \mathbb{Z}$,

$$\lim_{k \to \infty} \widetilde{H}_{\widetilde{\Lambda}} \psi_k' = 0 .$$

In other words, letting G_Λ be the projection onto the ground state space of $\widetilde{H}_{\widetilde{\Lambda}}$, that

$$\lim_{k \to \infty} \|G_\Lambda \psi_k'\| = 1 . \tag{5.10}$$

We note that for $\Lambda = [-R+1, R]$, the projections $\mathcal{F}_R$ and G_Λ commute, and in fact their product is the projection onto the normalized ground state vector

$$\Psi_0'([-R+1, R] \times [1, 2J], N) .$$

By Lemma 5.8 and equation (5.10) we see that

$$\lim_{R \to \infty} \liminf_{k \to \infty} |\langle \Psi_0'([-R+1, R] \times [1, 2J], N) | \psi_k' \rangle|^2 = 1 .$$

Since $\Psi_0'([-R+1, R] \times [1, 2J], N)$ converges in norm to $\Psi_0'(\mathbb{Z} \times [1, 2J], N)$ as $R \to \infty$, we have

$$\liminf_{k \to \infty} |\langle \Psi_0'(\mathbb{Z} \times [1, 2J], N) | \psi_k' \rangle|^2 = 1 . \tag{5.11}$$

Now comes the contradiction. We know, by virtue of the fact that $\psi_k' \in \widetilde{\mathcal{H}}_{0, \perp}([1, L_k] \times [1, 2J], M_k)$, that $\psi_k' \perp \Psi_0'([1, L_k] \times [1, 2J], N)$. But on the other hand, we know that $\Psi_0'([1, L_k] \times [1, 2J], N)$ converges strongly to $\Psi_0'(\mathbb{Z} \times [1, 2J], N)$, so

$$\limsup_{k \to \infty} |\langle \Psi_0'(\mathbb{Z} \times [1, 2J], N) | \psi_k' \rangle|^2 = 0 ,$$

clearly contradicting (5.11). ∎

Proof: (of Lemma 5.7) We define D_R to be the projection onto all those vectors in $\mathcal{H}(\mathbb{Z} \times [1, 2J], \text{kink})$ with at most $2J - 1$ down spins shared between the sites $(-R + 1, 1), \ldots, (-R + 1, 2J)$, and at least one down spin shared between the sites $(R, 1), \ldots, (R, 2J)$. Let

$$\widetilde{\Psi}_0(\widetilde{\Lambda}, m) = \frac{\Psi_0'(\widetilde{\Lambda}, m)}{\|\Psi_0'(\widetilde{\Lambda}, m)\|} \, .$$

Let $\Lambda_R = [-R + 1, R]$. It is clear that if

$$\psi = \sum_{m \in \mathcal{M}(J, M)} C(m) \widetilde{\Psi}_0(\widetilde{\Lambda}_R, m)$$

then

$$\langle \psi | D_R \psi \rangle = \sum_m |C(m)|^2 \|D_R \widetilde{\Psi}_0(\widetilde{\Lambda}_R, m)\|^2$$

$$\geq \sum_{m \in \mathcal{M}(J, M) \setminus \mathcal{M}_R(J, M)} |C(m)|^2 \|D_R \widetilde{\Psi}_0(\widetilde{\Lambda}_R, m)\|^2$$

$$\geq \frac{1}{2} \sum_{m \in \mathcal{M}(J, M) \setminus \mathcal{M}_R(J, M)} |C(m)|^2$$

the second line owing to the fact that D_R commutes with $S^3_{[-L+1, L] \times \{j\}}$ for each leg j and all $L \in \mathbb{N}$. The last inequality is the result from to the following consideration: if one of the m_j is greater than R or less than $-R + 1$, then with probability at least $1/2$ one finds the state with at least one down spin at R, or at least one up spin at $-R + 1$, respectively. Thus

$$\sum_{m \in \mathcal{M}_R(J, M)} |C(m)|^2 \geq 1 - 2\langle \psi | D_R \psi \rangle \, .$$

Now suppose that ψ is a ground state vector of $\widetilde{\widetilde{H}}_{\widetilde{\Lambda}_R}$. Then, because D_R commutes with $S^3_{\widetilde{\Lambda}_R}$ we have

$$\langle \psi | D_R \psi \rangle \leq \max_{M \in [-2JR, 2JR]} \langle \Psi_0(\widetilde{\Lambda}_R, M) | D_R \Psi_0(\widetilde{\Lambda}_R, M) \rangle \, .$$

We can make the following crude but simple estimate

$$\max_{M \in [-2JR, 2JR]} \|D_R \Psi_0(\widetilde{\Lambda}_R, M)\|^2 \leq \frac{4J^2 R q^{2R}}{1 - 4J^2 R q^{2R}} \, . \tag{5.12}$$

We prove this estimate for $M \leq 0$, and the $M \geq 0$ follows by spin flip/reflection symmetry. Of course if $M = -2JR$, then the estimate is trivial because Ψ_0 has all down spins, so the expectation with D_R is zero. Suppose $-2JR < M \leq 0$. Then there is at least one down spin and at most $2JR$ down spins. We write $\mathbb{M}(\widetilde{\Lambda}_R, n)$ for all the classical Ising configurations on the lattice $\widetilde{\Lambda}_R$ with exactly n down spins.

We write $\mathbb{M}(\widetilde{\Lambda}_R, n, j)$ for all the configurations with the extra constraint that the number of down spins on the sites $(R, 1), \ldots, (R, 2\mathrm{J})$ is j. The normalized ground state $\Psi_0(\widetilde{\Lambda}_R, 2\mathrm{J}R - n)$ is

$$\Psi_0(\widetilde{\Lambda}_R, 2\mathrm{J}R - n) = Z^{-1} \sum_{\{m(\alpha, j)\} \in \mathbb{M}(\widetilde{\Lambda}_R, n)} W(\{m(\alpha, j)\}) |\{m(\alpha, j)\}\rangle,$$

where

$$W(\{m(\alpha, j)\}) = \prod_{(\alpha, j)} q^{-\alpha m(\alpha, j)}$$

and

$$Z^2 = \sum_{\{m(\alpha, j)\} \in \mathbb{M}(\widetilde{\Lambda}_R, n)} W(\{m(\alpha, j)\})^2$$

On the other hand, defining $E_{R,j}$ to be the projection onto those states with exactly j down spins on the sites $(R, 1), \ldots, (R, 2\mathrm{J})$, we have

$$\|E_{R,j} \Psi_0([-R+1, R] \times [1, 2\mathrm{J}], 2\mathrm{J}R - n)\|^2 = \frac{Z_j^2}{Z^2}$$

where Z_j is the same as Z but with the sum over classical configurations restricted to $\mathbb{M}(\widetilde{\Lambda}_R, n, j)$.

The inequality comes from recognizing that $Z_{j+1}^2 \leq 4\mathrm{J}^2 R q^{2R} Z_j^2$. This is a straightforward estimate. Define a lexicographic order on $\widetilde{\Lambda}_R$ by $(\alpha_1, j_1) < (\alpha_2, j_2)$ if either $\alpha_1 < \alpha_2$ or $\alpha_1 = \alpha_2$ and $j_1 < j_2$. Define a map $f : \mathbb{M}(\widetilde{\Lambda}_R, n, j+1) \to \mathbb{M}(\widetilde{\Lambda}_R, n, j)$ where the down spin at the greatest site (α, j) with a down spin, is exchanged for the up spin at the least site (β, k) with an up spin. Note that since there are at most $2\mathrm{J}R$ down spins, the point (β, k) must lie in the subset $[-R+1, 0] \times [1, 2\mathrm{J}]$, so there are at most $2\mathrm{J}R$ choices of (β, k). Similarly, since $j + 1 \geq 1$, we know there is at least one down spin in the sites $(R, 1), \ldots, (R, 2\mathrm{J})$. So there are at most $2\mathrm{J}$ choices for $(\alpha, j) = (R, j)$. Thus, $\#f^{-1}(\{m(\alpha, j)\}) \leq 4\mathrm{J}^2 R$ for any configuration $\{m(\alpha, j)\}$. We see that

$$W(f(\{m(x, j)\})) \geq q^{-R} W(\{m(x, j)\})$$

because the down spin at site $(\alpha, j) = (R, j)$ has moved at least R units to the left to (β, k), $\beta \leq 0$. So

$$\begin{aligned}
Z_{j+1}^2 &= \sum_{\{m(\alpha, j)\} \in \mathbb{M}(\widetilde{\Lambda}_R, n, j+1)} W(\{m(\alpha, j)\})^2 \\
&\leq q^{2R} \sum_{\{m(\alpha, j)\} \in \mathbb{M}(\widetilde{\Lambda}_R, n, j+1)} W(f(\{m(\alpha, j)\}))^2 \\
&\leq 4\mathrm{J}^2 R q^{2R} \sum_{\{m(\alpha, j)\} \in \mathbb{M}(\widetilde{\Lambda}_R, n, j)} W(\{m(\alpha, j)\})^2 \\
&= 4\mathrm{J}^2 R q^{2R} Z_j^2 \, .
\end{aligned}$$

The crude estimate is proved.

Now we know that as $k \to \infty$, the vectors ψ_k come closer and closer to the ground state space of $\widetilde{H}_{\widetilde{\Lambda}_R}$. So our estimate implies

$$\liminf_{k \to \infty} \sum_{m \in \mathcal{M}_R(\mathrm{J},M)} |C_k(m)|^2 \geq 1 - \frac{8\mathrm{J}^2 R q^{2R}}{1 - 4\mathrm{J}^2 R q^{2R}}.$$

Hence

$$\lim_{R \to \infty} \liminf_{k \to \infty} \sum_{m \in \mathcal{M}_R(\mathrm{J},M)} |C_k(m)|^2 \geq 1 - \lim_{R \to \infty} \frac{8\mathrm{J}^2 R q^{2R}}{1 - 4\mathrm{J}^2 R q^{2R}} = 1,$$

and this concludes the proof.   ∎

6   Numerical Approximation

We now find an explicit representation of

$$\mathrm{Proj}(\mathcal{H}_0(\widetilde{\Lambda}, M)) P_\Lambda \mathrm{Proj}(\mathcal{H}_0(\widetilde{\Lambda}, M)).$$

From this we numerically calculate $1 - \delta(L, \mathrm{J}, M)$. We begin with some definitions. First of all, we will always have $\Lambda = [1, L]$ in this section, and hence $\widetilde{\Lambda} = [1, L] \times [1, 2\mathrm{J}]$. For $N \in [0, 2\mathrm{J}L]$, define

$$\widetilde{P}(\widetilde{\Lambda}, N) = \mathrm{Proj}(\mathcal{H}_0(\widetilde{\Lambda}, \mathrm{J}L - N)) P_\Lambda \mathrm{Proj}(\mathcal{H}_0(\widetilde{\Lambda}, \mathrm{J}L - N)).$$

Also, define the "classical Ising configurations" to be

$$\mathbb{M}(L, 2\mathrm{J}, N) = \{A \in [0, 1]^{\widetilde{\Lambda}} : \sum_{(x,j) \in \widetilde{\Lambda}} A(x, j) = N\}.$$

These are $\{0, 1\}$-matrices with $2\mathrm{J}$ rows, L columns, and N ones. For any $A \in \mathbb{M}(L, 2\mathrm{J}, N)$ we define

$$\phi_A = \prod_{(x,j) \in \widetilde{\Lambda}} (S^-_{(x,j)})^{A(x,j)} \, \Omega$$

where $\Omega = \bigotimes_{(x,j) \in \widetilde{\Lambda}} |1/2\rangle_{(x,j)}$. Then it is clear that $\mathcal{H}(\widetilde{\Lambda}, \mathrm{J}L - N)$ has an orthonormal basis $\{\phi_A : A \in \mathbb{M}(L, 2\mathrm{J}, N)\}$. For any matrix A, we define two vectors $\boldsymbol{r}_A \in \mathbb{C}^{2\mathrm{J}}$ and $\boldsymbol{c}_A \in \mathbb{C}^L$ by

$$r_A(j) = \sum_{x=1}^{L} A(x, j), \qquad c_A(x) = \sum_{j=1}^{2\mathrm{J}} A(x, j).$$

Finally we define

$$M_{r,c} = \#\{A \in \mathbb{M}(L, 2\mathrm{J}, N) : \boldsymbol{r}_A = \boldsymbol{r}, \ \boldsymbol{c}_A = \boldsymbol{c}\}. \qquad (6.13)$$

Note that by its definition $M_{r,c}$ is unchanged if one permutes the components of $\boldsymbol{r}$ or $\boldsymbol{c}$. We mention that there is no known formula for $M_{r,c}$ although it has useful characterizations in terms of generating functions. (C.f. [27] §7.4 for more details.)

The definitions immediately lead to the following result.

Lemma 6.1. *The following are true identities:*

$$\Psi_0\left(\Lambda, J, \frac{1}{2}Le - n\right) = \sum_{\substack{A \in \mathbb{M}(L, 2J, N) \\ r_A = n}} \phi_A q^{x \cdot c_A} \tag{6.14}$$

$$\left\|\Psi_0\left(\Lambda, J, \frac{1}{2}Le - n\right)\right\|^2 = \sum_{\substack{c \in [0, 2J]^L \\ \sum_x c(x) = N}} q^{2x \cdot c} M_{n, c} \tag{6.15}$$

$$P_\Lambda \phi_A = \prod_{x=1}^L \binom{2J}{c_A(x)} \sum_{\substack{B \in \mathbb{M}(L, 2J, N) \\ c_B = c_A}} \phi_B \tag{6.16}$$

$$\left\langle \Psi_0\left(\Lambda, J, \frac{1}{2}Le - m\right) \middle| P_\Lambda \Psi_0\left(\Lambda, J, \frac{1}{2}Le - n\right) \right\rangle$$

$$= \sum_{\substack{c \in [0, 2J]^L \\ \sum_x c(x) = N}} M_{m, c} M_{n, c} q^{2x \cdot c} \prod_{x=1}^L \binom{2J}{c(x)} \tag{6.17}$$

∎

We can define an action of $\mathfrak{S}_{2J}$ on $\mathcal{H}_0(\widetilde{\Lambda}, JL - N)$ by $U(\pi) \cdot \phi_A = \phi_{\pi A}$, where $\pi A(x, j) = A(x, \pi^{-1}(j))$. By (6.17), we know that the range of $\widetilde{P}(\widetilde{\Lambda}, N)$ is a trivial representation of $\mathfrak{S}_{2J}$. We define $\mathbb{P}_0(L, 2J, N)$ to be the set of all sequences $\mu = (\mu_1, \ldots, \mu_{2J})$ such that

$$L \geq \mu_1 \geq \mu_2 \geq \cdots \geq \mu_{2J} \geq 0$$

and $\mu_1 + \cdots + \mu_{2J} = N$. These are restricted partitions, but allowing parts equal to zero. (We mention this fact for consistency. The interested reader can consult [2], [11], or [27] for more information about partitions.) Then the range of $\widetilde{P}(\widetilde{\Lambda}, N)$ is spanned by the linearly independent vectors

$$\psi_\mu = \frac{1}{(2J)!} \sum_{\pi \in \mathfrak{S}_{2J}} U(\pi) \Psi(\widetilde{\Lambda}, JL - \mu), \qquad \mu \in \mathbb{P}_0(L, 2J, N).$$

We note that we can define an action of $\mathfrak{S}_{2J}$ on $\mathbb{Z}^{2J}$ in the obvious way, with the outcome that

$$\Psi(\widetilde{\Lambda}, JL - \pi n) = U(\pi) \Psi(\widetilde{\Lambda}, JL - n).$$

The orthogonal basis $\{\psi_\mu : \mu \in \mathbb{P}_0(L, 2J, N)\}$ is not yet orthonormal. We observe that

$$\|\psi_\mu\|^2 = ((2J)!)^{-2} \|\Psi(\widetilde{\Lambda}, JL - \mu)\|^2$$
$$\times \#(\text{orbit of } \mu) \times \#(\text{stabilizer of } \mu)^2.$$

Since $\#(\text{stabilizer}) \times \#(\text{orbit}) = \#\mathfrak{S}_{2J} = (2J)!$, we have

$$
\begin{aligned}
\|\psi_\mu\|^2 &= \#(\text{orbit of } \mu)^{-1}\|\Psi(\widetilde{\Lambda}, JL - \mu)\|^2 \\
&= \binom{2J}{n_0(\mu), n_1(\mu), n_2(\mu), \ldots, n_L(\mu)}^{-1} \sum_{\substack{c \in [0,2J]^L \\ \sum_x c(x) = N}} q^{2x \cdot c} M_{n,c}
\end{aligned}
\tag{6.18}
$$

where $n_k(\mu)$ is the number of parts of μ equal to k.

By (6.17), and the fact that the inner product is invariant under permutations of m and n, we obtain

$$
\langle \psi_\mu | P_\Lambda \psi_\nu \rangle = \sum_{\substack{c \in [0,2J]^L \\ \sum_x c(x) = N}} M_{m,c} M_{n,c} q^{2x \cdot c} \prod_{x=1}^{L} \binom{2J}{c(x)}.
$$

for all $\mu, \nu \in \mathbb{P}_0(L, 2J, N)$. Therefore $\widetilde{P}(\widetilde{\Lambda}, N)$ is represented, on its range, by a matrix $\mathcal{P} = (\mathcal{P}(\mu, \nu) : \mu, \nu \in \mathbb{P}_0(L, 2J, N))$, where

$$
\begin{aligned}
\mathcal{P}(\mu, \nu) &= \binom{2J}{n_0(\mu), \ldots, n_L(\mu)}^{1/2} \binom{2J}{n_0(\nu), \ldots, n_L(\nu)}^{1/2} \\
&\quad \times \left(\sum_{\substack{c \in [0,2J]^L \\ \sum_x c(x) = N}} M_{m,c} M_{n,c} q^{2x \cdot c} \prod_{x=1}^{L} \binom{2J}{c(x)} \right) \\
&\quad \Big/ \left(\sum_{\substack{c \in [0,2J]^L \\ \sum_x c(x) = N}} q^{2x \cdot c} M_{n,c} \right).
\end{aligned}
\tag{6.19}
$$

This is quite a complicated looking formula. There are two nice features about it. First, the powers of q grow quite rapidly. Second, the matrix $(M_{\mu,\nu'} : \mu, \nu \in \mathbb{P}_0(L, 2J, N))$ is upper triangular with respect to dominance order, where ν' is the transpose of the partition ν. (Dominance order is the natural partial order on partitions.) These two facts insure that the matrix components of $\mathcal{P}$ decay exponentially with the distance from the diagonal. (More details and an equivalent expression are found in [28].)

We have not attempted a rigorous analysis of $\mathcal{P}$, but we have obtained very convincing numerical data, by simply numerically diagonalizing the matrix. The main qualitative feature of the lower bound for the spectral gap is that it is not always maximized at the Ising limit. In particular, if $J > 3/2$ and the number of down spins N satisfies $N = 2J \lfloor |\Lambda|/2 \rfloor$, then the local maximum for the lower bound of the spectral gap occurs somewhere other than the Ising limit. The Ising limit is a classical model, whose energy levels can be calculated explicitly, and doing so it is easy to see that the lower bound for the spectral gap is actually equal to the true spectral gap at the Ising limit. So the true spectral gap of the XXZ spin chain with

$J > 3/2$ has a local maximum somewhere other than the Ising limit in finite volumes as long as the number of down spins satisfies $N \approx J|\Lambda|$ and $N \equiv 0(\mathrm{mod}\ 2J)$. One can take $N \approx J|\Lambda|$ and $N \equiv 0(\mathrm{mod}\ 2J)$ because of the approximate periodicity of the spectral gap in N. This same result is also obtained by Ising perturbation series, where we show that the curve for the spectral gap is concave up at the Ising limit. Also, the asymptotic analysis of Section 7 verifies the qualitative picture of the spectral gap when $J \gg 1$.

We now give an alternative description of $\mathcal{P}$ in terms of representations. Recall that the ground state space of the spin 1/2 XXZ model is the highest dimensional irreducible representation of $SU_q(2)$. On the other hand, the symmetric tensors form the highest dimensional irreducible representation of $SU(2)$. Consider the array $\widetilde{\Lambda} = [1, L] \times [1, 2J]$. At each site put a two dimensional representation of $SU(2)$ and $SU_q(2)$. Note that this is possible because the two dimensional representations of $SU(2)$ and $SU_q(2)$ coincide. Now tensor all the representations in a single row, considering them as representations of $SU_q(2)$. For each row, define an operator $R_j(q)$ which projects onto the highest dimensional irreducible representation of $SU_q(2)$. Next tensor all the representations in a single column, considering them as representations of $SU(2)$. Define C_x to project onto the highest dimensional irreducible representation. Then the operator $\sum_N \widetilde{P}(\widetilde{\Lambda}, N)$ is identical to $\prod_{x=1}^{L} C_x \prod_{j=1}^{2J} R_j(q)$, modulo null spaces. If one turns the procedure around, first projecting on columns then on rows, one almost (but not quite) recovers the original problem of the spin J XXZ chain.

6.1   Perturbation Series about Ising Limit

We now perform a perturbation analysis for $\gamma([1, L], J, M, \Delta^{-1})$ about the point $\Delta^{-1} = 0$, i.e. the Ising limit. We write

$$H(\Delta^{-1}) = H^{(0)} + \Delta^{-1} H^{(1)}$$

$$H^{(0)} = \sum_{x=1}^{L-1} (J + S_x^3)(J - S_{x+1}^3)$$

$$H^{(1)} = \sum_{x=1}^{L-1} \left(-\frac{1}{2} S_x^+ S_{x+1}^- - \frac{1}{2} S_x^- S_{x+1}^+ \right).$$

We have left out of $H^{(1)}$ the first order corrections to the boundary terms. However since all our vectors are local perturbations of an Ising kink, the first order corrections to the boundary terms will act as a multiple of the identity. We will include these trivial corrections after we perform the perturbation theory with $H^{(1)}$ as above. We note that $H(\Delta^{-1})$ is unitarily equivalent to $H(-\Delta^{-1})$, where the unitary transformation is

$$U = \exp \left(2\pi i \sum_{j=1}^{\lceil L/2 \rceil} S_{2j-1}^3 \right).$$

This proves that the point $\Delta^{-1} = 0$ is always either a local maximum or a local minimum of $\gamma([1, L], \mathrm{J}, M, \Delta^{-1})$. If $\gamma([1, L], \mathrm{J}, M, \Delta^{-1})$ is differentiable near $\Delta^{-1} = 0$, the first derivative is zero, and we proceed to second order perturbation theory. The reason $\gamma([1, L], \mathrm{J}, M, \Delta^{-1})$ may not be differentiable near $\Delta^{-1} = 0$ is that the first excited state may be infinitely degenerate in the Ising limit. This is the case for spin $1/2$ and for $\mathrm{J} = 1$ when M is odd. For $\mathrm{J} = 1/2$ and any $x \in \mathbb{Z}$ there is an Ising ground state

$$\Psi_0(x) = \left(\bigotimes_{y \leq x} |-1/2\rangle_y \right) \otimes \left(\bigotimes_{y \geq x+1} |1/2\rangle_y \right) .$$

It is easy to see that there are infinite families of first excitations, for example $\prod_{j=1}^{L} S_{x+1-j}^+ S_{y+j-1}^- \Psi_0(x)$ for any $L \geq 1$ and $y \geq x+2-L$. For $\mathrm{J} = 1$ and M odd, the ground state is

$$\Psi_0(x) = \left(\bigotimes_{y < x} |-1\rangle_y \right) \otimes |0\rangle_x \otimes \left(\bigotimes_{y > x} |1\rangle_y \right) ,$$

and there are two classes of excitations, each infinitely degenerate: $S_y^+ S_x^- \Psi_0(x)$ for any $y < x$; and $S_x^+ S_y^- \Psi_0(x)$ for any $y > x$. These are the only cases where the first excitations are infinitely degenerate. The only cases where there is a finite degeneracy for the first excited state are $\mathrm{J} = 2, 3, 4, \ldots$ and M congruent to J modulo $2\mathrm{J}$. Then the ground state is

$$\Psi_0(x) = \left(\bigotimes_{y < x} |-\mathrm{J}\rangle_y \right) \otimes |0\rangle_x \otimes \left(\bigotimes_{y > x} |\mathrm{J}\rangle_y \right) ,$$

and the two first excitations are $S_{x-1}^+ S_x^- \Psi_0(x)$ and $S_x^+ S_{x+1}^- \Psi_0(x)$. The other most interesting case, which has unique first excitations are $\mathrm{J} \geq 1$ and M divisible by $2\mathrm{J}$. Then

$$\Psi_0(x) = \left(\bigotimes_{y \leq x} |-\mathrm{J}\rangle_y \right) \otimes \left(\bigotimes_{y > x} |\mathrm{J}\rangle_y \right) ,$$

and the unique first excitation is $S_x^+ S_{x+1}^- \Psi_0(x)$. There are ground states with infinitely degenerate second excitations, and so on, but this does not interest us.

We now consider the results of second order perturbation theory, assuming the first order excitation is non-degenerate. The kink ground states of the Ising model are all of the form

$$\Psi_0(x, n) = \left(\bigotimes_{y < x} |-\mathrm{J}\rangle_y \right) \otimes |-\mathrm{J}+n\rangle_x \left(\bigotimes_{y > x} |\mathrm{J}\rangle_y \right) ,$$

where one can assume that $0 \leq n \leq \lfloor \mathrm{J} \rfloor$. The first excited state is then

$$\Psi_1(x, n) = \left(\bigotimes_{y < x} |-\mathrm{J}\rangle_y \right) \otimes |-\mathrm{J}+n+1\rangle_x \otimes |\mathrm{J}-1\rangle_{x+1} \left(\bigotimes_{y > x+1} |\mathrm{J}\rangle_y \right) ,$$

	$n = 0$	1	2	3
$J = 1/2$	$-\infty$			
1	$-1/3$	$-\infty$		
3/2	11/12	$-9/4$		
2	7/3	$-1/4$	$-46/5$	
5/2	97/24	4/3	$-39/20$	
3	91/15	3	0	$-26/3$

Table 1: Some values of the curvature of the gap in the Ising limit. For $J = 1/2$, $n = 0$, and $J = 1$, $n = 1$, the excited state is infinitely degenerate, and the curvature is infinite as well.

which has energy $E^{(0)} = n + 1$. We now expand to determine the corrections for small but nonzero Δ^{-1}. In particular we write $E(\Delta^{-1}) = E^{(0)} + \Delta^{-1} E^{(1)} + \ldots$. The perturbation series is standard, so we omit details. The results are that $E^{(1)} = 0$ and

$$E^{(2)} = -\frac{1}{2} \left(2J(J-1) + n - \frac{2(J+1)(2J-1)}{n+3} + \frac{4J^2}{2J - n - 1} \right) .$$

This is not an accurate description of the kink Hamiltonian because we have not included the correct boundary fields. To fix this situation we must add $J(\sqrt{1 - \Delta^{-2}} - 1)(S_1^3 - S_L^3)$. It is obvious that for a long enough spin chain, and excitations which are localized at the interface, the extra boundary fields act just as $-2J^2(\sqrt{1 - \Delta^{-2}} - 1)$ times the identity. Note that this is $\Delta^{-2} J^2 + o(\Delta^{-2})$. So for $0 \le M < J$,

$$\left. \frac{d^2}{d(\Delta^{-1})^2} \right|_{\Delta^{-1}=0} \gamma([1, L], J, M, \Delta^{-1})$$
$$= J - \frac{M}{2} + \frac{(J+1)(2J-1)}{M+3} - \frac{2J^2}{2J - M - 1} . \tag{6.20}$$

The finitely degenerate case is $J \in \mathbb{Z}$ and $M \equiv J \mod (2J)$, as mentioned before. Then the first excitation of the Ising ground state is doubly degenerate, and we perform degenerate perturbation theory. As soon as $\Delta^{-1} > 0$, the degeneracy lifts and there are two branches. It is easily verified that the curvature of both branches is negative, but we are only concerned with the lowest branch which gives

$$\left. \frac{d^2}{d(\Delta^{-1})^2} \right|_{\Delta^{-1}=0} \gamma([1, L], J, J, \Delta^{-1}) = -8 - \frac{3}{J-1} - \frac{J}{2} + \frac{14}{J+3} . \tag{6.21}$$

We list some values for the curvature of γ in Table 6.1. In the Ising limit, the minimum gap occurs for $n = 0$. One can see from this table that for $M = 0$ and $J > 1$, the gap is concave up at $\Delta^{-1} = 0$. This is the basis for Conjecture 2.4.

7 Boson Model

We now give a heuristic derivation of the free Bose gas model for the XXZ spin system in the limit $J \to \infty$. This is an approximation to the full XXZ Hamiltonian

H_Λ^J on a finite chain $\Lambda = [1, L]$. Our approach is similar to that of [13], although we would suggest to the reader to look at [9, 10] and [8] instead. We are interested in the classical limit, $J \to \infty$. Lieb, [19], proved that for the Heisenberg model one obtains the classical partition function as a scaled limit of quantum partition functions. Lieb's method used coherent states to obtain rigorous upper and lower bounds on the partition function. In [8], the same result was derived without coherent states, and then it was shown that with a sufficiently large external magnetic field the large J limit of the XXX model can be viewed as a free Bose gas, which verified predictions of Dyson in [9, 10]. A more recent proof of the Bose gas limit has been obtained by Michoel and Verbeure [23], where the spin J operator is viewed as a sum of 2J spin 1/2 operators, (using a spin ladder), and then a noncommutative central limit theorem is applied.

The physical requirement of a large external field to obtain the Bose gas limit in the isotropic case is easy to understand. All the approximations (including our own) rely on a spin wave description of the elementary excitations. In order for this to be valid, the ground state must be very nearly saturated, i.e. the ground state should satisfy $|\langle S_\alpha^3 \rangle| - J \ll J$. To accomplish this for the isotropic Heisenberg model, one must place a rather large external magnetic field. This is an important difference between the isotropic and anisotropic ferromagnets. The XXZ model with $\Delta > 1$ possesses kink ground states, which the isotropic model does not. For the kink ground states, there is a quantum interface separating two regions, which we can assume to be located at $\alpha = 1/2$. For sites $\alpha \leq 0$ one has $\langle S_\alpha^3 \rangle \leq -J + Cq^{-\alpha}$ and for $\alpha \geq 1$, $\langle S_\alpha^3 \rangle \geq +J - Cq^\alpha$. Thus the spin is saturated well away from the interface, with exponentially small corrections. The XXZ model exhibits saturation with just a boundary field, and the boundary field vanishes in the thermodynamic limit. Moreover the boundary field is known to give the correct ground states (cf [16]). So the boson picture is quite natural for the XXZ model.

The energy–momentum dispersion relation is different for the XXZ model than for the isotropic model, as one would expect. The most important difference is that the lowest energy spin wave is not actually localized in momentum space, but in position space. It is localized at the interface, instead of being spread out uniformly over a large region. (There is one other spin wave with lower energy, in fact zero energy. But this is the spin wave which simply moves one ground state to the other, owing to the fact that all ground states in all sectors of total S^3 have equal energy. We remove this boson by restricting to a single sector.) Moreover, there is a spectral gap between the lowest spin wave, and the others. The next independent spin wave boson does have a well-defined momentum, and from there on the usual picture of spin waves prevails. These are the results for one dimension, but the Bose gas model also holds for excitations of the $(1, \ldots, 1)$ interface ground states in dimensions $d \geq 2$. In dimensions higher than one, the low lying spectrum is more complex, having a continuous band of interface excitations at the bottom, as proved in [5, 4]. An interesting recent result by Caputo and Martinelli [6] gives a rigorous lower bound for the spectral gap in a large but finite system Λ, whose power law is $|\Lambda|^{-2/d}$ in agreement with [5]. This gives strong evidence that the only excitations beneath a certain energy are interface excitations. The Bose gas approximation implies more, that for large J the interface excitations are separated from all other

spin wave excitations by a spectral gap of order J. The $d \geq 2$ results will be elucidated in a forthcoming paper [24], as will be the rigorous proof of the spin wave Boson model for the XXZ model. For now we provide a heuristic argument.

We begin by considering the simplest case, namely $\Lambda = [1, 2]$. It is convenient to work in the dual space to $\mathcal{H}(\Lambda, J)$. Namely, for $\psi : [-J, J] \times [-J, J] \to \mathbb{C}$, define

$$|\psi\rangle = \sum_{m_1, m_2 \in [-J, J]} \psi(m_1, m_2)|m_1, m_2\rangle .$$

Then $H_\Lambda^J |\psi\rangle = |G_J \psi\rangle$ where G_J is an operator on $\mathbb{C}^{[-J, J]^2}$

$$G_J \psi(m_1, m_2) = (J^2 - m_1 m_2 + A(\Delta)J(m_1 - m_2))\psi(m_1, m_2)$$
$$- \frac{1}{2\Delta}[J(J+1) - m_1(m_1 + 1)]^{1/2}$$
$$[J(J+1) - m_2(m_2 - 1)]^{1/2}\psi(m_1 + 1, m_2 - 1)$$
$$- \frac{1}{2\Delta}[J(J+1) - m_1(m_1 - 1)]^{1/2}$$
$$[J(J+1) - m_2(m_2 + 1)]^{1/2}\psi(m_1 - 1, m_2 + 1)$$

where $A(\Delta) = \sqrt{1 - \Delta^{-2}}$, and we define $\psi(m_1, m_2) = 0$ for any (m_1, m_2) not in $[-J, J] \times [-J, J]$. All we have done is to explicitly write down the action of the spin matrices. Next, for any real numbers $-1 < \mu_i < 1$, $i = 1, 2$, let us define a linear operator $T_{\mu_1, \mu_2, J} : \mathcal{C}^\infty(\mathbb{R}^2) \to \mathbb{C}^{[-J, J]^2}$, where $T_{\mu_1, \mu_2, J} \Psi = \psi$,

$$\psi(m_1, m_2) = \Psi(J^{-1/2}(m_1 - \mu_1 J), J^{-1/2}(m_2 - \mu_2 J)) .$$

This operator has a very large null space. But if for fixed μ_1, μ_2 one knows that $T_{\mu_1, \mu_2, J} \Psi = 0$ for every J, then Ψ must obviously also be zero.

There are many choices of operators $\mathcal{H}_J$ on $\mathcal{C}^\infty(\mathbb{R}^2)$ which satisfy $G_J T_{\mu_1, \mu_2, J} = T_{\mu_1, \mu_2, J} \mathcal{H}_J$. One particularly good choice is the following

$$\mathcal{H}_J \Psi(x_1, x_2) = J^2 \left(1 - (\mu_1 + x_1 J^{-1/2})(\mu_2 + x_2 J^{-1/2}) \right.$$
$$\left. + A(\Delta) \left((\mu_1 - \mu_2) + (x_1 - x_2)J^{-1/2} \right) \right) \Psi(x_1, x_2)$$
$$- \frac{1}{2\Delta} \sum_{\varepsilon = \pm 1} \left(\prod_{i=1,2} \left[J(J+1) - (\mu_i J + x_i J^{1/2})(\mu_i J + x_i J^{1/2} + (-1)^{i+1}\varepsilon) \right]^{1/2} \right. \quad (7.22)$$
$$\left. \Psi \left(x_1 + \varepsilon J^{-1/2}, x_2 - \varepsilon J^{-1/2} \right) \right),$$

which is the same as the definition of G_J, but now allowing the operator to act on smooth functions instead of discrete functions. One can formally expand

$$\mathcal{H}_J = J^2 \mathcal{H}^{(2)} + J^{3/2} \mathcal{H}^{(3/2)} + J \mathcal{H}^{(1)} + \ldots$$

considering the shift by $\pm J^{-1/2}$ as $e^{\pm J^{-1/2}\partial}$, and expanding in the small parameter

$J^{-1/2}$. The resulting expressions for $\mathcal{H}^{(2)}$, $\mathcal{H}^{(3/2)}$ and $\mathcal{H}^{(1)}$ are as follows

$$\mathcal{H}^{(2)} = 1 - \mu_1\mu_2 + A(\Delta)(\mu_1 - \mu_2) - \Delta^{-1}[1 - \mu_1^2]^{1/2}[1 - \mu_2^2]^{1/2} , \qquad (7.23)$$

$$\mathcal{H}^{(3/2)} = A(\Delta)(x_1 - x_2) - \mu_1 x_2 - \mu_2 x_1$$
$$+ \Delta^{-1} \left(\frac{\sqrt{1 - \mu_2^2}}{\sqrt{1 - \mu_1^2}} \mu_1 x_1 + \frac{\sqrt{1 - \mu_1^2}}{\sqrt{1 - \mu_2^2}} \mu_2 x_2 \right) , \qquad (7.24)$$

$$\mathcal{H}^{(1)} = -x_1 x_2 - \frac{1}{2\Delta}[1 - \mu_1^2]^{1/2}[1 - \mu_2^2]^{1/2}$$
$$\left((\partial_{x_1} - \partial_{x_2})^2 - \frac{x_1^2}{(1 - \mu_1^2)^2} - \frac{x_2^2}{(1 - \mu_2^2)^2} + \frac{2\mu_1\mu_2 x_1 x_2}{(1 - \mu_1^2)(1 - \mu_2^2)} \right.$$
$$\left. + \frac{1}{1 - \mu_1^2} + \frac{1}{1 - \mu_2^2} \right) \qquad (7.25)$$

Let us now use the parameter $\eta = \log(1/q)$, which is related to Δ by

$$\Delta^{-1} = \operatorname{sech}(\eta) , \qquad A(\Delta) = \tanh(\eta) .$$

Then (7.23) shows that $\mathcal{H}^{(2)}$ is a multiplication operator, multiplying by the non-negative constant

$$\operatorname{sech}(\eta) \left(e^{\eta/2}\sqrt{(1 + \mu_1)(1 - \mu_2)} - e^{-\eta/2}\sqrt{(1 + \mu_2)(1 - \mu_1)} \right)^2 .$$

Therefore, $\mathcal{H}^{(2)}\Psi = 0$ iff

$$\exists r \in \mathbb{R} \text{ s.t. } \forall \alpha \in \Lambda , \; \mu_\alpha = \tanh(\eta(\alpha - r)) . \qquad (7.26)$$

The number r is determined by $\mu_1 + \mu_2$, implicitly. Note that $\mathcal{H}^{(3/2)}$ is also a multiplication operator, but given (7.26) we know that it vanishes identically, as well. So the first non-vanishing term is $\mathcal{H}^{(1)}$. We use (7.26) to rewrite (7.25)

$$\mathcal{H}^{(1)} = \frac{1}{2\Delta} \operatorname{sech}(\eta(1 - r)) \operatorname{sech}(\eta(2 - r))$$
$$\times \left(-\partial_{x_1}^2 + \cosh^4(\eta(1 - r))x_1^2 - \partial_{x_2}^2 + \cosh^4(\eta(2 - r))x_2^2 \right.$$
$$+ 2\partial_{x_1}\partial_{x_2} - 2\cosh^2(\eta(1 - r))\cosh^2(\eta(2 - r))x_1 x_2 \qquad (7.27)$$
$$\left. - \left[\cosh^2(\eta(1 - r)) + \cosh^2(\eta(2 - r))\right] \right) .$$

Now we notice the following: $\mathcal{H}^{(1)}$ is a second order differential operator which is homogeneous in ∂_{x_1}, ∂_{x_2}, x_1 and x_2 except for a constant (the zero point energy). Therefore, $\mathcal{H}^{(1)}$ can be regarded as the Hamiltonian for a two-mode Boson system with quadratic interaction. Thus, for $\alpha = 1, 2$, we define

$$\hat{a}_\alpha = \frac{1}{\sqrt{2}} \left(\cosh(\eta(\alpha - r))x_\alpha + \operatorname{sech}(\eta(\alpha - r))\partial_{x_\alpha} \right) ,$$
$$\hat{a}_\alpha^\dagger = \frac{1}{\sqrt{2}} \left(\cosh(\eta(\alpha - r))x_\alpha - \operatorname{sech}(\eta(\alpha - r))\partial_{x_\alpha} \right) , \qquad (7.28)$$

which satisfy the Canonical Commutation Relations

$$[\hat{a}_\alpha, \hat{a}_\beta] = [\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger] = 0, \qquad [\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha,\beta}, \qquad (7.29)$$

and also

$$\hat{a}_\alpha^\dagger \hat{a}_\alpha = \frac{1}{2} \left(\cosh^2(\eta(\alpha - r)) x_\alpha^2 - \operatorname{sech}^2(\eta(\alpha - r)) \partial_{x_\alpha}^2 - 1 \right). \qquad (7.30)$$

One sees that

$$\hat{a}_n + \hat{a}_n^\dagger = \sqrt{2} \cosh(\eta(n - r)) x_n$$

and

$$\hat{a}_n - \hat{a}_n^\dagger = \sqrt{2} \operatorname{sech}(\eta(n - r)) \partial_{x_n} \quad .$$

These relations imply

$$2 \cosh(\eta(1 - r)) \cosh(\eta(2 - r)) x_1 x_2 = (\hat{a}_1 + \hat{a}_1^\dagger)(\hat{a}_2 + \hat{a}_2^\dagger)$$

and

$$2 \operatorname{sech}(\eta(1 - r)) \operatorname{sech}(\eta(2 - r)) \partial_{x_1} \partial_{x_2} = (\hat{a}_1 - \hat{a}_1^\dagger)(\hat{a}_2 - \hat{a}_2^\dagger),$$

respectively. Hence

$$\begin{aligned} 2\partial_{x_1} \partial_{x_2} &- 2 \cosh^2(\eta(1 - r)) \cosh^2(\eta(2 - r)) x_1 x_2 \\ &= -2 \cosh(\eta(1 - r)) \cosh(\eta(2 - r))(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1). \end{aligned} \qquad (7.31)$$

All of these algebraic manipulations allow us to rewrite (7.27) as

$$\mathcal{H}^{(1)} = \frac{1}{\Delta} \left[\frac{\cosh(\eta(1 - r))}{\cosh(\eta(2 - r))} \hat{a}_1^\dagger \hat{a}_1 + \frac{\cosh(\eta(2 - r))}{\cosh(\eta(1 - r))} \hat{a}_2^\dagger \hat{a}_2 - \hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1 \right]. \qquad (7.32)$$

One can verify that one of the two eigenmodes of this system has zero energy, while the other is positive. The zero mode is a direct consequence of the infinitely many ground states, corresponding to different values of M, the third component of the total spin. If one considers the canonical picture, restricting the total magnetization to have a fixed quantity, then that boson disappears.

The above results extend directly to a chain of arbitrary length. One has $\mu_1, \ldots, \mu_L$ satisfying (7.26). This is required for $\mathcal{H}^{(2)}$ to vanish, and sufficient for $\mathcal{H}^{(3/2)}$ to vanish. The definition of the single site Bosons is just as in (7.28), for each $\alpha \in \Lambda = [1, L]$, and the definition of $\mathcal{H}^{(1)}$ becomes

$$\mathcal{H}_\Lambda^{(1)} = \sum_{\alpha, \beta \in \Lambda} \mathcal{J}_{\alpha, \beta} \hat{a}_\alpha^\dagger \hat{a}_\beta, \qquad (7.33)$$

where $\mathcal{J}_{\alpha,\beta} = 0$ if $|\alpha - \beta| > 1$, $\mathcal{J}_{\alpha,\beta} = -\Delta^{-1}$ if $|\alpha - \beta| = 1$, and

$$\mathcal{J}_{1,1} = \Delta^{-1} \frac{\cosh(\eta(1 - r))}{\cosh(\eta(2 - r))}$$

$$\mathcal{J}_{L,L} = \Delta^{-1} \frac{\cosh(\eta(L - r))}{\cosh(\eta(L - 1 - r))}$$

$$\mathcal{J}_{\alpha,\alpha} = \Delta^{-1} \Big(\frac{\cosh(\eta(\alpha - r))}{\cosh(\eta(\alpha + 1 - r))}$$

$$+ \frac{\cosh(\eta(\alpha - r))}{\cosh(\eta(\alpha - 1 - r))} \Big), \qquad \text{for } 1 < \alpha < L.$$

The single site Bosons are coupled, but the coupling matrix can be diagonalized. We obtain new Bose operators $\hat{b}_n$, in terms of which the Hamiltonian is diagonal quadratic:

$$\mathcal{H}^{(1)} = \sum_{n=0}^{L-1} \lambda_n \hat{b}_n^\dagger \hat{b}_n \, ,$$

where $\hat{b}_n = \sum_\alpha v_\alpha^{(n)} \hat{a}_\alpha$ with $v^{(n)}$ the eigenvector of $\mathcal{J}$ corresponding to the eigenvalue λ_n. Again there is one zero-mode, $\lambda_0 = 0$, and $\lambda_i > 0$, for $1 \le i \ge L-1$. λ_1 remains isolated in the limit $L \to \infty$, for $0 < q < 1$.

By considering only the leading order terms for the bottom of the spectrum, we have exchanged a quantum many body Hamiltonian H_Λ^J to an L body Hamiltonian $\mathcal{J}$. For sufficiently high spin this drastic simplification describes the physics at low energies very well.

In Figure 5 we compare our predictions to the spectrum of H_Λ as obtained through numerical diagonalization. The comparison is good, particularly along the first excited state and near the isotropic limit. The reason that the Ising limit compares poorly is that the quantum fluctuations have the effect of regularizing the eigenstates ψ, whereas for the Ising model these states are definitely not smooth. However, for any $q > 0$, if J is made large enough, then we believe that these asymptotics eventually dominate. In Figure 6, we have plotted the spectrum of $\mathcal{J}$ for fifty sites and $r = 0$, which corresponds to the magnetization for which one has a minimal gap. It is clear that there is only a single isolated eigenvalue beneath the branch of (what would in infinite volumes be) continuous spectrum. Of course, to recover the spectrum of $\mathcal{H}^{(1)}$ one must take all (nonnegative) integer valued linear combinations of these lines, since each line corresponds to the first excited energy of an independent boson. In Figure 7, we have plotted several multiples of the eigenvalue line, to show how many eigenvalues lie beneath the continuous spectrum. There is also interesting behavior for other values of r. In Figure 4 we have plotted the spectral gap of $\mathcal{J}$ as a function of r and Δ^{-1} Finally we mention that this analysis can be done for any dimension, not just one. Thus one may obtain, at least heuristic, information about the low spectrum of quantum spin systems in higher dimensions by analyzing $\mathcal{J}_\Lambda$, which is the first order quantum correction to the classical ground states for large but finite J. The higher-dimensional case, where the low-lying spectrum is known to exhibit additional structure [5], is the subject of a separate paper [24]

Acknowledgements

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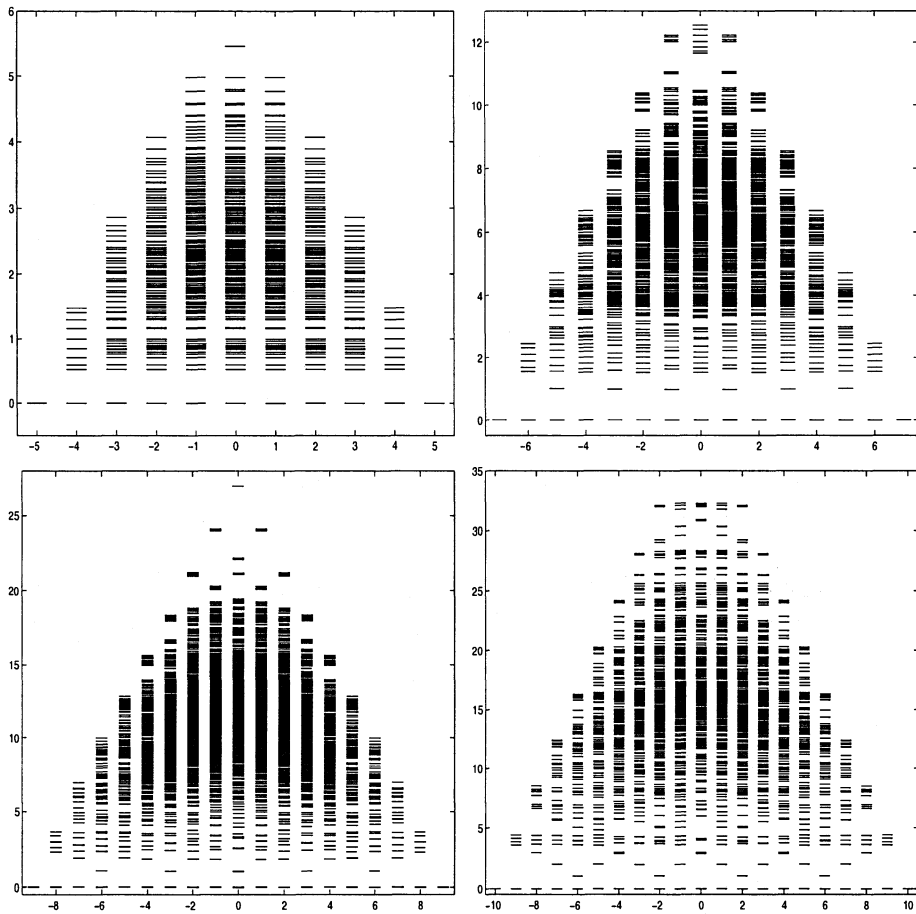
Figure 1: The spectrum of the XXZ spin chain for various finite spin chains. The horizontal axis is the total magnetization S^3_{tot} of a sector: the lines above each number show the eigenvalues in that sector. The spin systems are, from left to right and top to bottom, $(J, L, \Delta) = (1/2, 10, 2); (1, 7, 4); (3/2, 6, 4); (2, 5, 8)$.
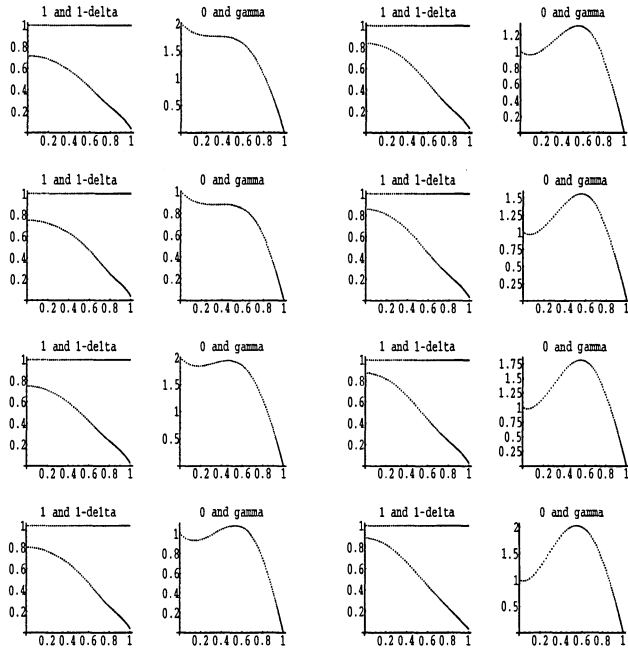
Figure 2: Plot of 1, $1 - \delta$ (left) and 0, γ (right) versus Δ^{-1}, for (J, n, L) equal to: First column $(7/2, 1, 4)$, $(2, 0, 6)$, $(4, 1, 4)$, $(5/2, 0, 5)$; Second column $(3, 0, 4)$, $(7/2, 0, 4)$, $(4, 0, 4)$, $(9/2, 0, 3)$
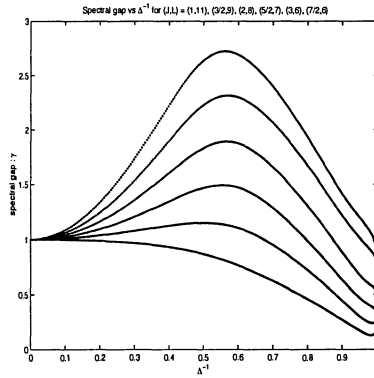
Figure 3: Some plots of the spectral gap using Lanczos iteration. For all three curves, $n \equiv 0 \mod 2J$.
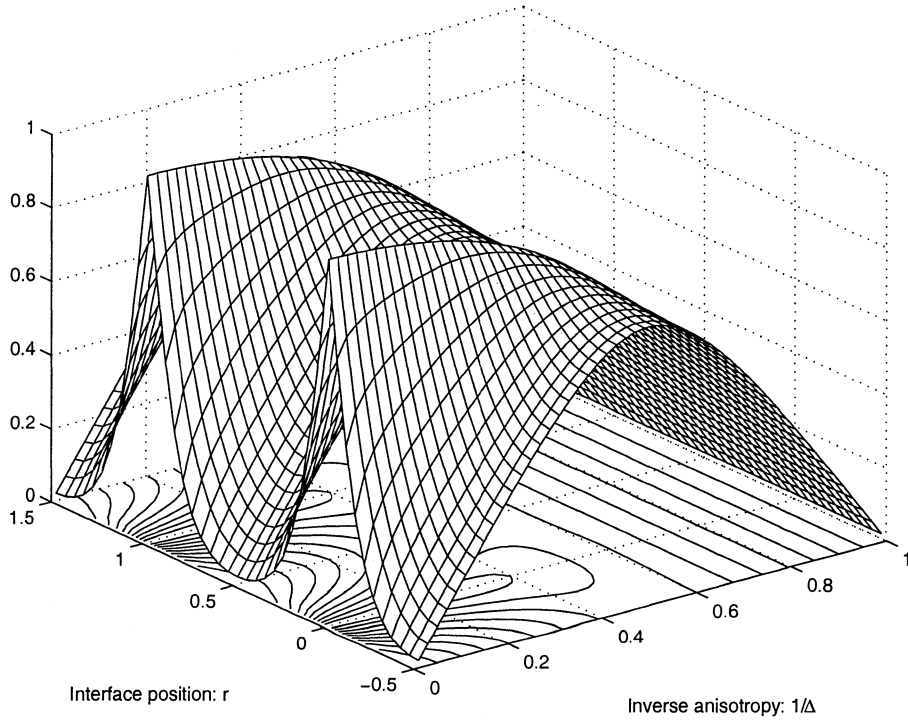
Figure 4: Surface and contour plot for the function γ_∞ versus r and Δ^{-1}
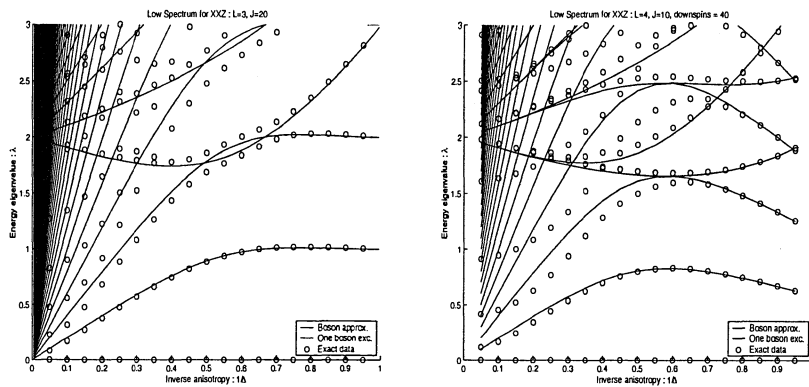
Figure 5: Solid lines are the predicted values of spectrum according to Boson gas model, circles are actual values of the spectrum for full XXZ as obtained by Lanczos
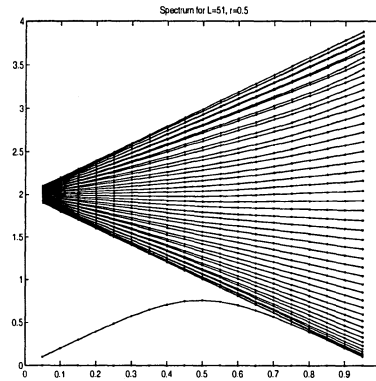
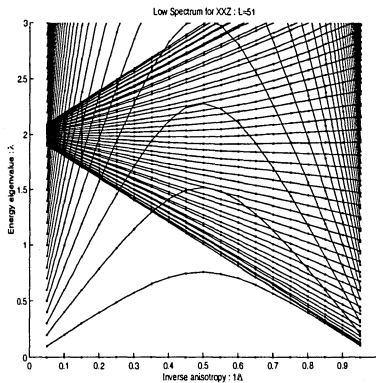Figure 6: The spectrum of the Boson coupling matrix versus anisotropy

Figure 7: The spectrum of the Boson coupling matrix, with multiples of the lowest boson energy included