Low Temperature Results for the Heisenberg XXZ and XY Models

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Abstract

This thesis contains two results for the low temperature behavior of quantum spin systems. First, we present a lower bound for the spin-1 XXZ chain in finite volumes in terms of the gap of the two-site Hamiltonian. The estimate is derived by a method developed by Nachtergaele in [22] called the Martingale Method. Our bound relies on an assumption which we have, as yet, been unable to verify analytically in all cases. We present numerical evidence that strongly indicates our assumption is valid.

The second result is a proof that the spin-1/2 d-dimensional XY model in the presence of an external magnetic field does not undergo a phase transition at low temperature, provided that the strength of the field is great enough. Using a contour expansion inspired by Kennedy in [12], we show that the weights of contours satisfy a condition of Kotecký and Preiss [18] which allows us to express the free energy of the system as a cluster expansion. As part of the setup we give a simple proof that the all-spin-up state is the unique ground state when the external magnetic field has strength at least 2d.
Chapter 1

Introduction

This thesis contains two results in the statistical mechanics of quantum spin systems. The first is an explicit lower bound bound for the spectral gap of the one dimensional, spin-1, XXZ ferromagnet. The estimate is obtained using a method developed by Nachtergaele in [22]. The second result is a proof on the absence of a phase transition for the Heisenberg XY model in an external magnetic field. In general the XXZ and XY models have very different behavior, ironically however, the techniques used in Chapter 3 were developed by Kennedy in [12] to treat the low temperature XXZ model.

The XXZ Hamiltonian on a domain $\Lambda \subset \mathbb{Z}^d$ is given by

$$H_{\Lambda}^{XXZ} = - \sum_{\{x,y\} \subset \Lambda, |x-y|=1} \frac{1}{\Delta} S_x^1 S_y^1 + \frac{1}{\Delta} S_x^2 S_y^2 + S_x^3 S_y^3$$

(1.0.1)

where the operators $S_x^\alpha$ are the spin operators in the direction $\mathbf{e}_\alpha$ at the site $x \in \Lambda$, $\Delta > 1$, and $| \cdot |$ is the standard $\ell^1$-norm on $\mathbb{Z}^d$. Ferromagnets are of general physical interest, and are not uncommon in nature. However there are other reasons to study ferromagnets as opposed to antiferromagnets or ferrimagnets. The first, and perhaps least serious, is that it tends to be very difficult to extract information from antiferromagnetic models. There are good results on antiferromagnets though. For
example in Dyson, Lieb, and Simon used reflection positivity to prove the existence of long range order in dimension two or greater. However, the XXZ model is not, in general, reflection positive.

For the ferromagnet much more is known. In Alcaraz, Salinas, and Wreszinski gave a formula for the ground states of the XXZ chain for any spin. Koma and Nachtergaele showed that in the thermodynamic limit, the spin-1/2 XXZ model has a spectral gap above the ground state, and were able to calculate an exact expression for the gap. Later, Matsui used the existence of the gap to prove that for any anisotropy \( \Delta > 1 \), the list of ground states given in is indeed a complete list. Matsui’s result was then improved upon by Koma and Nachtergaele in where they used the intrinsic quantum group symmetry of the XXZ chain to extend Matsui’s result to the case \( \Delta = 1 \).

The existence of a quantum group symmetry of the finite volume spin-1/2 chain, initially noted by Pasquier and Saleur in, is still another reason for studying the XXZ model. Physicists generally associate any symmetry with physical meaning, while mathematicians tend to view it as a special but interesting situation that is deserving of further investigation. In Koma and Nachtergaele not only calculated the spectral gap of the spin-1/2 infinite volume chain, but proved a sort of ordering of energy levels (à la Lieb and Mattis in) for the finite chain. Specifically they showed that not only is the ground state of \( H^{XXZ}_L \) the \( L + 1 \) dimensional irreducible representation of \( SU_q(2) \), but any first excited state must lie in an \( L - 1 \) dimensional irreducible representation. The quantum group symmetry does have some limitations however. It only exists in a restricted setting, i.e. for spin-1/2 chains in one dimension.

In this paper we are interested in the spin-1 chain, so other tools must be used.

The low-energy spectrum of the XXZ chain is also fairly well understood. This is relevant because the low-energy spectrum, and in particular the spectral gap, have direct implications for the low-temperature behavior, e.g. the decay of correlation
functions, of the physical systems modeled by the Hamiltonian. As stated before, Koma and Nachtergaele calculated the spectral gap of the spin-1/2 chain in [15]. For spins greater than 1/2 Koma, Nachtergaele, and Starr showed that there is a non-vanishing gap in one dimension in [17]. These results were extended by Caputo and Martinelli. In [18] they showed that the gap grows linearly with the spin. This confirmed a conjecture of Starr in [20]. The techniques of Caputo and Martinelli are limited however, in the sense that they do not give an explicit value for a lower bound of the spectral gap. In Chapter 2 we seek to remedy this in a small way. We present a method by Nachtergaele for estimating the gap of finite chains in terms of the gap of the nearest-neighbor interaction $\frac{1}{\Delta} \sum_{x,y} S_x^1 S_y^1 + \frac{1}{\Delta} S_x^2 S_y^2 + S_x^3 S_y^3$. The method relies on an assumption (2.4.8) that we believe to be satisfied for the spin-1 (and larger $J$) chain. We have much numerical evidence to suggest that the assumption is satisfied, but not an analytic proof of the fact. For this reason the lower bound for the gap of the spin-1 chain is only a conjecture, but we are confident that it is accurate and will soon be rigorously verified.

As stated before the second result in this thesis concerns the isotropic XY model in the presence of an external magnetic field for dimensions 2 or greater. The Hamiltonian is given by

$$H_{\Lambda}^{XY} = - \sum_{\{x,y\} \in \Lambda, |x-y|=1} \frac{1}{2} (\sigma_x^1 \sigma_y^1 + \sigma_x^2 \sigma_y^2) + h \sum_{x \in \Lambda} \frac{1}{2} (\mathbb{1} - \sigma_x^3)$$

where the $\sigma^\alpha$, $\alpha = 1, 2, 3$ are the Pauli spin matrices and $\Lambda$ is a finite subset of $\mathbb{Z}^d$ with $d \geq 2$. In a paper dated 1961, [20], Lieb, Shultz, and Mattis studied the general anisotropic one dimensional, spin-1/2, XY model without an external magnetic field ($h = 0$). They rigorously established the equivalence of the XY model with a free fermion model via the Jordan-Wigner transformation, and proved the existence of long-range order for the anisotropic model using a method they developed for calculating two point correlation functions. In the isotropic case the order vanishes. They
were also able to establish the uniqueness of a gapless ground state in the thermodynamic limit for the isotropic case. Later, Dyson, Lieb, and Simon, using reflection positivity, proved that the spin-1/2 XY model has a phase transition in three and higher dimensions \[7\]. Finally, in 1988, Kennedy, Lieb, and Shastry demonstrated the existence of long-range order for the ferromagnetic XY model in dimensions two and greater, regardless of spin. This then proved the existence of Bose-Einstein condensation for the hardcore gas on the same lattice at half filling \[13\].

In Chapter 3 we show that for magnetic fields with \( h > 2d \), there exists a range of non-zero temperatures where the XY model does not have a phase transition in two and higher dimensions. This case is not treated in the above papers since the presence of the magnetic field destroys the reflection positivity of the model. In \[14\] Kennedy and Tasaki study a much larger class of Hamiltonians, using similar techniques and with similar results. At this point, though, it remains unclear if there results cover the case with which we are interested. We employ a contour expansion, inspired by Kennedy in \[12\], to show that the free energy of the system is analytic for some values of inverse temperature \( \beta \) and magnetic field \( h > 2d \). Specifically we are able to show that the weights of our contours satisfy a condition of Kotecký and Preiss \[18\] which allows us to write the free energy using a cluster expansion.

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Chapter 2

XXZ Model

For many spin systems interesting behaviors (e.g. phase transitions) only occur in dimensions greater than one. However, in the case of the XXZ model, phase transitions do exist in dimension one. This remarkable fact is closely connected to the symmetry of the spin-1/2 chain under the action of the quantum group $SU_q(2)$.

In [15], Koma and Nachtergaele calculated the exact spectral gap for the spin-1/2 XXZ chain. The goal of this chapter is a lower bound for the spectral gap of the 1-dimensional spin-1 model. This is obtained using a method developed by Nachtergaele in [22], which was later improved by Spitzer and Starr in [29], for estimating the spectral gap of frustration free systems.

We will start by introducing the Hamiltonian for the XXZ chain. Since the method we use to find a lower bound requires one to know the ground states of the finite volume Hamiltonian, we will introduce these, and prove that they are indeed ground states for all values of spin. For completeness, we also present a brief account of the infinite volume ground states, although this is a much more sophisticated subject. Next we will give a proof, due to Koma and Nachtergaele, that the spectral gap of the infinite volume spin-1/2 chain is given by $1 - \Delta^{-1}$, where $\Delta$ is the anisotropy parameter in the XXZ Hamiltonian. In the last section we introduce the method
used to obtain the lower bound and present our results.

## 2.1 The Model

Initially we consider only finite intervals \( \Lambda \subset \mathbb{Z} \). For each \( x \in \Lambda \) we let \( H_x = \mathbb{C}^{(2J+1)} \) be the configuration space for the individual spin at site \( x \). The Hilbert space for the entire chain is given by \( H_{\Lambda} = \bigotimes_{x \in \Lambda} H_x \). The spin arises by way of a \((2J+1)\)-dimensional irreducible representation of \( SU(2) \) on each \( H_x \). This is generated by three operators \( S^1_x, S^2_x, S^3_x \), which are determined relative to a basis \( \{|-J\rangle_x, |-J+1\rangle_x, \ldots, |J\rangle_x\} \) by

\[
S^3_x|m\rangle_x = m|m\rangle_x
\]

and

\[
S^\pm_x|m\rangle_x = \sqrt{J(J+1) - m(m \pm 1)}|m \pm 1\rangle_x
\]

where \( S^\pm_x = S^1_x \pm iS^2_x \). The 1-dimensional spin-\( J \) XXZ Hamiltonian is then given by

\[
H_{XXZ}^L = -\sum_{x=1}^{L-1} \frac{1}{\Delta} (S^1_x S^1_{x+1} + S^2_x S^2_{x+1}) + S^3_x S^3_{x+1}
\]

where \( \Delta > 1 \) is the anisotropy parameter. The overall negative sign makes this a ferromagnetic model, while the inclusion of the anisotropy forces low energy states to have large regions in which spins are aligned along the 3-axis. Notice that in the limit \( \Delta \to 1 \) we obtain the isotropic Heisenberg, or XXX, model, while as \( \Delta \to \infty \) the model tends to an Ising like Hamiltonian.

As with many things in mathematics, the truly interesting behavior comes when we add boundary terms. To this end, we consider the so called “kink” boundary conditions. Let \( A(\Delta) = \sqrt{1 - \Delta^{-2}} \) and define \( H_{L}^{\pm} \) by

\[
H_{L}^{\pm} = H_{XXZ}^L + JA(\Delta)(S^3_L - S^3_1) + J^2 (L - 1)
\]
The last term, $J^2(L - 1)$, is added so that the ground state energy is zero. If we let

$$h_{x,x+1} = -\frac{1}{\Delta} \left( S_x^1 S_{x+1}^1 + S_x^2 S_{x+1}^2 \right) + S_x^3 S_{x+1}^3 + JA(\Delta)(S_{x+1}^3 + S_x^3) + J^2$$

then $H_L^{+-}$ can be expressed as the sum over translates of a single two-body interaction:

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

The choice of $A(\Delta)$ is such that the spin-1/2 Hamiltonian will commute with representations of the quantum group $SU_q(2)$ where $2\Delta = q + q^{-1}$ and $q \in (0, 1)$. If we define the operator $K$ to be

$$K = q^{-2S^3}$$

then $K$, $S^+$, $S^-$ satisfy the commutation relations

$$[S^+, S^-] = \frac{K - K^{-1}}{q^{-1} - q} \quad \text{and} \quad KS^\pm = q^{\mp 2} S^\pm K$$

$K$ and $S^\pm$ are the generators of an irreducible representation of $SU_q(2)$. Amazingly, there is a way to define tensor products of representations of $SU_q(2)$. For a chain of $L$ sites we write

$$S_x^3[1,L] = \sum_{x=1}^{L} \mathbb{1}_1 \otimes \cdots \otimes \mathbb{1}_{x-1} \otimes S_x^3 \otimes \mathbb{1}_{x+1} \otimes \cdots \otimes \mathbb{1}_L$$

$$S_x^+[1,L] = \sum_{x=1}^{L} K_1 \otimes \cdots \otimes K_{x-1} \otimes S_{x}^+ \otimes \mathbb{1}_{x+1} \otimes \cdots \otimes \mathbb{1}_L$$

$$S_x^-[1,L] = \sum_{x=1}^{L} \mathbb{1}_1 \otimes \cdots \otimes \mathbb{1}_{x-1} \otimes S_x^- \otimes K_{x+1}^{-1} \otimes \cdots \otimes K_L^{-1}$$

For spin-1/2 these operators commute with the XXZ Hamiltonian and were at the heart of the initial discovery of the ground states of the XXZ model. We will not use the quantum group symmetry much here and only mention the existence of the symmetry for completeness. Someone who is interested in learning more about quantum groups and their representations should consult the reference [11].
2.2 Finite Volume Ground States

Perhaps the first, or most basic question, one can ask when given a Hamiltonian like \( (2.1.4) \) is: does it have any non-trivial ground states and if so, what are they? This question was first answered by Alcaraz, Salinas and Wreszinski in [1]. As earlier indicated, they were able to realize the ground state of \( (2.1.4) \) in the spin-1/2 case as the highest weight irreducible representation of the quantum group \( SU_q(2) \). They were able to generalize the result for spins \( J > 1/2 \). Here we present their result, but the proof provided is due to Starr in [30].

**Theorem 2.2.1** (Alcaraz, Salinas, and Wreszinski) For each eigenvalue \( m \) of \( \sum_{x=1}^L S_x^3 \), \( m \in \{-JL, \ldots, +JL\} \) there is a unique (up to normalisation) state \( \Psi^m_0 \) in the sector of magnetization \( m \), such that \( H^+_L - \Psi^m_0 = 0 \). \( \Psi^m_0 \) is given by

\[
\Psi^m_0 = \sum_{\{m_x\} \in \{-J, \ldots, J\}^L} \prod_{x=1}^L q^{-x(j-m_x)} \left( \frac{2J}{J + m_x} \right)^{1/2} |\{m_x\}\rangle
\]

where \( |\{m_x\}\rangle \) is just the simple tensor

\[
|\{m_x\}\rangle = |m_1\rangle \otimes |m_2\rangle \otimes \cdots \otimes |m_L\rangle
\]

with respect to the natural basis for the spin operators given in \( (2.1.1) \).

**Proof:** The goal is to calculate all states \( \varphi \) such that \( H^+_L - \varphi = 0 \), that is we want to calculate \( \ker (H^+_L - \varphi) \). But by \( (2.1.6) \), \( H^+_L - \varphi \) is the sum of non-negative operators, thus if \( \varphi \in \ker (H^+_L - \varphi) \) then \( \varphi \in \ker (h_{x,x+1}) \) for \( 1 \leq x \leq L - 1 \). This gives

\[
\ker (H^+_L - \varphi) = \bigcap_{x=1}^{L-1} \ker (h_{x,x+1})
\]

Models with this property are often referred to as **frustration free**, since any state that minimizes the energy of the global interaction also minimizes the energy of every local interaction and hence are not “frustrated”. 


We begin by calculating \( \bigcap_{x=1}^{L-1} \ker (h_{x,x+1}) \) for \( J = 1/2 \). For other values of \( J \) we embed the spin-J chain into a longer spin-1/2 chain and use representation theory to obtain the desired result. For \( J = 1/2 \), \( \mathcal{H}_L \) is the \( 2^L \) dimensional space \( \otimes_{x=1}^{L} C^2 \). The simplest basis for \( \mathcal{H}_L \) is given by

\[
|\{m_x\}\rangle = \bigotimes_{x=1}^{L} |m_x\rangle
\]

where \( \{m_x\} \in \{\pm1/2\}^L \). Often we will use the convention that \( |1/2\rangle = |\uparrow\rangle \) and \( |-1/2\rangle = |\downarrow\rangle \). It is a short calculation to show that

\[
h_{x,x+1} = -\frac{1}{\Delta} (S^1_{x} S^1_{x+1} + S^2_{x} S^2_{x+1}) + S^3_{x} S^3_{x+1} + A(\Delta) (S^3_{x+1} - S^3_{x}) + J^2
\]

is the orthogonal projection onto the vector

\[
|\xi\rangle = \frac{1}{\sqrt{1 + q^2}} (|\uparrow\downarrow\rangle_{x,x+1} - |\downarrow\uparrow\rangle_{x,x+1})
\]

where \( q \) is the unique solution to the equation \( 2\Delta = q + q^{-1} \) on the interval \((0, 1)\).

Thus, we can write

\[
h_{x,x+1} = |\xi\rangle \langle \xi |
\]

To motivate our argument for general \( q \) consider the case when \( q = 1 \). Then \( |\xi\rangle_{x,x+1} \) is the spin singlet, or the anti-symmetric tensor, in \( \mathcal{H}_x \otimes \mathcal{H}_{x+1} \). If \( \tau(x, x+1) \in \mathcal{S}_L \) is just the transposition of \( x \) and \( x+1 \) then again for \( q = 1 \) we can write \( h_{x,x+1} \) as

\[
h_{x,x+1} = \frac{1}{2} (1 - P_{\tau(x,x+1)})
\]

where for \( \pi \in \mathcal{S}_L \), \( P_\pi \) represents the standard action of \( \mathcal{S}_L \) on \( \mathcal{H}_L \) given by

\[
P_\pi \bigotimes_{x=1}^{L} |\phi_x\rangle_x = \bigotimes_{x=1}^{L} |\phi_{\pi^{-1}(x)}\rangle_x
\]

Hence, for the isotropic model \( (\Delta = 1) \), if \( \psi \) is a ground state of \( h_{x,x+1} \), then \( P_{\tau(x,x+1)} \psi \) is also a ground state for all \( 1 \leq x \leq (L - 1) \). Since the nearest-neighbor transpositions generate the entire group \( \mathcal{S}_L \), we see that kernel of the isotropic Hamiltonian is
invariant under permutations, i.e. it is made up of symmetric tensors. This is quite evident when it is noted that the XXX Hamiltonian has full $SU(2)$ symmetry, so that its ground state coincides with the highest weight irreducible representation of $SU(2)$ in $\otimes_{x=1}^{L} \mathbb{C}^2$.

For $q \neq 1$ we again realize the ground states as symmetric tensors, however not with respect to the standard action $P_{\pi}$. Let $\omega : \{\pm 1/2\}^L \rightarrow \mathbb{Z}$ be given by

$$\omega(\{m_x\}) = \sum_{x=1}^{L} -x \left(\frac{1}{2} - m_x\right)$$

and consider the basis for $\mathcal{H}_L$ given by

$$|\{m_x\}\rangle^{(q)} = q^{\omega(\{m_x\})} |\{m_x\}\rangle$$

Now, let $P^{(q)} : SL \rightarrow GL(\mathcal{H}_L)$ be the standard representation of the symmetric group, but with respect to the basis $|m_x\rangle^{(q)}$. Thus we have

$$P_{\pi}^{(q)}|\{m_x\}\rangle^{(q)} = |\{m_{\pi^{-1}(x)}\}\rangle^{(q)}$$

but with respect to the standard basis we get

$$P_{\pi}^{(q)}|\{m_x\}\rangle = P_{\pi}^{(q)} \left(q^{-\omega(\{m_x\})} |\{m_x\}\rangle^{(q)}\right)$$

$$= q^{-\omega(\{m_x\})} |\{m_{\pi^{-1}(x)}\}\rangle^{(q)}$$

$$= q^{\omega(\{m_{\pi^{-1}(x)}\}) - \omega(\{m_x\})} |\{m_{\pi^{-1}(x)}\}\rangle$$

This formula looks a little complicated, but it is exactly what we want. If we restrict our attention to the space $\mathcal{H}_x \otimes \mathcal{H}_{x+1}$ then the symmetric group only consists of two elements, the identity $e$ and the transposition $\tau(x,x+1) \equiv \tau$. A short calculation shows that

$$P_{\tau}^{(q)}|\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle \quad P_{\tau}^{(q)}|\downarrow\downarrow\rangle = q^{-1}|\downarrow\downarrow\rangle$$

$$P_{\tau}^{(q)}|\downarrow\uparrow\rangle = |\downarrow\uparrow\rangle \quad P_{\tau}^{(q)}|\uparrow\downarrow\rangle = q|\uparrow\downarrow\rangle$$
Then we can immediately write down the symmetric tensors as
\[
|\uparrow\uparrow\rangle, \ |\downarrow\downarrow\rangle, \ \frac{|\uparrow\downarrow\rangle + q|\downarrow\uparrow\rangle}{\sqrt{1 + q^2}}
\]
while the anti-symmetric tensor is given by
\[
\frac{|\uparrow\downarrow\rangle - q|\downarrow\uparrow\rangle}{\sqrt{1 + q^2}}
\]
Thus, by (2.2.4), \(h_{x,x+1}\) is the orthogonal projection onto the anti-symmetric tensor of the representation \(P(q)\), and hence we write
\[
h_{x,x+1} = \frac{1}{2} \left( \mathbb{1} - P(q)_{\tau(x,x+1)} \right)
\]
where the anisotropy parameter \(\Delta\) in \(h_{x,x+1}\) and \(q \in (0,1)\) are related by \(2\Delta = q + q^{-1}\). So, just as in the isotropic case, we are able to conclude that any frustration free state of \(H_L^{+^-}\) is invariant under nearest-neighbor transpositions. But nearest-neighbor transpositions generate the symmetric group, so the ground states of \(H_L^{+^-}\) are symmetric with respect to the representation \(P(q)\). Since \(P(q)\) is identical to the standard representation with respect to the basis \(|\{m_x\}\rangle^{(q)}\) we can immediately write down the symmetric states with respect to this basis:
\[
\Psi_0^m = \sum_{\{m_x\} \in \{\pm 1/2\}^L} \sum_{\sum m_x = m} |\{m_x\}\rangle^{(q)}
\]
where \(m \in \{-L/2, -(L/2 + 1), \ldots, L/2\}\). Expressing this in terms of the standard basis gives
\[
\Psi_0^m = \sum_{\{m_x\} \in \{\pm 1/2\}^L} q^{\omega(\{m_x\})} |\{m_x\}\rangle
= \sum_{\{m_x\} \in \{\pm 1/2\}^L} q^{\sum_{-x(1/2-m_x)} |\{m_x\}\rangle}
= \sum_{\{m_x\} \in \{\pm 1/2\}^L} \prod_{x=1}^{L} q^{-x(1/2-m_x)} |\{m_x\}\rangle
\]
(2.2.7)
which is the correct formula for $J = 1/2$.

For $J > 1/2$ we let $\mathcal{H}_x^{(J)} = \mathbb{C}^{2J+1}$ as above. $\mathcal{H}_x^{(J)}$ can be realized as the highest-weight space in the representation $\otimes_{j=1}^{2J} \mathbb{C}^{2}$. In other words $\mathcal{H}_x^{(J)}$ consists of the symmetric tensors in $\otimes_{j=1}^{2J} \mathcal{H}_x^{(1/2)}$. But we have $L$ copies of $\mathcal{H}_x^{(J)}$ thus the space we want is

$$\mathbb{H}_L^{(J)} = \bigotimes_{i=1}^{L} \left( \otimes_{j=1}^{2J} \mathcal{H}_x^{(1/2)} \right)_i$$

(2.2.8)

Again, suppose that $P : S_{2J} \rightarrow GL(\mathcal{H}_x^{(1/2)})$ is the standard representation of $S_{2J}$ on $\mathcal{H}_x^{(1/2)}$ with respect to the basis $\{|{m}_x\rangle\}$. Let $S_{2J}^{\times L}$ be the direct product of $L$ copies of the symmetric group on $2J$ elements. Define a representation $\Pi$ of $S_{2J}^{\times L}$ onto $\mathbb{H}_L^{(J)}$ by

$$\Pi_{(\pi_1, \ldots, \pi_L)} \left( \bigotimes_{i=1}^{L} \{m_{x,j,i}\} \right)_i = \bigotimes_{i=1}^{L} P_{\pi_i} \{m_{x,j,i}\}_i$$

so that the $i^{th}$ copy of $S_{2J}$ acts in the standard way on the $i^{th}$ copy of $\otimes_{j=1}^{2J} \mathcal{H}_x^{(1/2)}$ in $\mathbb{H}_L^{(J)}$. Let $\text{Sym}_\Pi[\mathbb{H}_L^{(J)}] \subset \mathbb{H}^{(J)}$ denote the subspace of $\mathbb{H}^{(J)}$ which is invariant under the action of $\Pi$. This space coincides with $\mathcal{H}_L^{(J)}$ because

$$\text{Sym}_\Pi[\mathbb{H}_L^{(J)}] = \text{Sym}_\Pi \left[ \bigotimes_{i=1}^{L} \left( \otimes_{j=1}^{2J} \mathcal{H}_x^{(1/2)} \right)_i \right]$$

(2.2.9)

$$= \bigotimes_{i=1}^{L} \left( \text{Sym}_P \left[ \otimes_{j=1}^{2J} \mathcal{H}_x^{(1/2)} \right] \right)_i$$

(2.2.10)

since $\Pi$ only acts on individual factors in $\mathbb{H}_L^{(J)}$ via $P$. But

$$\text{Sym}_P \left[ \otimes_{j=1}^{2J} \mathcal{H}_x^{(1/2)} \right] = \mathcal{H}_i^{(J)}$$

and hence

$$\text{Sym}_\Pi[\mathbb{H}_L^{(J)}] = \bigotimes_{i=1}^{L} \mathcal{H}_i^{(J)} = \mathcal{H}_L^{(J)}$$

Next, we define a spin-1/2 Hamiltonian on $\mathbb{H}^{(J)}$ which reduces to the Hamiltonian $H_L^{+-,(J)}$. We consider $L$ distinct and disjoint copies of the set $\{1, 2, \ldots, 2J\}$ which we
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denote by \([1, 2J]_i, i = 1, \ldots, L\). Then define \(H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)}\) by

\[
H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)} = \frac{L-1}{2} \sum_{i=1}^{L-1} \sum_{\{x_i, x_{i+1}\} \in \{1,2J\}_i, \ x_{i+1} \in \{1,2J\}_{i+1}} h_{x_i, x_{i+1}} \tag{2.2.11}
\]

\(H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)}\) is clearly invariant under the action of \(\Pi\). Therefore, setting \(P_{\text{Sym}}\) as the orthogonal projection onto \(\text{Sym}[\Pi^{(J)}_L]\), gives

\[
H^{+-,(J)}_L = P_{\text{Sym}} H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)} P_{\text{Sym}}
\]

However, the construction of \(\Pi\) was such that \(H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)}\) commutes with the entire action, thus

\[
H^{+-,(J)}_L = H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)} P_{\text{Sym}}
\]

This means that \(\ker(H^{+-,(J)}_L) = \ker(H^{+-,(1/2)}_{2J_1, \ldots, 2J_L} \cap \text{ran}(P_{\text{Sym}})\). However, by the argument for the spin-1/2 case, the ground state of \(H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)}\) is invariant under the action \(P^{(q)}\). Therefore

\[
\ker(H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)}) \subset \text{ran}(P_{\text{Sym}})
\]

which implies

\[
\ker(H^{+-,(J)}_L) = \ker(H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)}) \cap \text{ran}(P_{\text{Sym}}) = \ker(H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)})
\]

that is, the ground state of \(H^{+-,(J)}_L\) is just the ground state of \(H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)}\). But the formula for the ground states of \(H^{+-,(1/2)}_{(2J_1, \ldots, 2J_L)}\) is given by (2.2.7). Writing these in terms of symmetric tensors; doing so yields

\[
\Psi^m_0 = \sum_{\{m_{x_j}\} \in \{\pm 1/2\}^{2JL}, \sum_j m_{x_j} = m} \prod_{j=1}^{2JL} q^{-j(1/2-m_{x_j})} |\{m_{x_j}\}\rangle
\]

\[
= \sum_{\{m_{x_j}\} \in \{\pm 1/2\}^{2JL}, \sum_j m_{x_j} = m} \bigotimes_{j=1}^{2JL} q^{-j(1/2-m_{x_j})} |m_{x_j}\rangle_j
\]
Next, we rewrite the single sum as two sums; first over the L chains of length \(2J\), and then over the bases of the individual chains. This gives

\[
\Psi^m_0 = \sum_{\{x\} \in \{-J, \ldots, J\}^L} \left( \prod_{x=1}^L q^{-x(J-m_x)} \right) \left( \prod_{\sum_j b_{j,x} = m_x} \sum_{\{b_j\} \in \{\pm \frac{1}{2}\}^L} \right) \left| \begin{array}{c}
\{b_j\} \\
\end{array} \right|_j
\]

which is the same as (2.2.1).

\[
2.3 \text{ Infinite Volume Ground States}
\]

In infinite volume the problem of determining the ground states for the Hamiltonian is much more subtle; even defining the Hamiltonian turns out not to be as simple as one might think. For \(\Lambda \subset \mathbb{Z}, |\Lambda| < \infty\) the algebra of observables is \(\mathcal{A}_\Lambda \equiv \mathcal{B}(\mathcal{H}_\Lambda)\). In infinite volume the algebra of quasi-local observables \(\mathcal{A}_\infty\) is defined by

\[
\mathcal{A}_\infty \equiv \left( \bigcup_{\Lambda \subset \mathbb{Z}, |\Lambda| < \infty} \mathcal{A}_\Lambda \right)
\]

where the completion is taken in the operator norm topology. Note that if \(\Lambda' \subset \Lambda\) then there is a natural way to embed \(\mathcal{A}_\Lambda'\) as a subalgebra of \(\mathcal{A}_\Lambda\), namely

\[
\mathcal{A}_{\Lambda'} \ni \mathcal{A}' \otimes \mathbb{1}_{\Lambda \setminus \Lambda'} \in \mathcal{A}_\Lambda
\]

(2.3.12)

In the infinite volume \(H_\mathbb{Z}\) is determined by a derivation \(\delta\) on \(\mathcal{A}_\infty\). For any \(A \in \mathcal{A}_\Lambda, |\Lambda| < \infty\)

\[
\delta(A) = \lim_{\Lambda'/\mathbb{Z}} [H_{\Lambda'}, A]
\]
A state, $\omega$, on $A_\infty$ is a positive (normalized) linear functional. A ground state is one that satisfies the local stability property

$$\omega(A^*\delta(A)) \geq 0 \quad A \in A_\Lambda; \; |\Lambda| < \infty$$

This condition becomes much more intuitive if we go to the GNS representation corresponding to the state $\omega$: $(\pi, \mathcal{H}, \Omega)$. For the XXZ Hamiltonian with $+-$ boundary condition the GNS Hilbert space, $\mathcal{H}_{+-}$, can be understood in a simple way. Let $\Omega^{+-}$ be given by

$$\Omega^{+-} = \bigotimes_{x \in \mathbb{Z}} \Omega^+_x, \quad \Omega^+_x = \begin{cases} \langle \uparrow \rangle & x \leq 0 \\ \langle \downarrow \rangle & x \geq 1 \end{cases} \tag{2.3.13}$$

Then the set of vectors of the form

$$\psi = A\Omega^{+-} \text{ where } A \in \bigcup_{\Lambda \subset \mathbb{Z}} A_\Lambda, \; |\Lambda| < \infty \tag{2.3.14}$$

is a dense subset of $\mathcal{H}_{+-}$. For a local observable $A$, the stability condition (2.3.12) becomes

$$\omega(A^*\delta(A)) = \langle \Omega^{+-} | \pi(A^*)\delta(\pi(A))\Omega^{+-} \rangle$$

$$= \langle \Omega^{+-} | \pi(A^*)[\pi(H), \pi(A)]\Omega^{+-} \rangle$$

$$= \langle \Omega^{+-} | \pi(A^*)\pi(H)\pi(A)\Omega^{+-} \rangle - \langle \Omega^{+-} | \pi(A^*)\pi(A)\pi(H)\Omega^{+-} \rangle$$

$$= \langle \pi(A)\Omega^{+-} | \pi(H) |\pi(A)\Omega^{+-}\rangle \geq 0$$

Thus we see that (2.3.12) designates a ground state as one for which any local change coincides with some increase in energy; which is exactly what a ground state should be.

A closely related, but stronger, notion in the infinite volume is that of a zero energy state. For a model like the XXZ, we can define this in the following way. Let $H_\Lambda = \sum_{\{x,x+1\} \subset \Lambda} h_{x,x+1}$ where $h_{x,x+1}$ is the translate of some nearest-neighbor
interaction $h_{1,2}$ for all $(x, x + 1)$. Then $\omega$ is a zero energy state iff

$$\omega(h_{x,x+1}) = \min_{\omega' \in A^\infty} \omega'(h_{x,x+1})$$

for all \{x, x + 1\} $\subset \mathbb{Z}$ where here the states are all normalized. This is also called frustration free as in the finite volume case. If $A \in A_{[1,L]}$, then

$$\omega(A^*\delta(A)) = \lim_{\Lambda \nearrow \mathbb{Z}} \omega(A^*(H_{\Lambda}A - AH_{\Lambda}))$$

$$= \sum_{x=0}^{L} \omega(A^*(h_{x,x+1}A - Ah_{x,x+1}))$$

$$= \sum_{x=0}^{L} \omega(A^*(h_{x,x+1} - \lambda_0)A)$$

$$= \sum_{x=0}^{L} \omega_A(h_{x,x+1} - \lambda_0) \geq 0$$

where $\lambda_0$ is the smallest eigenvalue of $h_{x,x+1}$ and $\omega_A(\cdot) = \omega(A^* \cdot A)$. Therefore, if $\omega$ is a zero energy state then it is also a ground state, however the reverse is not in general true. For the XXZ chain Gottstein and Werner found all zero energy states in [8]. Their results and techniques were quite general and will not be presented here, although they obtained very nice results connecting zero energy states and VBS states. Moreover, they predicted correctly that for the XXZ and XXX chains the zero energy states are the only ground states. Recalling the definition of $\Omega^{+-}$ in (2.3.13), the zero energy states for the XXZ Hamiltonian are given by

$$\Psi_0(n) = \sum_{k=0}^{\infty} \sum_{\{x_1, \ldots, x_k\} \subset \mathbb{Z} \leq 0} \sum_{\{y_1, \ldots, y_{n+k}\} \subset \mathbb{Z} \geq 1} q^{-(x_1 + \cdots + x_k) + (y_1 + \cdots + y_{n+k})} \prod_{j=1}^{k} S_{x_j}^- \prod_{j=1}^{n+k} S_{y_j}^+ \Omega^{+-} \quad (2.3.15)$$

It was shown by Matsui in [21] that the zero energy states defined above along with those obtained from $-+$, $++$ and $--$ boundary conditions account for all ground states of the XXZ chain. Later, Koma and Nachtergaele in [16] gave an alternative proof of this fact with the added result that their techniques could be applied to the
XXX chain as well. This is a major difference between Koma and Nachtergaele’s and Matsui’s results. Their results not only apply to spin-1/2, but to all $J$.

2.4 The Spectral Gap

2.4.1 Spin-1/2

The spectral gap of the spin-1/2 XXZ chain was first calculated by Koma and Nachtergaele in [15]. Their proof is a truly beautiful piece of work that makes use of standard tools of statistical mechanics, such as the transfer matrix, while also employing newer phenomena such as the quantum group symmetry of the XXZ model. Together with S. Starr they later showed for all $J$ there is a non-zero spectral gap in the thermodynamic limit, although they did not provide an estimate [17]. For completeness, we provide the proof of the existence of the gap in the spin-1/2 case.

For $\alpha, \beta \in \{+, -\}$, let $\Omega^{\alpha \beta}$ be the generalizations of $\Omega^{+-}$ given in (2.3.13), that is

$$
\Omega^{\alpha \beta} = \bigotimes_{x \in \mathbb{Z}} \Omega^{\alpha \beta}(x) \text{ where } \Omega^{\alpha \beta}(x) = \begin{cases} 
|\alpha\rangle & \text{if } x \leq 0 \\
|\beta\rangle & \text{if } x \geq 1
\end{cases} \quad (2.4.1)
$$

and similarly the GNS space $\mathcal{H}^{\alpha \beta}$ has a dense set of vectors of the form

$$
\psi = A \Omega^{\alpha \beta} \quad \text{where } A \in \bigcup_{A \subseteq \mathbb{Z}} \mathcal{A}_A, \quad |A| < \infty \quad (2.4.2)
$$

The cyclic vector of the GNS representation, $\Omega_{GNS}^{\alpha \beta}$ is then given by a generalization of equation (2.3.15)

$$
\Omega_{GNS}^{\alpha \beta} = Z^{-1}(q) \sum_{k=0}^{\infty} \sum_{\{x_1, \ldots, x_k\} \subseteq \mathbb{Z}_{\leq 0}} q^{\sum_{j=1}^{k}(y_j - x_j)} \prod_{j=1}^{k} S_{x_j}^{\beta} S_{y_j}^{\alpha} \Omega^{\alpha \beta} \quad (2.4.3)
$$

where $Z^{-1}(q)$ is a normalization factor. The Hamiltonian $H_{GNS}^{\alpha \beta}$ is then defined by
the equation
\[ H_{GNS}^{\alpha\beta} A \Omega_{GNS}^{\alpha\beta} = \lim_{\Lambda \rightarrow \mathbb{Z}} [H_{\Lambda}^{\alpha\beta}, A] \Omega_{GNS}^{\alpha\beta} \] (2.4.4)

Note that the set of vectors in (2.4.2) are in the domain of \( H_{GNS}^{\alpha\beta} \).

Theorem 2.4.1 (Koma and Nachtergaele) For all \( \Delta > 1 \) and for any choice of GNS sector \((\pm\pm), (-+), (++)\) let \( \Gamma^{\alpha\beta} \) be the set of all \( \lambda \in \mathbb{R} \) such that
\[ \langle \Omega^{\alpha\beta} | A^* \left( H_{GNS}^{\alpha\beta} \right)^3 A \Omega^{\alpha\beta} \rangle \geq \lambda \langle \Omega^{\alpha\beta} | A^* \left( H_{GNS}^{\alpha\beta} \right)^2 A \Omega^{\alpha\beta} \rangle \] (2.4.5)
for all \( A \in \cup_{\Lambda} A_{\Lambda} \). Then
\[ \sup \Gamma^{\alpha\beta} = 1 - \Delta^{-1} \] (2.4.6)
onlyor, in other words, if \( \gamma_{\alpha\beta} \) is the spectral gap of \( H_{GNS}^{\alpha\beta} \) then
\[ \gamma_{\alpha\beta} = 1 - \Delta^{-1}. \] (2.4.7)

The proof of theorem 2.4.1 consists of two main parts: first an estimate on a lower bound for \( \gamma \) and then an argument to show that this is also an upper bound.

**Proof:** In order to bound \( \gamma \) from below by \( 1 - \Delta^{-1} \) we show for all local observables \( A \)
\[ \langle \Omega^{\alpha\beta} | A^* \left( H_{GNS}^{\alpha\beta} \right)^3 A \Omega^{\alpha\beta} \rangle \geq (1 - \Delta^{-1}) \langle \Omega^{\alpha\beta} | A^* \left( H_{GNS}^{\alpha\beta} \right)^2 A \Omega^{\alpha\beta} \rangle \] (2.4.8)
that is, for every \( \psi \) in the range of \( H_{GNS}^{\alpha\beta} \)
\[ \langle \psi | H_{GNS}^{\alpha\beta} \psi \rangle \geq (1 - \Delta^{-1}) \langle \psi | \psi \rangle \] (2.4.9)

But, if \( A \in A_{\Lambda} \) with \( \Lambda \) finite, then
\[ \langle \Omega^{\alpha\beta} | A^* \left( H_{GNS}^{\alpha\beta} \right)^k A \Omega^{\alpha\beta} \rangle = \langle \Omega^{\alpha\beta} | A^* \left( H_{\Lambda+\{0,1\}}^{+\{0,1\}} \right)^k A \Omega^{\alpha\beta} \rangle \] (2.4.10)
The operator \( A^* \left( H_{\Lambda+\{0,1\}}^{+\{0,1\}} \right)^k A \) is in \( A_{\Lambda+\{0,1\}} ^+ \), and thus we can write
\[ \langle \Omega^{\alpha\beta} | A^* \left( H_{\Lambda+\{0,1\}}^{+\{0,1\}} \right)^k A \Omega^{\alpha\beta} \rangle = \text{Tr} \left[ \rho_{\Lambda+\{0,1\}} A^* \left( H_{\Lambda+\{0,1\}}^{+\{0,1\}} \right)^k A \right] \] (2.4.11)
where $\rho_{\Lambda^+\{-1,0,1\}}$ is a density matrix. Hence, we have shown the infinite volume gap $\gamma$ is greater than or equal to $1 - \Delta^{-1}$ if, for all finite volumes $\Lambda$, the spectral gap of $H_{\Lambda}^{\alpha\beta}$ is greater than $1 - \Delta^{-1}$. This is the result of the following proposition.

**Proposition 2.4.2** Let $\gamma_L$ denote the spectral gap of $H_L^{+-}$. Then for all $\Delta \geq 1$ and $L \geq 2$ we have

$$\gamma_L = 1 - \Delta^{-1} \cos(\pi/L) \quad (2.4.12)$$

To prove Proposition 2.4.2 we calculate the first non-zero eigenvalue in the subspace of $\mathcal{H}_L$ corresponding to eigenvectors of $S_{\text{tot}}^3$ with eigenvalue $L/2 - 1$, i.e. the sector with one downspin, and show that this is also a lower bound for the smallest non-zero eigenvalue in all other sectors.

Let $D_x = S_x^- |\uparrow\rangle^L$ where $|\uparrow\rangle^L = \otimes_{x=1}^{L} |\uparrow\rangle_x$. Then if $\psi$ is a vector in the sector with one downspin

$$\psi = \sum_{x=1}^{L} a_x D_x \quad (2.4.13)$$

Now suppose that $\psi$ is an eigenvector with eigenvalue $\mathcal{E}$, then

$$H_L^{+-} \psi = \sum_{x=1}^{L} a_x H_L^{+-} D_x = \mathcal{E} \psi \quad (2.4.14)$$

On the other hand computing $H_L^{+-}$ gives

$$H_L^{+-} D_1 = \frac{1 + A(\Delta)}{2} D_1 - \frac{1}{2\Delta} D_2$$
$$H_L^{+-} D_x = D_x - \frac{1}{2\Delta} (D_{x-1} + D_{x+1}) \quad \text{for } 2 \leq x \leq L$$
$$H_L^{+-} D_L = \frac{1 - A(\Delta)}{2} D_L - \frac{1}{2\Delta} D_{L-1} \quad (2.4.15)$$

Putting (2.4.13)-(2.4.15) together we get the equations

$$a_{x+1} = 2\Delta(1 - \mathcal{E})a_x - a_{x-1} \quad \text{for } 2 \leq x \leq L - 1, \quad (2.4.16)$$
$$a_2 = 2\Delta(1/2 + A(\Delta)/2 - \mathcal{E})a_1 \quad (2.4.17)$$
$$a_{L-1} = 2\Delta(1/2 - A(\Delta)/2 - \mathcal{E})a_L \quad (2.4.18)$$
Notice that if $a_1 = 0$ then the above implies $\psi = 0$, so we can assume from now on that $a_1 \neq 0$. Equation (2.4.16) can be written as

$$
\begin{pmatrix}
a_{x+1} \\
a_x
\end{pmatrix} = T
\begin{pmatrix}
a_x \\
a_{x-1}
\end{pmatrix}
$$

where $T = \begin{pmatrix} 2\Delta(1 - \mathcal{E}) & -1 \\ 1 & 0 \end{pmatrix}$ is called the transfer matrix. Iterating this gives

$$
\begin{pmatrix}
a_L \\
a_{L-1}
\end{pmatrix} = T^{L-2}
\begin{pmatrix}
a_2 \\
a_1
\end{pmatrix}
$$

So taking into account (2.4.17), (2.4.18), and (2.4.20) we arrive at

$$
a_L \begin{pmatrix} 1 \\ \Delta[1 - A(\Delta) - \mathcal{E}] \end{pmatrix} = a_1 T^{L-2} \begin{pmatrix} \Delta[1 + A(\Delta) - \mathcal{E}] \\ 1 \end{pmatrix}
$$

Equation (2.4.21) can be solved using the eigenvectors and eigenvalues of $T$. The characteristic equation of $T$ is

$$
\lambda^2 - 2\Delta(1 - \mathcal{E})\lambda + 1 = 0
$$

which has roots

$$
\lambda_{\pm} = \Delta(1 - \mathcal{E}) \pm \sqrt{\Delta^2(1 - \mathcal{E})^2 - 1}
$$

Initially, let us consider the case when $T$ does not have degenerate eigenvalues, that is $\Delta(1 - \mathcal{E}) \neq \pm 1$. The eigenvectors of $T$ are

$$
e_{\pm} = \begin{pmatrix} \lambda_{\pm} \\ 1 \end{pmatrix}
$$

We want to solve equation (2.4.21) so we must decompose each vector into a sum of $e_+$ and $e_-$. Projecting the vector on the left of (2.4.21) onto $e_{\pm}$ gives

$$
\begin{pmatrix} 1 \\ \Delta[1 - A(\Delta) - \mathcal{E}] \end{pmatrix} = \mu_+ \lambda_- e_+ + \mu_- \lambda_+ e_-
$$
where
\[ \mu_\pm = \frac{1}{2} \left[ 1 \pm \Delta \frac{A(\Delta) + \mathcal{E}}{\sqrt{\Delta^2(1 - \mathcal{E})^2 - 1}} \right] \] (2.4.26)
and the one on the right hand side of (2.4.21) gives
\[
\begin{pmatrix}
\Delta [1 + A(\Delta) - \mathcal{E}] \\
1
\end{pmatrix} = \eta_+ e_+ + \eta_- e_-
\] (2.4.27)
where
\[ \eta_\pm = \frac{1}{2} \left[ 1 \pm \Delta \frac{A(\Delta) - \mathcal{E}}{\sqrt{\Delta^2(1 - \mathcal{E})^2 - 1}} \right] \] (2.4.28)
Now we can substitute (2.4.25) and (2.4.27) back into (2.4.21) to get
\[
a_L (\mu_+ \lambda_+ e_+ + \mu_- \lambda_+ e_-) = a_1 T_L^{-2} (\eta_+ e_+ + \eta_- e_-)
\] (2.4.29)
\[
= a_1 (\eta_+ \lambda_+ L^{-2} e_+ + \eta_- T_L^{-2} e_-)
\] (2.4.30)
\[
= a_1 (\eta_+ \lambda_+ L^{-2} e_+ + \eta_- \lambda_- L^{-2} e_-)
\] (2.4.31)
But \(e_+\) and \(e_-\) are linearly independent thus we get the equations
\[
\frac{a_L}{a_1} \mu_+ = \frac{\lambda_+ L^{-2}}{\lambda_-} = \lambda_+ L^{-1}
\] (2.4.32)
\[
\frac{a_L}{a_1} \mu_- = \frac{\lambda_- L^{-2}}{\lambda_+} = \lambda_- L^{-1}
\] (2.4.33)
where we have used the fact that \(\lambda_+ \lambda_- = 1\). Simplifying (2.4.32) and (2.4.33) further gives
\[
\lambda^{2L-2} = \frac{\mu_+}{\mu_-} \times \frac{\eta_-}{\eta_+}
\] (2.4.34)
where we have assumed that \(\eta_- \neq 0\). This assumption is not restrictive since
\[
\eta_- = 0 \iff \frac{1}{2} \left[ 1 - \Delta \frac{A(\Delta) - \mathcal{E}}{\sqrt{\Delta^2(1 - \mathcal{E})^2 - 1}} \right] = 0
\] (2.4.35)
\[
\iff \Delta [A(\Delta) - \mathcal{E}] = \sqrt{\Delta^2(1 - \mathcal{E})^2 - 1}
\] (2.4.36)
\[
\iff \mathcal{E} \sqrt{\Delta^2 - 1} = \Delta \mathcal{E}
\] (2.4.37)
\[
\iff \mathcal{E} = 0
\] (2.4.38)
thus $\eta_- = 0$ corresponds to the ground state in the $L/2 - 1$ sector. Moreover, $\eta_- \neq 0$ guarantees that all $\mu_\pm$ and $\eta_\pm$ are non-zero, so we see that equation (2.4.34) is indeed valid in the setting we want. Using (2.4.26), (2.4.28), and (2.4.23), we can write

$$\frac{\mu_+}{\mu_-} = \frac{\Delta + \sqrt{\Delta^2 - 1}}{\lambda_+} \times \frac{\lambda_+ - (\Delta - \sqrt{\Delta^2 - 1})}{\lambda_+ - (\Delta + \sqrt{\Delta^2 - 1})}$$

(2.4.39)

and

$$\frac{\eta_-}{\eta_+} = \frac{\Delta - \sqrt{\Delta^2 - 1}}{\lambda_+} \times \frac{\lambda_+ - (\Delta + \sqrt{\Delta^2 - 1})}{\lambda_+ - (\Delta - \sqrt{\Delta^2 - 1})}$$

(2.4.40)

Together with (2.4.34) this gives

$$\lambda_+^2 L = 1$$

(2.4.41)

which implies

$$\lambda_+ = e^{i\pi \ell / L} \quad \ell \in \mathbb{Z}$$

(2.4.42)

Returning now to (2.4.23) and solving for $\mathcal{E}_L(\ell)$ gives

$$\mathcal{E}_L(\ell) = 1 - \frac{\lambda_+ + \lambda_-}{2\Delta} = 1 - \Delta^{-1} \cos(\pi \ell / L) \quad \ell = 1, 2, \ldots, L - 1$$

(2.4.43)

where the condition on $\ell$ comes from the assumption that (2.4.22) has non-degenerate roots. Furthermore, we see that equation (2.4.43) gives $L - 1$ distinct eigenvalues, which gives us a total of $L$ distinct eigenvalues of $H^+_L$ in the $(L/2 - 1)$ sector when we add the ground state energy $\mathcal{E} = 0$. More to the point, there are not any solutions with $\Delta(1 - \mathcal{E}) = \pm 1$.

The above proves Proposition 2.4.2, that is in the $(L/2 - 1)$ sector the smallest non-zero eigenvalue is given by $1 - \Delta^{-1} \cos(\pi / L)$. To finish the proof of Theorem 2.4.1 we must show that this is same for all other sectors. In order to accomplish this we utilize the quantum group symmetry of the model. Note that any irreducible representation of $SU_q(2)$ of dimension $L - 1$ must intersect the sector with one overturned spin. Thus if the first excited state, $\varphi^m_1$, lies in an $L - 1$ irreducible representation for any choice of magnetization $m$, $1 < m < L$, we can raise it to a state, $\phi^m_1$, in the $L/2 - 1$ sector by way of the quantum group raising operator. The state $\phi^m_1$ has energy greater than or
equal to $1 - \Delta^{-1} \cos(\pi/L)$ by the argument above. However, since the quantum group commutes with the Hamiltonian $H_L^{+-}$, $\phi_1^m$ has the same energy as the original ground state, $\phi_1^m$, and Theorem 2.4.1 follows. Thus we must show that the lowest excitations lie in the $L - 1$ dimensional irreducible representations of $SU_q(2)$. To this end we present the following lemma without proof. The proof makes use of straightforward applications of the quantum group symmetry as well techniques similar to those in Section 2.4.2.

Consider an arbitrary spin chain of length $n$. Let $\mathcal{H}_{S_{tot}^3 \geq nJ - s}$ be the span of eigenvectors of $S_{tot}^3$ with eigenvalue greater than $nJ - s$ (less than $nJ$.) Let $H_n = \sum_{x=1}^{n-1} h_{x,x+1}$ be an $SU_q(2)$ invariant Hamiltonian on a spin $J$ chain with $n$ sites. Let $\gamma_n$ denote the spectral gap of $H_n$ and let $\epsilon_n^{(s)}$ be given by

$$
\epsilon_n^{(s)} = \min_{0 \neq \psi \perp \ker H_n} \frac{\langle \psi | H_n \psi \rangle}{\| \psi \|^2}
$$

(2.4.44)

Then the following holds

**Lemma 2.4.3 (Koma and Nachtergaele [15])** Let $H_L$ be as above. Suppose that $h_{x,x+1} \geq 0$ and that $\ker(H_L)$ is non-empty. Furthermore, suppose that $\ker(H_n)$ coincides with the irreducible representation of $SU_q(2)$ with maximal spin ($=nJ$,) for $2 \leq n \leq L$. If

$$
\epsilon_n^{(2J)} \leq \epsilon_{n+1}^{(2J)}
$$

(2.4.45)

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

$$
\gamma_L = \epsilon_L^{(2J)}
$$

(2.4.46)

The calculation with the transfer matrix, combined with Lemma 2.4.3 completes the proof of Proposition 2.4.2. Thus, for all $L \geq 2$, the spectral gap of $H_L^{+-}$ is given by

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

(2.4.47)
Thus $1 - \Delta^{-1}$ is indeed a lower bound for $\gamma$.

In order to complete the proof of Theorem 2.4.1 we must show that $\gamma$ is less than or equal to $1 - \Delta^{-1}$. This is a little subtle; upon initial inspection one can see that the gaps for $H_{GNS}^{++}$ and $H_{GNS}^{-}$ are the same by spin flip symmetry, and that the gaps for $H_{GNS}^{-}$ and $H_{GNS}^{+}$ are the same by left-right symmetry. However, the ground state of $H_{GNS}^{++}$ is non-degenerate but the ground state of $H_{GNS}^{+}$ is infinitely degenerate, so it is not so clear that the gap for $H_{GNS}^{++}$ and the gap for $H_{GNS}^{+}$ are the same. It is known that the translation invariant states are weak limits of the (anti-) kink states.

Thus,

$$\inf_{\Lambda, A \in A} \frac{\langle \Omega^{\alpha\beta} | A^* (H_{A+}^{+-}(-1,0,1))^3 A \Omega^{\alpha\beta} \rangle}{\langle \Omega^{\alpha\beta} | A^* (H_{A+}^{+-}(-1,0,1))^2 A \Omega^{\alpha\beta} \rangle} \leq \inf_{\Lambda, A \in A} \lim_{n \to \pm\infty} \frac{\langle \Omega^{\alpha\beta} | A^* (H_{A+}^{+-}(-1,0,1))^2 A \Omega^{\alpha\beta} \rangle}{\langle \Omega^{\alpha\beta} | A^* (H_{A+}^{+-}(-1,0,1))^2 A \Omega^{\alpha\beta} \rangle}$$

so $\gamma^{+-} \leq \gamma^{++}$ and hence we must only show that $1 - \Delta^{-1}$ is greater that or equal to $\gamma^{++}$ in order to finish the proof of Theorem 2.4.1. Towards this end we start with the variational principle

$$\gamma^{++} = \inf_{\psi \perp \ker H_{GNS}^{++}, \psi \in \text{dom} H_{GNS}^{++}} \frac{\langle \psi | H_{GNS}^{++} \psi \rangle}{\| \psi \|^2} \quad (2.4.49)$$

In addition we note that since $h_{x,x+1} \geq 0$, for any sequence of sets $\Lambda_1 \subset \Lambda_2 \subset \cdots, n \in \mathbb{N}$, $\mathcal{H}^{++} \supset \ker H_{\Lambda_1}^{++} \supset \ker H_{\Lambda_2}^{++} \supset \cdots$. So, if $\psi$ must be in a space orthogonal to $\ker H_{GNS}^{++}$, $\psi$ need only satisfy $\psi \perp \ker H_{\Lambda}^{++}$ for some particularly well chosen $\Lambda$.

Let $\Lambda = [1, n] \subset \mathbb{Z}$. Define the spin wave operators, $X_k$, $k \in \mathbb{Z}_n \{1, 2, \ldots, n - 1\}$ by

$$X_k = \frac{1}{\sqrt{n}} \sum_{x=1}^{k} e^{ikx} S_{x}^- \quad (2.4.50)$$
where we multiply by $1/\sqrt{n}$ so that
\[
\langle \Omega^+ | X_k^* X_l \Omega^+ \rangle = \delta_{k,l}
\] (2.4.51)

To get the upper bound we take $\psi = (c_1 X_{k_1} + c_2 X_{k_2}) \Omega^+$. Notice that $\psi$ is in the subspace of $\mathcal{H}_{++}$ with one overturned spin; specifically, $\sum_{x=1}^n S^3_x \psi = (n/2 - 1) \psi$. But for each eigenvalue $m$ of $\sum_{x=1}^n S^3_x$ there is exactly one ground state $\psi^m_0$ of $H^-_{[1,n]}$ such that $\sum_{x=1}^n S^3_x \psi^m_0 = m \psi^m_0$. Therefore for fixed distinct $k_1$ and $k_2$ we can pick $c_1$, $c_2$ such that $\psi \perp \psi^{(n-2)/2}$. But this implies that
\[
\inf_{n,k_1,k_2,c_1,c_2} \sup \frac{\langle \psi | H_{GNS}^+ \psi \rangle}{\| \psi \|^2} \geq \gamma^+
\] (2.4.52)

However, we will show that
\[
\inf_{n,k_1,k_2,c_1,c_2} \sup \frac{\langle \psi | H_{GNS}^+ \psi \rangle}{\| \psi \|^2} = 1 - \Delta^{-1}
\] (2.4.53)

which together with (2.4.52) establishes $1 - \Delta^{-1}$ as an upper bound for $\gamma^+$. For $1 \leq x, y \leq n$ define $T_{x,y}$ by
\[
T_{x,y} = \langle \Omega^+ | S^+_x H^+_{[0,n+1]} S^-_y \Omega^+ \rangle = \frac{1}{2\Delta} (2\Delta \delta_{x,y} - \delta_{x,y} - 1 - \delta_{x,y+1})
\] (2.4.54)

Then a simple, messy computation shows that the sup in (2.4.53) gives the norm of the matrix $M(n, k_1, k_2)$ whose matrix elements
\[
M(n, k_1, k_2)_{i,j} = M_n(k_i, k_j)
\]
are given by
\[
M_n(k, l) = \frac{1}{n} \sum_{x,y=1}^n e^{-ikx} T_{x,y} e^{ily} = \delta_{k,l}(1 - \Delta^{-1} \cos k) + \frac{e^{i(l-k)}}{2\Delta n}
\] (2.4.55)

for $k, l = 2\pi m/n$. Thus we have
\[
\inf_{n,k_1,k_2,c_1,c_2} \sup \frac{\langle \psi | H_{GNS}^+ \psi \rangle}{\| \psi \|^2} = \inf_{n,k_1,k_2} \| M(n, k_1, k_2) \| = 1 - \Delta^{-1}
\] (2.4.56)

which finishes the proof that $\gamma^+ \leq 1 - \Delta^{-1}$, which in turn gives us Theorem 2.4.1.

\[\blacksquare\]
2.4.2 Spin-1

For spins greater than one-half, the quantum group symmetry, which was instrumental in the calculation of the spectral gap in the spin-1/2 model, is lost. Although this makes questions about the gap for spins greater than one-half harder, it does not make them untreatable. In [17], Koma, Nachtergaele, and Starr showed that for all values of spin, there is a non-vanishing gap in the thermodynamic limit. They also conjectured that the gap grew linearly with the spin. This prediction was confirmed in [5] by Caputo and Martinelli as a corollary to results on interacting particle systems. Using the equivalence of the Markov generators for certain reaction-diffusion processes and Hamiltonians of quantum spin models, Caputo and Martinelli were able to show that for all values of anisotropy parameter $\Delta > 1$ there is a constant $\delta$ such that

$$\delta J \leq \text{gap} \left( H_{L}^{+,-,(J)} \right) \leq \delta^{-1} J$$

for all values of spin-$J$ and chains of length $L \geq 2$. Here we use techniques developed by Nachtergaele to give a concrete lower bound for the gap in the case $J = 1$. We begin by introducing the techniques for a slightly more general class of Hamiltonians than the XXZ; specifically the method will work for any Hamiltonian with frustration free ground states, so we only assume this. The method presented here has been significantly improved by Spitzer and Starr in [29], but there method is a bit more complicated, so for simplicity we present the original method here. We then give the estimate and then seek to justify it through a series of Lemmas.

The Martingale Method

We start with a spin chain on $L$ sites and label the Hilbert space as $\mathcal{H}_{L} = (\mathbb{C}^{d})^{\otimes L}$. Let $h_{1,2} \geq 0$ be a two-site Hamiltonian acting non-trivially on the first two sites, and let $h_{x,x+1}$ denote the translate of $h_{1,2}$ acting non-trivially on the factors at sites
{x, x + 1}. We consider the Hamiltonian

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

and assume that the kernel of $H_L$ is non-trivial. If $1 \leq a < b \leq L$ then we denote by $G_{[a,b]}$ the orthogonal projection onto the kernel of $\sum_{x=a}^{b-1} h_{x,x+1}$, and use the convention that $G_{\{x\}} = I$. More generally, for $\Lambda \subset [1, L]$ we set $G_{\Lambda}$ to be the orthogonal projection onto

$$\ker \sum_{x,(x,x+1) \subset \Lambda} h_{x,x+1}$$

Then the $G_{\Lambda}$ satisfy

$$G_{\Lambda_1} G_{\Lambda_2} = G_{\Lambda_2} G_{\Lambda_1} = G_{\Lambda_2} \text{ if } \Lambda_1 \subset \Lambda_2$$

$$G_{\Lambda_1} G_{\Lambda_2} = G_{\Lambda_2} G_{\Lambda_1} \text{ if } \Lambda_1 \cap \Lambda_2 = \emptyset$$

The above follows directly from the assumption that $h_{1,2} \geq 0$, and thus we have for any $\Lambda \subset [1, L]$

$$\ker H_{\Lambda} = \bigcap_{x,(x,x+1) \subset \Lambda} \ker h_{x,x+1}$$

Moreover if $\gamma$ is the smallest non-zero eigenvalue of $h_{1,2} = H_2$ then

$$h_{x,x+1} \geq \gamma (I - G_{[x,x+1]})$$

Next define the family of orthogonal projections $\{E_n : 1 \leq n \leq L\}$ by

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

Using (2.4.57) and (2.4.58) it is clear that the $E_n$'s are self-adjoint and satisfy

$$E_n E_m = \delta_{n,m} E_n$$

$$\sum_{n=1}^{L} E_n = I$$
Theorem 2.4.4 (The Martingale Method) Assume that $H$ is a Hamiltonian satisfying the properties above. Furthermore, assume that for each $n$, $1 \leq n \leq L - 1$,

$$
\|G_{[n,n+1]}E_n\| < 1/\sqrt{2} \tag{2.4.63}
$$

Then for all $\psi$ such that $G_{[1,n]}\psi = 0$

$$
\langle \psi | H \psi \rangle \geq \gamma (1 - \sqrt{2}\varepsilon)^2 \|\psi\| \tag{2.4.64}
$$

where $\varepsilon = \max_n \|G_{[n,n+1]}E_n\|$ and $\gamma$ is the spectral gap of the nearest-neighbor Hamiltonian $h_{1,2}$.

**Proof:** Take $\psi$ such that $G_{[1,n]}\psi = 0$. By (2.4.61) and (2.4.62)

$$
\|\psi\|^2 = \sum_{n=1}^{L} \|E_n\|^2
$$

but $E_n = G_{[1,n]}$ so

$$
\|\psi\|^2 = \sum_{n=1}^{L-1} \|E_n\|^2
$$

We then use $\langle \psi | h_{x,x+1} \psi \rangle$ to estimate $\|E_n\|$ by writing:

$$
\|E_n\|^2 = \langle \psi | (1 - G_{[n,n+1]})E_n \psi \rangle + \langle \psi | G_{[n,n+1]}E_n \psi \rangle
$$

then, we insert the resolution of the identity given by (2.4.62) into the second term noting that $G_{[n,n+1]}\psi = 0$ to get

$$
\|E_n\|^2 = \langle \psi | (1 - G_{[n,n+1]})E_n \psi \rangle + \langle \psi | \sum_{m=1}^{L-1} E_m G_{[n,n+1]}E_n \psi \rangle \tag{2.4.65}
$$

The second term simplifies further.

$$
E_m G_{[n,n+1]} = (G_{[1,m]} - G_{[1,m+1]})G_{[n,n+1]} = G_{[n,n+1]}(G_{[1,m]} - G_{[1,m+1]}) = G_{[n,n+1]}E_m
$$
for $m < (n - 1)$ or $m > n + 1$ by (2.4.58). But if $m \neq n$, then $E_mE_n = 0$ by (2.4.61) so that

$$
\|E_n\psi\|^2 = \langle \psi | (\mathbb{1} - G_{[n,n+1]})E_n\psi \rangle \\
+ \langle \psi | (E_{n-1} + E_n)G_{[n,n+1]}E_n\psi \rangle \\
= \langle \psi | (\mathbb{1} - G_{[n,n+1]})E_n\psi \rangle \\
+ \langle (E_{n-1} + E_n)\psi | G_{[n,n+1]}E_n\psi \rangle
$$

(2.4.66)

We now estimate both terms in (2.4.67) using the identity

$$
|\langle \varphi_1 | \varphi_2 \rangle| \leq \frac{1}{2c} \|\varphi_1\|^2 + \frac{c}{2} \|\varphi_2\|^2
$$

for $c > 0$. Hence

$$
\|E_n\psi\|^2 = \langle (\mathbb{1} - G_{[n,n+1]})\psi | E_n\psi \rangle + \langle (E_{n-1} + E_n)\psi | G_{[n,n+1]}E_n\psi \rangle
$$

(2.4.68)

$$
\leq \frac{1}{2c_1} \langle \psi | (\mathbb{1} - G_{[n,n+1]})\psi \rangle + \frac{c_1}{2} \langle \psi | E_n\psi \rangle
$$

$$
+ \frac{1}{2c_2} \langle \psi | E_nG_{[n,n+1]}E_n\psi \rangle + \frac{c_2}{2} \langle \psi | (E_{n-1} + E_n)^2\psi \rangle
$$

(2.4.69)

$$
= \frac{1}{2c_1} \langle \psi | (\mathbb{1} - G_{[n,n+1]})\psi \rangle + \frac{c_1}{2} \|E_n\psi\|^2
$$

$$
+ \frac{1}{2c_2} \|G_{[n,n+1]}E_n\psi\|^2 + \frac{c_2}{2} \|(E_{n-1} + E_n)\psi\|^2
$$

The first term in (2.4.69), $\frac{1}{2c_1} \langle \psi | (\mathbb{1} - G_{[n,n+1]})\psi \rangle$, can be estimated using (2.4.59) and gives

$$
\frac{1}{2c_1} \langle \psi | (\mathbb{1} - G_{[n,n+1]})\psi \rangle \leq \frac{1}{2c_1\gamma} \langle \psi | h_{n,n+1}\psi \rangle
$$

(2.4.70)

The third term is then treated using (2.4.63) to get

$$
\frac{1}{2c_2} \|G_{[n,n+1]}E_n\psi\|^2 \leq \frac{\varepsilon^2}{2c_2} \|E_n\psi\|^2
$$

(2.4.71)

Finally the last term can be split up as

$$
\frac{c_2}{2} \|(E_{n-1} + E_n)\psi\|^2 = \frac{c_2}{2} (\|E_{n-1}\psi\|^2 + \|E_n\psi\|^2)
$$

(2.4.72)
since $E_{n-1}$ and $E_n$ are mutually orthogonal projections. Thus by (2.4.69)-(2.4.72) we have

$$\|E_n\psi\|^2 \leq \frac{1}{2c_1\gamma} \langle \psi | h_{n,n+1} \psi \rangle + \frac{c_1}{2} \|E_n\psi\|^2 + \frac{\varepsilon^2}{2c_2}\|E_n\psi\|^2 + \frac{c_2}{2} (\|E_{n-1}\psi\|^2 + \|E_n\psi\|^2)$$

Summing over $n$ gives

$$\|\psi\|^2 \leq \frac{1}{2c_1\gamma} \langle \psi | H \psi \rangle + \left( \frac{c_1}{2} + \frac{\varepsilon^2}{2c_2} + c_2 \right) \|\psi\|^2$$

where we note that there is not an $E_0$ term and that $E_L\psi = 0$. Rearranging this expression gives the inequality

$$\langle \psi | H \psi \rangle \geq \gamma c_1 \left( 2 - c_1 - \frac{2c_2}{c_2} - 2c_2 \right) \|\psi\|^2$$

(2.4.73)

Maximizing $c_1 \left( 2 - c_1 - \frac{2c_2}{c_2} - 2c_2 \right)$ over $c_1 > 0$, $c_2 > 0$ gives $c_1 = 1 - \varepsilon / \sqrt{2}$ and $c_2 = \varepsilon / \sqrt{2}$. Substituting these into (2.4.73) gives (2.4.64).

---

**Main Result and Conjectures**

We present here an explicit lower bound of the spin-1 XXZ Hamiltonian based on the Martingale Method given above. The result relies on an, as yet, unverified assumption (2.4.63). Since the projections $G_\Lambda$ and $E_n$ all commute with $S^3_{\text{tot}} = \sum_{x=1}^{L} S^3_x$, we can first project into each sector of $S^3_{\text{tot}}$, and then check to see if assumption (2.4.63) is true. This is the strategy we employ and it is the substance of Lemma 2.4.7 and conjecture (2.4.8). We are able to verify that for a spin-1 chain of $L + 1$ sites that (2.4.63) holds in the sector of magnetization $L$. For the remainder of the sectors we are unable to verify (2.4.63) analytically, but we do have numerical evidence to support it.
We proceed as follows: In Theorem 2.4.5 we apply the Martingale Method to get a lower bound for the gap of the spin-1 XXZ Hamiltonian as a function of the two-site gap $\gamma$. In Lemma 2.4.6 we calculate the gap, $\gamma$, of the two site Hamiltonian. In Lemma 2.4.7 we calculate $\|G_{[L,L+1]} E_L\|$ in the sector with one overturned spin and show that it is less than $1/\sqrt{2}$ for all $L$, followed by the conjecture, along with numerical support, that the maximum $\|G_{[L,L+1]} E_L\|$ is achieved in the sector with one overturned spin.

**Theorem 2.4.5** Consider the spin-1 XXZ chain on $L + 1$ sites, and assume that Conjecture 2.4.8 holds. Let $\psi \neq 0$ be such that $G_{[1,L+1]} \psi = 0$. Then
\[
\inf_{\psi} \frac{\langle \psi | H_{L+1} \psi \rangle}{\| \psi \|^2} \geq \gamma \left( 1 - \sqrt{\frac{2q^2}{1 + q^2} \cdot \frac{1 - q^{2L}}{1 - q^{2L+2}}} \right)^2
\]
(2.4.74)
where $\gamma$ is the gap of the two-site Hamiltonian given by $\frac{5}{2} - \sqrt{\frac{9}{4} - \frac{2}{\Delta^2}}$.

**Lemma 2.4.6 (\(\gamma\): gap of \(h_{1,2}\))** Let $h_{1,2}$ be given by
\[
h_{1,2} = -\frac{1}{\Delta} (S_1^1 S_2^1 + S_1^2 S_2^2) - S_1^3 S_2^3 - A(\Delta) (S_1^3 - S_2^3) + 1
\]
and let $\psi \neq 0$. Then
\[
\gamma = \min_{\psi: G_{[1,2]} \psi = 0} \frac{\langle \psi | h_{1,2} \psi \rangle}{\| \psi \|^2} = \frac{5}{2} - \sqrt{\frac{9}{4} - \frac{2}{\Delta^2}}
\]
(2.4.75)

**Proof:** This is really more of a calculation than a proof. The calculation proceeds in the following way: Let $P_m$ be the projection onto the subspace of $\mathcal{H}_2$ with total $S^3$ component equal to $m$. We calculate $\gamma_m = \text{gap}(P_m h_{1,2} P_m)$ for $m = -2, -1, \ldots, 2$, which is just the first non-zero eigenvalue since $h_{1,2}$ has a non-trivial kernel. Then $\gamma$ is just the minimum of the $\gamma_m$. For $m = \pm 2$ the subspaces are one dimensional and both vectors are ground states. For $m = \pm 1$ both $P_{\pm 1} h_{1,2} P_{\pm 1}$ can be expressed as the matrix
\[
P_{\pm 1} h_{1,2} P_{\pm 1} = \begin{pmatrix} 1 + A(\Delta) & -\frac{1}{\Delta} \\ -\frac{1}{\Delta} & 1 - A(\Delta) \end{pmatrix}
\]
(2.4.76)
where $A(\Delta) = \sqrt{1 - 1/\Delta^2}$. The matrix has eigenvalues 0 and 2, so we see that

$$\gamma_{\pm 1} = 2 \quad (2.4.77)$$

For $m = 0$, $P_0 h_{1,2} P_0$ the matrix is

$$P_0 h_{1,2} P_0 = \begin{pmatrix}
2(1 - A(\Delta)) & -\frac{1}{\Delta} & 0 \\
-\frac{1}{\Delta} & 1 & -\frac{1}{\Delta} \\
0 & -\frac{1}{\Delta} & 2(1 + A(\Delta))
\end{pmatrix} \quad (2.4.78)$$

Here the matrix also has a zero eigenvalue; when $\lambda$ is factored out of the characteristic equation we get

$$\lambda^2 - 5\lambda + \left(\frac{2}{\Delta^2} + 4\right) = 0$$

This has roots

$$\lambda = \frac{5}{2} \pm \sqrt{\frac{9}{4} - \frac{2}{\Delta^2}}$$

so we get

$$\gamma_0 = \frac{5}{2} - \sqrt{\frac{9}{4} - \frac{2}{\Delta^2}} \quad (2.4.79)$$

Taking the minimum of (2.4.77) and (2.4.79) we see that

$$\gamma = \frac{5}{2} - \sqrt{\frac{9}{4} - \frac{2}{\Delta^2}} \quad (2.4.80)$$

We now show that in the sector with magnetization $L$, $\|G_{[L,L+1]} E_L\| < 1/\sqrt{2}$ for all $q \in (0, 1)$. This is the first step in verifying (2.4.63) for the spin-1 chain. We mention that the calculation given here for the spin-1 case immediately generalizes to higher $J$, but we do not present that here. Let $P_m$ be the orthogonal projection onto the sector with total $S^3$ component equal to $m$. Then define $\varepsilon_m \equiv \|P_m G_{[L,L+1]} E_L P_m\|$. 

**Lemma 2.4.7** $\varepsilon_L = \left[\frac{(1-q^2)}{(1-q^2-1+q^2)} \cdot \frac{q^2}{1+q^2}\right]^{1/2} < \left[\frac{q^2}{1+q^2}\right]^{1/2}$. Thus for all values of $q$ in $(0, 1)$, $\varepsilon_L < 1/\sqrt{2}$. 
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Proof: To begin with we write

$$\psi_{L+1}^L = \psi_{L}^{L-1} \otimes |\uparrow\rangle + \sqrt{2q^{-L-1}} \psi_{L}^{L} \otimes |0\rangle$$ (2.4.81)

where $\psi_{N}^{M}$ is a spin-1 groundstate on a chain of length $N$ with total $S^3$ component $M$. Define

$$\varphi = \sqrt{2q^{-L-1}} \frac{\psi_{L}^{L-1} \otimes |\uparrow\rangle - \psi_{L}^{L} \otimes |0\rangle}{\|\psi_{L}^{L-1}\|^2}.$$ 

Now $\varepsilon_{L} = \frac{\|G[\varphi]\|}{\|\varphi\|}$, so we calculate $G[\varphi]$:

$$G[\varphi] = G[\psi_{L}^{L-1}] \left( \frac{\sqrt{2q^{-L-1}} \psi_{L}^{L-1} \otimes |\uparrow\rangle - \psi_{L}^{L} \otimes |0\rangle}{\|\psi_{L}^{L-1}\|^2} \right)$$

$$= \sqrt{2q^{-L-1}} \frac{\psi_{L}^{L-2} \otimes |m = 2\rangle + \frac{1}{\sqrt{1 + q^2}} \left( 2q^{-2L} - 1 \right) \psi_{L}^{L-1} \otimes |m = 1\rangle}{\|\psi_{L}^{L-1}\|^2}$$

$$= \sqrt{2q^{-L-1}} \frac{\psi_{L}^{L-2} \otimes |m = 2\rangle - \frac{1}{\sqrt{1 + q^2}} \frac{\|\psi_{L}^{L-1}\|^2}{\|\psi_{L}^{L-1}\|^2} \frac{\psi_{L}^{L-1} \otimes |m = 1\rangle}{\|\psi_{L}^{L-1}\|^2}}$$

where $|m = k\rangle$ is the ground state of $H_{L,L+1}$ such that

$$\langle S_{L}^3 + S_{L+1}^3 | m = k \rangle = k \cdot |m = k\rangle$$

Calculating $\|G[\varphi]\|^2$, we get

$$\|G[\varphi]\|^2 = \frac{1}{\|\varphi\|^2} \left( 2q^{-2L-2} \|\psi_{L}^{L-2}\|^2 + \frac{\|\psi_{L}^{L-2}\|^4}{1 + q^2} \right)$$

But $2q^{-2L-2} + 2q^{-2L} + \|\psi_{L}^{L-2}\|^2 = \|\psi_{L+1}^{L}\|^2$ so we have

$$\|G[\varphi]\|^2 = \frac{\|\psi_{L}^{L-1}\|^2 \|\psi_{L}^{L+1}\|^2}{\|\psi_{L}^{L+1}\|^4 (1 + q^2)}$$ (2.4.82)

On the other hand

$$\|\varphi\|^2 = \frac{\|\psi_{L+1}^{L}\|^2}{\|\psi_{L}^{L-1}\|^2}$$
so that
\[ \varepsilon^2_L = \frac{\|G_{[L,L+1]} \varphi\|^2}{\|\varphi\|^2} = \frac{\|\psi_{L-1}^L\|^2}{\|\psi_{L-1}^L\|^2} \cdot \frac{1}{1 + q^2}. \quad (2.4.83) \]
Substituting \( \|\psi_{L-1}^L\|^2 = 2 \sum_{x=1}^{L} q^{-2x} \) into (2.4.83) gives the expression
\[ \varepsilon^2_L = \frac{(1 - q^{2L})}{(1 - q^{2L+2})} \cdot \frac{q^2}{1 + q^2}. \quad (2.4.84) \]
Hence \( \varepsilon^2_L < 1/2 \) since for \( q \in (0, 1) \), \( (1 - q^{2L})/(1 - q^{2L+2}) < 1 \) and \( q^2/(1 + q^2) < 1/2 \).

What remains in order to verify assumption (2.4.63), is to show that in sectors with \( m < L \), \( \varepsilon_m \leq \varepsilon_L \). As stated previously this is really the hard part. At this point we are unable to prove this analytically, but we state the conjecture here and provide a little justification, both numeric and heuristic.

**Conjecture 2.4.8** \( \varepsilon_m \leq \varepsilon_L \) for all \( m \) such that \( -L \leq m < L \).

Some of the strongest evidence we have for this conjecture is numeric. We show here the values of \( \varepsilon_m \) in all sectors for a chain of length eight and various values of \( \Delta \).

The general shape persists for all values of \( L \) that we have tried (up to 11,) and moreover, for fixed \( \Delta \) the values of \( \varepsilon_m \) stabilize very quickly relative to the number of downspins, i.e. in the sector corresponding to \( k \) downspins for chains of length six, seven, or eight the \( \varepsilon_{L-k} \) varies no more that one part in a thousand. We include our code at the end of this paper in Appendix C.

It is easy to compute that in the Ising limit (\( \Delta \to \infty \)), we get \( \varepsilon_m = 0 \) for all \( m \). We hope to prove Conjecture 2.4.8 for at least most values of \( \Delta \) by performing perturbation around the Ising case. This should be possible since for long chains the ground states of the XXZ Hamiltonian can be thought of as perturbations of the Ising ground states. One also notices that \( \varepsilon_m \) becomes very small, i.e. close to the value in the Ising case, for relatively small values of \( \Delta \) (\( \Delta \approx 2 \)). This behavior gives us a hope of being able to prove Conjecture 2.4.8 for at least some values of \( \Delta \).
Figure 2.1: Some plots of $\varepsilon_m$ for a chain of length $L = 8$ for different values of $\Delta$.

The following is a plot comparing the true gap of the XXZ Hamiltonian for a chain of length $L$ to the lower bound given by Theorem 2.4.5. The anisotropy parameter $\Delta$ varies between 1 and 20.

The plot shows that the estimate captures the behavior of the true gap very well. Over the interval $1 \leq \Delta \leq 20$, the estimate is only off by 17% on average. The maximum error occurs for $\Delta$ close to 1 and at this point the estimate is off by about 70% from the true gap, but as $\Delta$ grows and gets closer to 20 the error shrinks to about 7% of the actual gap.
A comparison of the true gap of the XXZ Hamiltonian vs. the lower bound given the Martingale Method.

Figure 2.2: The upper plot is the true spectral gap of the XXZ chain on $L$ sites. The lower plot is the estimated gap from Theorem 2.4.5. ($1 \leq \Delta \leq 20$)
Chapter 3

XY Model

3.1 Introduction

Understanding phase transitions, for example ice to water, or non-magnetic to magnetic, is one of the central questions of statistical mechanics. Spin systems were initially introduced by Lenz in 1920 to try to explain the tendency of some materials to possess macroscopic magnetic fields. He proposed a simple model in which atoms in a crystal could assume two possible orientations which later came to be called the Ising model [3]. It was Ising’s failure, in 1925, to discover a phase transition in Lenz’s model which led Heisenberg to introduce quantum spin models in 1928. In 1935, Peierls gave an argument that demonstrated that the Ising model does exhibit phase transitions in two and greater dimensions [24]. Although Peierls’ argument was not completely rigorous it did contain all the essential ideas required for the desired result. The Peierls’ argument was later made rigorous by Griffiths [9], and Dobrushin [6].

Mathematically, phase transitions are associated with a singularity in some thermodynamic potential, generally the free energy. While the Ising model is a classical model, it has become the basis for understanding magnetic phase transitions in quan-
tum mechanical models. The Ising Hamiltonian is given by

\[ H_{\Lambda}(\{s_x\}) = -\sum_{x,y \in \Lambda, |x-y|=1} s_x s_y - h \sum_{x \in \Lambda} s_x \]  

(3.1.1)

where \( \Lambda \) is a finite subset of \( \mathbb{Z}^d \), \( h \) is some positive number, and \( \{s_x\} \) is in the set \( \Omega_{\Lambda} = \{\pm 1\}^\Lambda \). The partition function of the system \( Z_{\Lambda}(h, \beta) \) is given by

\[ Z_{\Lambda}(h, \beta) = \sum_{\{s_x\} \in \Omega_{\Lambda}} e^{-\beta H_{\Lambda}(\{s_x\})} \]  

(3.1.2)

For any thermodynamic variable, \( X \), defined on \( \Omega_{\Lambda} \), we define the expectation of \( X \) at inverse temperature \( \beta \) by

\[ \omega_{h,\beta}(X) = \lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{Z_{\Lambda}(h, \beta)} \sum_{\{s_x\} \in \Omega_{\Lambda}} X(\{s_x\}) e^{-\beta H_{\Lambda}(\{s_x\})} \]  

(3.1.3)

In dimension two and greater the Ising Model exhibits spontaneous magnetization. Consider the average magnetization at a particular site, \( m(h, \beta) = \omega_{h,\beta}(s_0) \). Then there is a constant \( \beta_c = \beta_c(d) \), such that for all \( \beta > \beta_c \), \( m(h, \beta) \) is discontinuous at \( h = 0 \). Specifically

\[ \lim_{h \to 0^-} m(h, \beta) = -\lim_{h \to 0^+} m(h, \beta) \]  

(3.1.4)

for all \( \beta > \beta_c(d) \). This implies that the free energy, \( f(h, \beta) \), is not analytic at \( h = 0 \) since

\[ m(h, \beta) = \left. \frac{\partial}{\partial h} (f(h, \beta)) \right|_\beta \]  

(3.1.5)

Physically, the discontinuity in \( m(h, \beta) \) at \( h = 0 \), can be interpreted as the system “remembering” the effects of an external magnetic field after the field has been removed, i.e. it continues to possess a macroscopic magnetic field.

The phase diagram of the XY model has been the subject of much study. For high temperature, one can use a high-temperature expansion to show that there is a unique phase. To see an excellent discussion of such techniques see [26]. In [4] Dyson, Lieb, and Simon showed that, in the absence of an external magnetic field, the spin-1/2
XY model does have a phase transition for positive temperature in dimensions greater than two. The Mermin-Wagner theorem shows that for positive temperature this result cannot be extended to dimension two. In a later paper, Kennedy, Lieb, and Shastry demonstrated that in dimensions two and greater the ground state of the XY model has off-diagonal long-range order.

![Phase Diagram](image)

Figure 3.1: The phase diagram for the XY Model. The numbered regions are: 1. \((h = 0)\) For dimension three and greater Dyson, Lieb, and Simon showed that LRO exists for \(T > 0\). 2. For spins bigger than one-half and dimensions two or greater, Kennedy, Lieb, and Shastry showed the groundstate has LRO. 3. The low-temperature/small \(h\) regime is the most interesting, but nothing is known (the shape of the curve is unknown.) 4. We show that there is a low-temperature/large \(h\) region in which there is no phase transition.

Here we show that the free energy of the XY model in the presence of an external magnetic field above a critical strength, is analytic for some region of non-zero temperature in dimension two and greater. The more interesting regime is when \(h < h_c = 2d\), where there is a connection to Bose-Einstein condensation.
results do not extend to this case.

We consider a perturbation of the spin-$\frac{1}{2}$ XY model by a uniform magnetic field in the $z$ direction. The strength of the magnetic field is great enough so that there is a unique ground state of all “up” spins. We use a contour expansion inspired by Kennedy in [12] to extend the uniqueness of phase to non-zero temperatures.

Take $\mathcal{H}_\Lambda = \left( \mathbb{C}^2 \right)^{\otimes |\Lambda|}$ where $\Lambda \subset \mathbb{Z}^d$, $d \geq 2$, and $|\Lambda| < \infty$. For $x, y \in \Lambda$ such that $|x - y| = 1$ we write $\{x, y\} \equiv (x, y)$. The Hamiltonian is defined as follows:

$$H'_\Lambda \equiv H^{XY}_\Lambda + h H^Z_\Lambda, \quad h \geq h_c(d) = 2$$ (3.1.6)

where

$$H^{XY}_\Lambda = -\sum_{(x,y) \subset \Lambda} \frac{1}{2} (\sigma_x^1 \sigma_y^1 + \sigma_x^2 \sigma_y^2) = \sum_{(x,y) \subset \Lambda} (\sigma_x^+ \sigma_y^- + \sigma_x^- \sigma_y^+)$$ (3.1.7)

and

$$H^Z_\Lambda = \sum_{x \in \Lambda} \frac{1}{2} (\mathbb{1} - \sigma_x^3)$$ (3.1.8)

The operators $\sigma^1$, $\sigma^2$, and $\sigma^3$ are the Pauli spin matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where the subscript denotes the site on which they act. We take the strength of the magnetic field $h$ to be greater than some $h_c(d)$ so that the unique state is the all up state $|\uparrow\rangle^\Lambda$ given by

$$|\uparrow\rangle^\Lambda = \bigotimes_{x \in \Lambda} |\uparrow\rangle_x$$ (3.1.9)

For the remainder of this chapter we will work with the scaled Hamiltonian

$$H_\Lambda \equiv (1 - \delta) H^{XY}_\Lambda + h_c H^Z$$ (3.1.10)

where the parameter $\delta$ is given by the equation

$$1 - \delta = \frac{h}{h_c}$$ (3.1.11)
By (3.1.6), $h > h_c$ so we have $\delta \in (0, 1)$.

Let

$$Z_\Lambda(\delta, \beta) = \text{Tr} e^{-\beta H_\Lambda}$$  \hspace{1cm} (3.1.12)

be the partition function. Our goal is to show that the free energy

$$f(\delta, \beta) = -\frac{1}{\beta} \lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \left[ \text{Tr} e^{-\beta H_\Lambda} \right]$$  \hspace{1cm} (3.1.13)

is analytic for all $(\delta, \beta)$ in some appropriate region, and hence that no first-order phase transition exists. In order to do this, we will express $Z_\Lambda(\delta, \beta)$ as a contour expansion. Then, we follow Kennedy in [12], and show that the partition function can be rewritten as a cluster expansion. The key to this is Theorem 3.3.2 which shows that the weights of the contours decay in an appropriate way. Once the cluster expansion is established the analyticity of $f(\delta, \beta)$ follows immediately, as the cluster expansion is a uniform limit of analytic functions.

### 3.2 Basic Definitions

A set $\mathcal{A} \subset \Lambda$ will be called a **contour**. This differs from the usual definition of contours as set of bonds separating lattice sites with opposite spins. This is okay though, because in the model we consider the ground state does not possess the spin-flip symmetry that generally introduces ambiguities. A connected set $P \subset \Lambda$ will be called a **polymer**. To each contour $\mathcal{A} \subset \Lambda$ let $|\mathcal{A}\rangle$ denote the basis vector of $\mathcal{H}_\Lambda$ such that

$$|\mathcal{A}\rangle = \otimes_{x \in \Lambda} |\mathcal{A}\rangle_x, \quad |\mathcal{A}\rangle_x = \begin{cases} |\uparrow\rangle & x \in \Lambda \setminus \mathcal{A} \\ |\downarrow\rangle & x \in \mathcal{A} \end{cases}$$  \hspace{1cm} (3.2.14)

Furthermore, if $(\sigma_x^+ \sigma_y^- + \sigma_x^- \sigma_y^+)|\mathcal{A}\rangle \neq 0$ then we will denote the corresponding contour by $(\sigma_x^+ \sigma_y^- + \sigma_x^- \sigma_y^+).$
Returning to $Z_\Lambda(\delta, \beta)$, by the Trotter product formula, we can express $e^{-\beta H}$ as

$$e^{-\beta H} = \lim_{N \to \infty} \left[ e^{-\frac{\beta \hbar}{N} \frac{\partial Z}{\partial \Lambda}} \left( 1 - \frac{\beta (1 - \delta)}{N} H_{XY}^{\Lambda} \right) \right]^N$$

so that

$$Z_\Lambda(\delta, \beta) = \text{Tr} e^{-\beta H} = Z_\Lambda = \lim_{N \to \infty} \sum_{\alpha \subset \Lambda} \langle \alpha | e^{-\frac{\beta \hbar}{N} \frac{\partial Z}{\partial \Lambda}} \left( 1 - \frac{\beta (1 - \delta)}{N} H_{XY}^{\Lambda} \right) \right] N \langle \alpha \rangle$$

inserting a resolution of the identity between each term in the product we can write the above as

$$\text{Tr} e^{-\beta H} = \lim_{N \to \infty} \sum_{\alpha_0, \ldots, \alpha_{N-1}} \langle \alpha_0 | e^{-\frac{\beta \hbar}{N} \frac{\partial Z}{\partial \Lambda}} \left( 1 - \frac{\beta (1 - \delta)}{N} H_{XY}^{\Lambda} \right) \right] \langle \alpha_1 | \ldots \langle \alpha_{N-1} | e^{-\frac{\beta \hbar}{N} \frac{\partial Z}{\partial \Lambda}} \left( 1 - \frac{\beta (1 - \delta)}{N} H_{XY}^{\Lambda} \right) \right] \langle \alpha_0 \rangle$$

Taking this new expression for $Z_\Lambda(\delta, \beta)$ we see that the non-zero terms in the sum are characterized by sequences of contours $\{\alpha_0, \alpha_1, \ldots, \alpha_N\}$ with the following properties

(i) $\alpha_0 = \alpha_N$

(ii) $\alpha_{i+1} = \begin{cases} \alpha_i \\ \text{or} \\ (\sigma_x^+ \sigma_y^- + \sigma_x^- \sigma_y^+) \alpha_i \end{cases}$ for some $\langle x, y \rangle$

This motivates the following definition

**Definition 3.2.1** A quantum contour $\Gamma = \{\Gamma_0, \Gamma_2, \ldots, \Gamma_N\}$ is a sequence of contours satisfying

(i) $\Gamma_0 = \Gamma_N$

(ii) $\Gamma_{n+1} = \begin{cases} \Gamma_n \\ \text{or} \\ (\sigma_x^+ \sigma_y^- + \sigma_x^- \sigma_y^+) \Gamma_n \end{cases}$ where $|x - y| = 1$
Figure 3.2: The spin-flips for the above quantum contour are \(1 \rightarrow 2: (C4, D4), 2 \rightarrow 3: (F4, G4), 3 \rightarrow 4: (F3, G3), 4 \rightarrow 5: (F3, F4), 5 \rightarrow 6: (G3, G4), 6 \rightarrow 1: (C4, D4)\)

We now write

\[
Z_\Lambda(\delta, \beta) = \lim_{N \to \infty} \sum_{\alpha_0, \ldots, \alpha_{N-1}} \langle \alpha_0 | e^{-\frac{\beta h c}{N} H_\Lambda^Z} \left( 1 - \frac{\beta (1 - \delta) N}{1 - \beta (1 - \delta) N} H_\Lambda^{XY} \right) | \alpha_1 \rangle \langle \alpha_1 | \ldots \langle \alpha_{N-1} | e^{-\frac{\beta h c}{N} H_\Lambda} \left( 1 - \frac{\beta (1 - \delta) N}{1 - \beta (1 - \delta) N} H_\Lambda^{XY} \right) | \alpha_0 \rangle
\]

\[
= \lim_{N \to \infty} \sum_{\Gamma} \omega(\Gamma)
\]

(3.2.16)

where

\[
\omega(\gamma) = e^{-\beta h c |\Gamma_0|} \left( \frac{\beta (1 - \delta) N}{1 - \beta (1 - \delta) N} \right)^{n(\Gamma)}
\]

(3.2.17)

and \(n(\Gamma)\) is the number of times \(\Gamma_{i+1} = (\sigma_x^+ \sigma_y^- + \sigma_x^- \sigma_y^+)\Gamma_i\) in the quantum contour \(\Gamma\).

Let \(S(\Gamma) = \bigcup \Gamma_n\) be called the support of a quantum contour \(\Gamma\). If \(S(\Gamma)\) is connected, then \(\Gamma\) will be called connected. We will use \(\gamma\) to denote a connected quantum contour. Two connected quantum contours \(\gamma^1\) and \(\gamma^2\) are disjoint if \(S(\gamma^1) \cup S(\gamma^2)\) is not connected.
For a given quantum contour $\Gamma$, $S(\Gamma)$ can be written as the disjoint union of connected parts

$$S(\Gamma) = \bigcup_{j=1}^{k} S^j(\Gamma)$$

Then, $\Gamma$ can be split up into connected parts by

$$\gamma^j_n = \Gamma_n \cap S^j(\Gamma)$$

and we write $\Gamma = \sqcup \gamma^j$. We call two general quantum contours $\Gamma_1$ and $\Gamma_2$ disjoint if all there connected components are disjoint in the sense of connected quantum contours defined above.

With these definitions fixed consider a quantum contour $\Gamma = \Gamma^1 \sqcup \Gamma^2$, then $\omega(\Gamma)$ will factorize in the following way

$$\omega(\Gamma) = e^{-\beta h_c |\Gamma_0|} \left( \frac{\beta(1 - \delta)}{N} \right)^{n(\Gamma)}$$

But, $\Gamma = \Gamma^1 \sqcup \Gamma^2$ so that

$$|\Gamma_0| = |\Gamma_0^1| + |\Gamma_0^2|$$

$$n(\Gamma) = n(\Gamma^1) + n(\Gamma^2)$$

Thus

$$\omega(\Gamma) = e^{-\beta h_c |\Gamma_0^1|} \left( \frac{\beta(1 - \delta)}{N} \right)^{n(\Gamma^1)} e^{-\beta h_c |\Gamma_0^2|} \left( \frac{\beta(1 - \delta)}{N} \right)^{n(\Gamma^2)}$$

$$= \omega(\Gamma^1)\omega(\Gamma^2)$$
CHAPTER 3. XY Model

So that

\[
\text{Tr } e^{-\beta H_N} = \lim_{N \to \infty} \sum_{\Gamma} \omega(\Gamma) = \lim_{N \to \infty} \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\gamma_1, \ldots, \gamma_n \text{ all disjoint}} \prod_{j=1}^{n} \omega(\gamma_j)
\]

(3.2.22)

Now, for a polymer \(P\), we define

\[
W(P) = \lim_{N \to \infty} \sum_{\gamma: S(\gamma) = P} \omega(\gamma)
\]

(3.2.23)

Using these new weights we can re-write the partition function as

\[
Z_\Lambda(\delta, \beta) = \lim_{N \to \infty} \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\gamma_1, \ldots, \gamma_n \text{ all disjoint}} \prod_{j=1}^{n} \omega(\gamma_j)
\]

(3.2.24)

\[
= \sum_{n=1}^{\infty} \sum_{\{P_1, \ldots, P_n\}} \prod_{i=1}^{n} W(P)
\]

(3.2.25)

These are all the basic definitions which we need to apply the cluster expansion

3.3 Cluster Expansion

Cluster expansions were introduced as a perturbative method for high-temperature gases. They apply to continuous systems, e.g. classical interacting particle systems, as well as discrete systems such as lattice particle models, polymer models, or, as in our case, spin models. There are many good references, perhaps the most accessible being Simon’s book on lattice gases [27], while the treatise by Brydges [4] is also excellent. Others include [10], [18], [25], [6], [2], and [26]. The basic goal of the cluster expansion is to give an expression for the partition function of some system that can be more easily manipulated that the standard expression as the sum of exponentials. Here we present a condition for the convergence of the cluster expansion attributed to Kotecky and Preiss [18]. The proof is taken from Ueltschi in [31]. Although the
setting of $\mathbb{R}^2$ is both continuous and discrete space, here we only need the discrete case.

Let $\mathbb{A}$ be a finite set whose elements are called polymers. Let $\iota$ be a symmetric and reflexive relation on $\mathbb{A} \times \mathbb{A}$. For polymers $A, A' \in \mathbb{A}$ we say that $A$ and $A'$ are incompatible if $A \iota A'$ and are compatible otherwise. The partition function of the polymer model is

$$Z(\mathbb{A}) = \sum_{n=1}^{\infty} \sum_{\{A_1, \ldots, A_n\}} \prod_{i=1}^{n} w(A_i)$$

(3.3.26)

where the $w$ is a complex function on $\mathbb{A}$ and the sum is over sets of polymers whose elements are pairwise compatible.

A sequence $C = (A_1, \ldots, A_n)$ of polymers is called a cluster if $\{A_1, \ldots, A_n\}$ can not be partitioned into two sets, all the elements in the first being compatible with all the elements in the second. We can make this definition more visual. Consider the graph $G(C)$ with $n$ vertices where there is an edge between $i$ and $j$ whenever $A_i \iota A_j$. $C$ is a cluster iff $G(C)$ is connected. We write $G \subset G(C)$ if $G$ is a graph with the same number of vertices as $G(C)$ and whose edges form a subset of the edges of $G(C)$; $|G|$ denotes the number of edges of $G$. Define a function, $\varphi(C)$, on clusters given by

$$\varphi(C) = \begin{cases} 1 & \text{if } n = 1 \\ \sum_{G \subseteq G(C), \text{connected}} (-1)^{|G|} & \text{if } n \geq 2 \end{cases}$$

(3.3.27)

and a function $\Phi(C)$ on clusters by

$$\Phi(C) = \frac{1}{n!} \varphi(C) \prod_{i=1}^{n} w(A_i)$$

(3.3.28)

where $C = (A_1, \ldots, A_n)$. The following theorem is due to Kotecky and Preiss [18]. It says that if the weight function on the polymers, $w$, satisfies some condition then the logarithm of the partition function $Z(\mathbb{A})$ can be given by a sum over clusters.

**Theorem 3.3.1** Let $a$ and $b$ be non-negative functions on $\mathbb{A}$ such that for all $A \in \mathbb{A}$

$$\sum_{A' : A' \iota A} |w(A')| e^{a(A') + b(A')} \leq a(A)$$

(3.3.29)
Then,
\[ Z(A) = \exp \left( \sum_C \Phi(C) \right) \] (3.3.30)
where the sum converges absolutely. Furthermore
\[ \sum_{C \cup A} |\Phi(C)| e^{b(C)} \leq a(A) \] (3.3.31)
where \( C \cup A \) means that \( A \) is incompatible with at least one polymer in \( C = (A_1, \ldots, A_n) \) and \( b(C) = \sum_{i=1}^{n} b(A_i) \).

So, in order to show that \( f(\delta, \beta) \) is analytic, we prove that the weights of the polymers \( W(P) \) given in (3.2.23) satisfies condition (3.3.29). Then Theorem 3.3.1 allows us to write
\[ f(\delta, \beta) = -\frac{1}{\beta} \lim_{\Lambda \to \mathbb{Z}^2} \frac{1}{|\Lambda|} \ln Z(\delta, \beta) \] (3.3.32)
which is the sum of analytic functions. Then the analtycity of \( f(\delta, \beta) \) follows from the uniform convergence of this sum. To this end we state and prove the following proposition and leave the proof of Theorem 3.3.1 to Appendix B.

**Proposition 3.3.2** Given \( \delta \) where \( 0 \leq \delta < 1 \), there exists a \( \beta_0 \) and an \( \varepsilon \) such that for all \( \beta \geq \beta_0 \)
\[ \sum_{P \ni y} W(P)e^{\varepsilon|P|} \leq \varepsilon \] (3.3.34)
where \( y \in \mathbb{Z}^2 \) is fixed.

Proposition (3.3.2) immediately gives us (3.3.29) since
\[ \sum_{P \ni y} W(P)e^{\varepsilon|P|} \leq \sum_{y \in P'} \sum_{P \ni y} W(P)e^{\varepsilon|P|} \leq \sum_{y \in P'} \varepsilon \leq \varepsilon|P'| \] (3.3.35)

**Proof:** Initially we will express the sum \( \sum_{P \ni y} W(P)e^{\varepsilon|P|} \) as a sum over contours. Recall that
\[ W(P) = \lim_{N \to \infty} \sum_{\gamma: S(\gamma) = P} \omega(\gamma) \]
So, $\sum_{P \ni y} W(P) e^{\varepsilon |P|}$ can be re-written as

$$\sum_{P \ni y} W(P) e^{\varepsilon |P|} = \sum_{P \ni y} \left( \lim_{N \to \infty} \sum_{\gamma : S(\gamma) = P} \omega(\gamma) \right) e^{\varepsilon |P|} \tag{3.3.36}$$

$$= \lim_{N \to \infty} \sum_{\gamma \ni y} \omega(\gamma) e^{\varepsilon |S(\gamma)|} \tag{3.3.37}$$

where we have written $\gamma : y$ for the condition $y \in S(\gamma)$. Let the new Hamiltonian $H^0_\Lambda$ be given by

$$H^0_\Lambda = \left( 1 - \frac{\delta}{2} \right) \left( H^{XY}_\Lambda + h_c H^Z_\Lambda \right) \tag{3.3.38}$$

and define the modified weights $\omega_0(\gamma)$ by

$$\omega_0(\gamma) = e^{-\beta(1-\delta/2)h_c|\gamma_0|} \left( \frac{(1-\delta/2)\beta}{N} \right)^{n(\gamma)} \tag{3.3.39}$$

which are just the weights of a quantum contour $\gamma$ when $H_\Lambda$ is replaced by $H^0_\Lambda$ in the expansion of the partition function $Z_\Lambda(\delta, \beta)$. The weights $\omega(\gamma)$ and $\omega_0(\gamma)$ are related by

$$\omega(\gamma) = m(\gamma) \omega_0(\gamma) \tag{3.3.40}$$

where the multiplier $m(\gamma)$ is

$$m(\gamma) = e^{-\beta \frac{\delta}{2} h_c |\gamma_0|} \rho^{n(\gamma)}, \quad \rho = \frac{1 - \delta}{1 - \delta/2} < 1 \tag{3.3.41}$$

Thus, the sum on the right side of equation (3.3.37) can be expressed as

$$\sum_{\gamma \ni y} \omega(\gamma) e^{\varepsilon |S(\gamma)|} = \sum_{\gamma \ni y} \omega_0(\gamma) e^{-\beta \frac{\delta}{2} h_c |\gamma_0|} \rho^{n(\gamma)} e^{\varepsilon |S(\gamma)|} \tag{3.3.42}$$

Let $F(\gamma)$ be the set of spins that flip at least once in $\gamma$ then $F(\gamma)$ satisfies the inequalities

$$|S(\gamma)| \leq |F(\gamma)| + |\gamma_0| \tag{3.3.43}$$

and

$$|F(\gamma)| \leq 2n(\gamma) \tag{3.3.44}$$
Inequality (3.3.43) follows since $F(\gamma)$ contains all the spins that flip and any $\gamma_i$ contains all the spins that never flip, and we get inequality (3.3.45) from the fact that for every occurrence of a spin flip in $\gamma$ two spins change, but it might be possible for certain spins to change more than once in the course of a quantum contour $\gamma$.

From inequalities (3.3.43) and (3.3.45) we get $|S(\gamma)| \leq 2n(\gamma) + |\gamma|$, which in turn implies
\[
e^{-\beta \delta h c} e^{\frac{\epsilon n(\gamma)}{2}} \leq e^{-\beta \delta h c} e^{\epsilon |\gamma|}.
\]

From the above inequality we can determine
\[
e^{-\beta \delta h c} e^{\frac{\epsilon n(\gamma)}{2}} \leq e^{(-\beta \delta h c + \epsilon) |\gamma|} \cdot \left( \rho^{1/2} e^{\epsilon} \right)^{n(\gamma)} \leq 1
\]
for $\beta$ large enough, and $\epsilon$ small enough. Applying this estimate to (3.3.42) we get
\[
\sum_{\gamma : y} \omega(\gamma) e^{\epsilon |S(\gamma)|} \leq \sum_{\gamma : y} \omega(\gamma) \rho^{\frac{n(\gamma)}{2}} e^{-\beta \delta h c |\gamma|}
\]
(3.3.47)

We now re-write the sum on the right side as a sum over initial configurations $\gamma_0$ and then a sum over quantum contours with that initial state. This gives the expression
\[
\sum_{\gamma : y} \omega(\gamma) \rho^{\frac{n(\gamma)}{2}} e^{-\beta \delta h c |\gamma|} = \sum_{G \subset \Lambda} \sum_{\gamma : \gamma_0 = G, y} \omega(\gamma) \rho^{\frac{n(\gamma)}{2}} e^{-\beta \delta h c |G|}
\]
(3.3.48)

where we have used $\gamma : G$ to indicate the sum is over quantum contours $\gamma$ such that $\gamma_0 = G$.

Let $D_y(G)$ be the number defined as follows: A set $K \subset \Lambda$ will be called $G, y$-connecting if the set $(K \cup G \cup \{y\}) \subset \Lambda$ is connected. $D_y(G)$ is then defined as
\[
D_y(G) = \min\{|K| : K \text{ is } G, y \text{- connecting}\}
\]
(3.3.49)

In other words, $D_y(G)$ is the minimum number of sites required to make $G \cup \{y\}$ a connected set. Since $\gamma$ is a connected contour, $F(\gamma)$ is $\gamma_0, y$-connecting, hence
\[
D_y(\gamma_0) \leq |F(\gamma)| \leq 2n(\gamma)
\]
(3.3.50)
This allows one to bound the term $\rho^{\gamma(\gamma)/2}$ by $\rho^{D_y(\gamma)/4}$. The advantage to this is that now the term does not depend on the choice of quantum contour, but only on its initial configuration. Therefore, in (3.3.48), we can write

$$\sum_{G \subset \Lambda} \sum_{\gamma: G, y} \omega_0(\gamma) \rho^{\gamma(\gamma)/2} e^{-\frac{\beta}{2} h_c |G|} \leq \sum_{G \subset \Lambda} \rho \frac{D_y(G)}{4} e^{-\frac{\beta}{2} h_c |G|} \sum_{\gamma: G} \omega_0(\gamma)$$

(3.3.51)

We can drop the condition that $\gamma$ be connected since adding more terms only increases the sum. Thus, by (3.3.47), (3.3.48), and (3.3.51), we have

$$\lim_{N \to \infty} \sum_{G \subset \Lambda} \omega(G) e^{\varepsilon |S(\gamma)|} \leq \lim_{N \to \infty} \sum_{G \subset \Lambda} \rho \frac{D_y(G)}{4} e^{-\frac{\beta}{2} h_c |G|} \sum_{\Gamma: G} \omega_0(\Gamma)$$

(3.3.52)

However, the only term on the right side of (3.3.52) which depends on the length of the quantum contour $\Gamma$ is

$$\sum_{\Gamma: G} \omega_0(\Gamma)$$

thus we can pass the limit through the initial sum to get

$$\lim_{N \to \infty} \sum_{\Gamma: G} \omega_0(\Gamma) = \text{Tr} \left( e^{-\beta H_0^\Lambda} \circ \mathbb{P}_G \right)$$

(3.3.53)

$$= e^{-\beta |G| H_0^\Lambda}$$

(3.3.54)

where $\mathbb{P}_G = |G\rangle \langle G|$. But $H_0^\Lambda \geq 0$, so $e^{-\beta |G| H_0^\Lambda} \leq 1$ Thus we have shown

$$\lim_{N \to \infty} \sum_{\gamma: y} \omega(\gamma) e^{\varepsilon |S(\gamma)|} \leq \sum_{G \subset \Lambda} \rho \frac{D_y(G)}{4} e^{-\frac{\beta}{2} h_c |G|} \lim_{N \to \infty} \sum_{\Gamma: G} \omega_0(\Gamma) \leq \sum_{G \subset \Lambda} \rho \frac{D_y(G)}{4} e^{-\frac{\beta}{2} h_c |G|}$$

(3.3.55)

The proof is then completed by the following lemma.

**Lemma 3.3.3** For fixed $\delta$, $0 < \delta \leq 1$

$$\sum_{G \subset \Lambda} \rho \frac{D_y(G)}{4} e^{-\frac{\beta}{2} h_c |G|} \leq r(\delta, \beta)$$

(3.3.56)

where $r(\delta, \beta) \to 0$ as $\beta \to \infty$
To prove Lemma 3.3.3 we follow Kennedy and think of $G$ as being generated by a random walk on points on the lattice in the following way: Let $F$ be a $G, y$-connecting set with $|F| = D_y(G)$. Consider a nearest-neighbor walk $\bar{\eta}$ on the elements of $F \cup G \cup \{y\}$ where $\bar{\eta}_0 = y$. We take $\bar{\eta}$ in such a way that it does not visit any site in $F \cup G \cup \{y\}$ more $c_0$ times, where $c_0$ is a constant that only depends on the dimension. We take $G$ to be generated by a walk $\eta$ where $\eta$ is the walk $\bar{\eta}$ with the steps on the set $F$ removed. Notice that in general $\eta$ is not a nearest-neighbor walk.

The product
\[
\rho \frac{D_y(G)}{4} e^{-\beta \frac{\delta h_c}{4} |G|} \quad (3.3.57)
\]
contains a factor $\rho^{1/4}$ for every site in $F$ and a factor $e^{-\beta \delta h_c} / 4^{c_0}$ for each site in $G$. Taking $\rho_0 = \rho^{1/4}$ and $\delta_0 = \frac{\delta h_c}{4c_0}$
\[
(3.3.58)
\]
gives
\[
\rho \frac{D_y(G)}{4} e^{-\beta \frac{\delta h_c}{4} |G|} \leq e^{-\beta \delta_0 |\eta|} \prod_{i=1}^{\frac{|\eta|}{\delta h_c}} N \rho_0^{d(\eta_{i-1}, \eta_i)} \quad (3.3.59)
\]
where $d(\eta_{i-1}, \eta_i)$ is the minimal number of sites required to connect $\eta_{i-1}$ and $\eta_i$.

Therefore
\[
\sum_{G \subset \Lambda} \rho \frac{D_y(G)}{4} e^{-\beta \frac{\delta h_c}{4} |G|} \leq \sum_{\eta} e^{-\beta \delta_0 |\eta|} \prod_{i=1}^{\frac{|\eta|}{\delta h_c}} N \rho_0^{d(\eta_{i-1}, \eta_i)} \quad (3.3.60)
\]
\[
= \sum_{n=1}^{\infty} e^{-\beta \delta_0 |\eta|} \sum_{|\eta| = n} \prod_{i=1}^{n} N \rho_0^{d(\eta_{i-1}, \eta_i)} \quad (3.3.61)
\]

But
\[
\sum_{|\eta| = n} \prod_{i=1}^{n} N \rho_0^{d(\eta_{i-1}, \eta_i)} = \sum_{b_0, \ldots, b_n \in \Lambda} \prod_{i=0}^{n} N \rho_0^{d(b_{i-1}, b_i)} \quad (3.3.62)
\]
\[
\leq \left( \sum_b N \rho_0^{d(b, b)} \right) \cdots \left( \sum_b N \rho_0^{d(b, b)} \right) \quad (3.3.63)
\]
So, let $K = \sup_{b'} \sum_b \rho_0^{d(b', b)}$. Then

$$\sum_{G \subset \Lambda} \rho \frac{D_G}{4} e^{-\beta \frac{\Delta h_c}{4} |G|} \leq \sum_{n=1}^{\infty} K^n e^{-\beta \delta_n} = r(\delta, \beta) \quad (3.3.64)$$

and we note that $r(\delta, \beta) \to 0$ as $\beta \to \infty$.

This completes the proof of Lemma 3.3.3 which in turn completes the proof of Proposition 3.3.2.
Appendix A

Calculation of critical magnetic field.

In Chapter 3 above we presented a contour expansion for the free energy of the system. In this expansion the contours that contribute the most are those that are close to the ground state of the Hamiltonian. They can be thought of as islands of down spins in a sea of up spins. The argument relies upon the fact that we only consider a region in which the all-up spin state is the unique ground state of the system. Here we present the proof that there is a critical magnetic field strength, $h_c = 2d$, such that for all $h > h_c$ the all spin up state is the unique ground state of the XY Hamiltonian

$$H^{XY} = -\sum_{|x-y|=y} (\sigma^+_x \sigma^-_y + \sigma^-_x \sigma^+_y) + h \sum_x \frac{1}{2} (1 - \sigma^3_x)$$

We show $h_c \geq 2d$ by calculating the energy of spin waves and comparing it to the energy of the all-up state. The inequality $h_c \leq 2d$ is obtained by writing the Hamiltonian as the sum over two-site interactions and then determining a condition on $h$ such that the all up state minimizes every two-site interaction.

**Proposition A.0.4** There is a critical value $h_c$ such that for $h \geq h_c$ the ground state of $H_1$ is the all ‘up’ state, while for $h < h_c$ this is no longer the case. Moreover
\( h_c = 2d \)

**Proof:** To find the critical value of \( h \) we first calculate when a spin wave has lower energy than the all up state. Let \( \psi^k = \sum_x a_x \sigma^- |\uparrow\rangle \) where \( a_x = e^{i k x}/|\Lambda|^{1/2} \). Then

\[
\langle \psi^k | H | \psi^k \rangle = \langle \psi^k | H^{XX} | \psi^k \rangle + \langle \psi^k | H^Z | \psi^k \rangle
\]

\[
= - \sum_{\langle x, y \rangle \neq \langle z, z' \rangle} \bar{a}_x a_y \langle \uparrow | \sigma_x^+ \sigma_y^- + s_x^+ s_y^- | \sigma_x^- \sigma_y^- | \uparrow \rangle + \frac{h}{2} \sum_{x, z, z'} \bar{a}_x a_{z'} \langle \uparrow | \sigma_x^+ (\mathbb{I} - \sigma^3_x) \sigma_y^- | \uparrow \rangle
\]

But \( \langle \uparrow | \sigma_x^+ \sigma_y^- \sigma_x^- \sigma_y^- | \uparrow \rangle = \delta_{x, z} \delta_{y, z} \) and \( \langle \uparrow | \sigma_x^+ \sigma_y^- \sigma_x^+ \sigma_y^- | \uparrow \rangle = \delta_{x, z} \delta_{y, z'} \), so

\[
\langle \psi^k | H | \psi^k \rangle = - \sum_{\langle x, y \rangle} \bar{a}_x a_y + h
\]

\[
= -2 \sum_{\langle x, y \rangle} \bar{a}_x a_y + h
\]

\[
= - \left[ \frac{2}{|\Lambda|} \sum_{x \in \Lambda} e^{-ikx} \frac{1}{2} \sum_{j=1}^d (e^{ik(x+e_j)} + e^{ik(x-e_j)}) + h \right]
\]

\[
= -2 \sum_{j=1}^d \cos k_j + h \geq -2d + h
\]

Therefore the spin wave \( \psi^k \) at least has variational energy \(-2d + h\). But the state \( |\uparrow\rangle \) has energy zero, so we are looking for the regime in which

\[-2d + h < 0 \iff h < 2d\]

This implies

\[ h_c \geq 2d \]

To get the other inequality we write

\[
H = \sum_{\langle x, y \rangle} \left( H^{(2)}_{x, y} + \frac{h}{2d} \mathbb{I} \right), \quad H^{(2)}_{x, y} = - (\sigma_x^+ \sigma_y^- + \sigma_x^- \sigma_y^+) - \frac{h}{4d} (\sigma_x^3 + \sigma_y^3)
\]

If we denote by \( E_0 \) and \( e_0 \) the ground state energies of \( H \) and \( H^{(2)}_{x, y} \) respectively, then we see

\[
E_0 \geq \sum_{\langle x, y \rangle} (e_0 + \frac{h}{2d})
\]
Then we can calculate for which values of $h$ the state $|↑⟩$ minimizes each $H^{(2)}_{x,y}$. For these values of $h$

$$E_0 = \sum_{(x,y)} (e_0 + \frac{h}{2d})$$

The eigenvalues of $H^{(2)}_{x,y}$ are $\pm 1$ and $\pm h/2d$. The eigenvalue $-h/2d$ corresponds to the state $|↑↑⟩$ at the sites $x$ and $y$. Hence, for $|↑⟩$ to minimize $H^{(2)}_{x,y}$ $h$ must satisfy

$$-\frac{h}{2d} < -1 \iff h > 2d \quad (A.0.9)$$

which gives the inequality

$$h_c \leq 2d \quad (A.0.10)$$

Therefore, we have $2d \leq h_c \leq 2d$ which implies $h_c = 2d$. \hfill \blacksquare
Appendix B

Proof of Theorem 3.3.1

We restate Theorem 3.3.1 here and present a proof due to Ueltschi [31]. The proof is very technical and is included here for the sake of completeness. Let \( \mathbb{A} \) be a finite set whose elements are called polymers. Let \( \iota \) be a symmetric and reflexive relation on \( \mathbb{A} \times \mathbb{A} \). For polymers \( A, A' \in \mathbb{A} \) we say that \( A \) and \( A' \) are incompatible if \( A \iota A' \) and are compatible otherwise. The partition function of the polymer model is

\[
Z(\mathbb{A}) = \sum_{n=1}^{\infty} \sum_{\{A_1, \ldots, A_n\}} \prod_{i=1}^{n} w(A_i)
\]

where \( w \) is a complex function on \( \mathbb{A} \) and the sum is over sets of polymers whose elements are pairwise compatible.

**Theorem B.0.5** Let \( a \) and \( b \) be non-negative functions on \( \mathbb{A} \) such that for all \( A \in \mathbb{A} \)

\[
\sum_{A', A \iota A} |w(A')| e^{a(A') + b(A')} \leq a(A) \quad (B.0.1)
\]

Then,

\[
Z(\mathbb{A}) = \exp \left( \sum_{C} \Phi(C) \right) \quad (B.0.2)
\]

where the sum converges absolutely. Furthermore

\[
\sum_{C \iota A} |\Phi(C)| e^{b(C)} \leq a(A) \quad (B.0.3)
\]
where \( C \setminus A \) means that \( A \) is incompatible with at least one polymer in \( C = (A_1, \ldots, A_n) \) and \( b(C) = \sum_{i=1}^{n} b(A_i) \).

The sequence of the proof is out of order with the statements of the theorem. We first prove inequality (B.0.3) as this follows from the assumption (B.0.1). We then use (B.0.3) to prove the convergence of the cluster expansion on the right hand side of (B.0.2) and finally show that the partition function \( Z(A) \) can indeed be written as the cluster expansion.

**Proof:** In order to prove inequality (B.0.3) we induct on number of elements in the cluster. For \( n = 1 \), \( C = (A_1) \) then by assumption (B.0.1) we have

\[
\sum_{C \setminus A, |C| = 1} |\Phi(C)| e^{b(C)} \leq a(C)
\]

Assume that for all \( k \leq n \)

\[
\sum_{C \setminus A, |C| \leq k} |\Phi(C)| e^{b(C)} \leq a(C)
\]  

(B.0.4)

and consider the sum over clusters with \( n + 1 \) elements or less. To bound this, first sum over polymers \( A_1 \) incompatible with \( A \) and then over remaining polymers. Thus, we have

\[
\sum_{C \setminus A, |C| \leq n + 1} |\Phi(C)| e^{b(C)} \leq \sum_{A_1 \setminus A} \sum_{j=2}^{n+1} \frac{1}{(j-1)!} \sum_{A_2, \ldots, A_j} \prod_{\ell=1}^{j} \left| w(A_\ell) e^{b(A_\ell)} \right| \sum_{G \subset G(A_1, \ldots, A_j) \text{ connected}} (-1)^{|G|}
\]  

(B.0.5)

For a given graph \( G \), let \((G_1, \ldots, G_k)\) be a sequence of connected subgraphs of \( G \). Let each subgraph \( G_i \) have vertex set \( V_i \) where \( V_i \cap V_j = \emptyset \) if \( i \neq j \). Furthermore, assume that \( V_1 \cup \cdots \cup V_k = \{2, \ldots, n\} \). The sequence \((G_1, \ldots, G_n)\) defines a disconnected
subgraph $G'$ of $G$ obtained by removing all edges emanating from vertex 1. Hence,

$$\left| \sum_{G \subset G(A_1, \ldots, A_j)} (-1)^{|G|} \right| \leq \sum_{k \geq 1} \frac{1}{k!} \left| \sum_{(G_1, \ldots, G_k)} \prod_{i=1}^k (-1)^{|G_i|} \sum_{G_i'} (-1)^{|G_i'|} \right|$$

$$= \sum_{k \geq 1} \frac{1}{k!} \left| \sum_{(G_1, \ldots, G_k)} \prod_{i=1}^k (-1)^{|G_i|} \right| \quad \text{(B.0.6)}$$

since $\sum_{G_i'} (-1)^{|G_i'|} = -1$. Next we expand the sum over sequences $(G_1, \ldots, G_k)$. First sum over the respective number of vertices $m_1, \ldots, m_k$ with the condition that $m_1 + \cdots + m_k = j - 1$, and then choose connected graphs for each choice of $m_1, \ldots, m_k$.

We can bound the sum over $A_2, \ldots, A_j$ by summing over clusters of length $k$ that are incompatible with the polymer $A_1$ such that $|C_i| = m_i$. This gives

$$\sum_{C \subset A, |C| \leq n+1} |\Phi(C)| e^{bc(C)} \leq \sum_{A_1 \subset A} w(A_1) e^{b(A_1)} \sum_{j=2}^{n+1} \sum_{k \geq 0} \frac{1}{k!} \left( \sum_{(m_1, \ldots, m_k) \vdash j-1} \sum_{C_1, \ldots, C_k} \prod_{i=1}^k |\Phi(C_i)| e^{b(C_i)} \right) \quad \text{(B.0.7)}$$

Relaxing the condition that $(m_1, \ldots, m_k) \vdash j - 1 \leq n$ to $m_i \leq n$ for all $i$ and then summing over $j$ gives

$$\sum_{C \subset A, |C| \leq n+1} |\Phi(C)| e^{bc(C)} \leq \sum_{A_1 \subset A} w(A_1) e^{b(A_1)} \sum_{k \geq 0} \frac{1}{k!} \left( \sum_{C \subset A, |C| \leq n} |\Phi(C)| e^{b(c)} \right)^k \quad \text{(B.0.8)}$$

We now use the induction hypothesis \[\text{B.0.4}\] to bound the term in the brackets by $a(A_1)$, which in turn bounds the sum over $k$ by $e^{a(A_1)}$. But, under the assumptions of the theorem \[\text{B.0.1}\]

$$\sum_{A_1 \subset A} |w(A_1)| e^{b(A_1)+a(A_1)} \leq a(A) \quad \text{(B.0.9)}$$

which give \[\text{B.0.3}\] by induction.
To get the convergence of the cluster expansion in (B.0.2), note that any cluster is incompatible with its first element, so

\[ \sum_C |\Phi(C)| \leq \sum_{A \in \mathcal{A}} \sum_{C \in A} |\Phi(C)| \leq \infty \]  

(B.0.10)

by (B.0.3). Thus we have established the convergence of the cluster expansion, what remains is to show

\[ Z(A) = \exp \left( \sum_C \Phi(C) \right) \]

This will be done by expanding \( Z(A) \) and correctly rearranging terms so that the sum over clusters becomes apparent.

\[
Z(A) = \sum_{\{A_1, \ldots, A_n\} \text{ compatible}} \prod_{i=1}^{\infty} w(A_i) \\
= 1 + \sum_{n \geq 1} \frac{1}{n!} \sum_{(A_1, \ldots, A_n)} \prod_{i=1}^{n} w(A_i) \prod_{j<i} (1 - \chi[A_i \cap A_j]) \\
= 1 + \sum_{n \geq 1} \frac{1}{n!} \sum_{(A_1, \ldots, A_n)} \prod_{i=1}^{n} w(A_i) \sum_{G \subset G(A_1, \ldots, A_n)} (-1)^{|G|} \\
\]

(B.0.13)

Again, we sum over partitions of the vertices \( m = (m_1, \ldots, m_k) \vdash n \), first summing over the size of the partition \( k \), considering sequences of graphs \( (G_1, \ldots, G_k) \) corresponding to the partition \( m \). This gives

\[
Z(A) = 1 + \sum_{n \geq 1} \sum_{k \geq 1} \frac{1}{k!} \sum_{(m_1, \ldots, m_k) \vdash n} \frac{1}{m_1! \cdots m_k!} \\
\prod_{i=1}^{k} \left[ \sum_{A_1, \ldots, A_{m_i}} \prod_{j=1}^{m_i} w(A_j) \sum_{G \subset G(A_1, \ldots, A_{m_i})} (-1)^{|G|} \right] \\
= 1 + \sum_{n \geq 1} \sum_{k \geq 1} \frac{1}{k!} \sum_{(m_1, \ldots, m_k) \vdash n} \prod_{i=1}^{n} \sum_{C \vdash \{1, \ldots, m_i\}} \Phi(C) \\
= \exp \left( \sum_C \Phi(C) \right) \\
\]

(B.0.14)
where the last line follows since by (B.0.10) we have absolute convergence of the cluster expansion.
Appendix C

Matlab Code

We include the Matlab code with which we produced the images in Chapter 2. There are two main programs spin1kink.m and spin1compare.m. In spin1kink.m we evaluate $\| G_{L,L+1} E_L \|$ for $L+1 = 8$ in each sector of $S_{tot}^3$. This is accomplished by building the XXZ Hamiltonian using the spin operators $S_z$, $S_x$, and $S_y$ defined below. The Matlab function $\text{kron}$ computes the tensor product of its inputs. The projections onto ground states are produced by calculating ground state vectors and then creating the operator $|v\rangle\langle v|$ where $v$ is the given ground state. Finally we compute the proper eigenvalues and plot them versus the $S_{tot}^3$ sector.

spin1kink.m

```matlab
%spin1kink.m
% SPIN 1 KINK HAMILTONIAN
clear;
delta = 50; q = delta -sqrt(delta^2-1);
A = sqrt(1-delta^(-2));
L = 8;
```
Sz=[1 0 0;0 0 0;0 0 -1];
Sx=[0 1 0;1 0 1;0 1 0]/sqrt(2);
Sy=[0 1 0;-1 0 1;0 -1 0]/(i*sqrt(2));

hdiag= kron(Sz,Sz);
hhop = kron(Sx,Sx) + kron(Sy,Sy);
hbdry= kron(Sz,eye(3)) - kron(eye(3),Sz);
HDIAG = sparse(3^L,3^L);
HHOP = sparse(3^L,3^L);
HBDRY = sparse(3^L,3^L);
Sztot = sparse(3^L,3^L);
for a=1:(L-1)
    HDIAG = HDIAG + kron(speye(3^(a-1)), kron(hdiag,speye(3^((L-1-a)))));
    HHOP = HHOP + kron(speye(3^(a-1)), kron(hhop,speye(3^((L-1-a)))));
    HBDRY = HBDRY + kron(speye(3^(a-1)), kron(hbdry,speye(3^((L-1-a)))));
    Sztot = Sztot + kron(speye(3^(a-1)),kron(Sz,speye(3^((L-a)))));
end
Sztot = Sztot + kron(speye(3^((L-1))),Sz);

Hkink = - HDIAG - 1/delta * HHOP - A*HBDRY;
H =  Hkink + (L-1) * speye(3^L);

% Projection G onto the last two sites, [L,L+1]
h2 = -hdiag-1/delta*hhop - A*hbdry + speye(3^2);
[v,d] = eigs(h2,5,'sm');
G=0;
for k=1:5
\begin{verbatim}
G = G + v(:,k)*transpose(v(:,k));
end
G = kron(speye(3^(L-1)), G);

for downspins = 1:2*L-1
    for m = downspins-1: downspins+1
        Proj =[];Proj = speye(3^L);
        for n=0:(2*L)
            if ne(n,m),
                Proj = Proj*(Sztot - (L-n)*speye(3^L))/(n-m);
            end;
        end;
        Hred = transpose(Proj)*(H - 0.2*speye(3^L))*Proj;
        [V,D] = eigs(Hred + 0.2*speye(3^L),1,'sm');
        psi(:,m-downspins+2) =V;
    end
end

Psi(:,1) = kron(psi(:,1),[0,0,1]');
Psi(:,2) = kron(psi(:,2),[0,1,0]');
Psi(:,3) = kron(psi(:,3),[1,0,0]');

A=[];
for i=1:3
    for j=1:3
        A(i,j)=transpose(Psi(:,i))*G*Psi(:,j);
    end
end
\end{verbatim}
epsi = eigs(A); e(:,downspins+1) = epsi(2);
end
e(:,1) = sqrt(q^2/(1+q^2)*(1-q^(2*L))/(1-q^(2*L+2)))
for i=1:2*L-1
    p(i)=e(2*L-i);
end

s=[-L+1:L-1];
plot(s,p,'b:*');

The program spin1compare.m is very straightforward. It calls two other programs, Hmltn.m and SectrProj.m. Hmltn.m produces the XXZ Hamiltonian of inputted spin on a chain whose length is passed to the program. SectrProj.m produces a projection onto the desired sector of $S^3_{tot}$. In spin1compare.m we loop through values of $\Delta$ between 1 and a specified number DeltaMax. For each value of $\Delta$ spin1compare.m calculate the spectral gap of the output from Hmltn.m by projecting into each sector of $S^3_{tot}$ and calculating the two smallest eigenvalues. In each sector, 0 is one of the eigenvalues and the other is the spectral gap. spin1compare.m then plots the spectral gap for each $\Delta$ along with the estimate from Theorem 2.4.5.

spin1compare.m

% spin1compare.m
%This code produces a graph that compares the true gap of the
%XXZ Hamiltonian with the estimate in this Thesis: Theorem 2.4.5
%The variables are:
% L = Length of the chain  J = spin of the system considered
% DeltaMax = this is the max value of Delta (anisotropy parameter)
clear;
L = 8;
J = 1;
DeltaMax = 20;

for i=10:(10*DeltaMax)
    Delta = (i/10);
    H = Hmltn(L,J,Delta); %Sets H to be the XXZ Hamiltonian
    % on spin-J chain of length L with
    % anisotropy Delta
    for j = -L+1:L-1
        P = SectrProj(L,J,j); %This sequence calculates the
        % gap of H by projecting into
        % different sectors and then
        smallH = transpose(P)*H*P; %finding the two smallest e-values.
        % Since there is a unique
        v = eigs(smallH,2,'sr'); %ground state in every sector the
        % first non-zero eigenvalue
        u(L+j) = v(2); %is the gap in that sector.
        smallH=[]; P = [];
    end
    gap(i-9) = min(u); %This asks now for the minimum
    % gap over all sectors
gamma = 2.5 - sqrt(2.25-(2/Delta^2)); %This is the gap of the
two-site Hamiltonian given
in 2.4.75

q = Delta - sqrt(Delta^2-1); %q solves equation
2Delta = q + q^(-1) on
interval (0,1)

epsilon = sqrt(((1-q^(2*L))/(1-q^(2*L+2))*(q^2/(1+q^2)));
%This is the value calculated
in Lemma 2.4.7

gapest(i-9) = gamma * (1-sqrt(2)*epsilon)^2;
%This is the lower bound
provided in Theorem 2.4.4

Deltavec(i-9) = Delta;

plot(Deltavec, gap, 'b')
hold on
plot(Deltavec, gapest, 'r')

We also include the programs Hmltn.m and SectrProj.m.

Hmltn.m

function Hmltn=Hmltn(L,J,Delta)

%A = 0.1; gives Delta = 1.005
DelInv = 1/Delta; \%sqrt(1-A*A);
A = sqrt(1-Delta^(-2));

\%Dimension of 1-site Hamiltonian
dim1 = 2*J+1;
\%Pauli Spin Matrix in third (or Z) direction
S3 = sparse(1:dim1,1:dim1,J-(0:2*J),dim1,dim1);
\%Spin-raising operator
Splus = sparse(dim1,dim1);
for j=0:(2*J-1)
    Splus = Splus + sparse(2*J-j,2*J-j+1,sqrt((2*J-j)*(j+1)),dim1,dim1);
end
\%Spin lowering operator
Sminus = transpose(Splus);

\%SS = Isotropic nearest neighbor interaction S(x).S(x+1)
SS = kron(S3,S3) + (1/2)*(kron(Splus,Sminus) + kron(Sminus,Splus));
\%Ising = Ising Nearest neighbor interaction S3(x)*S3(x)
Ising = kron(S3,S3);
\%h = nearest neighbor interaction
h = -DelInv*SS - (1-DelInv)*Ising+J^2*speye(dim1^2);
\%H = sum over all nearest neighbor pairs of h(x,x+1) = Hamiltonian
H = sparse(dim1^L,dim1^L);
for x=1:(L-1)
    H = H + kron(eye(dim1^(x-1)),kron(h,eye(dim1^(L-1-x))));
end
\%Bdry = boundary term A*(S3(x+1)-S3(x))

Bdry = J*A*(kron(speye(dim1^(L-1)),S3) - kron(S3,speye(dim1^(L-1))));
H = H +Bdry;

Hmltn=H;

\textbf{SectrProj.m}

function SectrProj=SectrProj(L,J,sector)

\%produces a projection matrix onto the the subspace of total S3 "sector"
\% for a spin J chain of length L

downspins = J*L-sector;

\%Dimension of 1-site Hamiltonian
dim1 = 2*J+1;
\%Pauli Spin Matrix in third (or Z) direction
S3 = sparse(1:dim1,1:dim1,J-(0:2*J),dim1,dim1);

\%S3tot = total third-component of spin operator
S3tot = sparse(dim1^L,dim1^L);
for x=1:L,
    S3tot = S3tot + kron(speye(dim1^(x-1)),kron(S3,speye(dim1^(L-x))));
end
We now define the projection to the sector specified by
\[ S_{3\text{tot}} = (J*L - \text{downspins}) \]

\[ \text{Proj} = \text{speye}(\text{dim}1^L); \]

for \( n=0:(2*J*L) \)

if \( \text{ne}(n, \text{downspins}) \),

\[ \text{Proj} = \text{Proj} \ast (S_{3\text{tot}} - (J*L-n) \ast \text{speye}(\text{dim}1^L))/(n-\text{downspins}); \]

end;

end;

Proj is the orthogonal projection onto sector with specified number
% of downspins. Next we want to define a projection from this subspace
% to a vector space of the same dimension.
% The command "find" finds the nonzero elements of Proj,
% which is what we need.

[I1,I2] = find(Proj);

dim = length(I1);

NewProj = sparse(I1,1:dim,ones(dim,1),dim1^L,dim);

SectrProj=NewProj;
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