Spectral Gap in the Ferromagnetic Heisenberg Spin-½ Quantum Spin Chain

By

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Abstract

The ferromagnetic Heisenberg spin-½ quantum spin chain describes a quantum spin system of spin-½ particles on a one-dimensional lattice. In the thermodynamic limit, the spectral gap of this system closes at rate of $\mathcal{O}\left(n^{-2}\right)$. We demonstrate this by proving an upper bound on the spectral gap using the variational principle and a lower bound using the martingale method.

1. Introduction

Determining the energy of a physical system is an ubiquitous problem in physics, and especially in quantum mechanics, where the possible energy values on are often discretized. Calculating the ground and first excited energies are often of particular importance, especially in areas such as molecular physics and thermodynamics. The gap between these two energies, and whether it remains open or closes in certain limiting cases, will determine many fundamental principles of a system; for example, systems with an open gap have correlation functions which decay exponentially [6, 11].

In a quantum spin chain, particles are fixed in space on the sites of the integer lattice $\mathbb{Z}$. These particles can not move and thus only interact through their spin. A particle of spin-s located at the site $x \in \mathbb{Z}$ is described by the Hilbert space $\mathcal{H}_{\{x\}} = \mathbb{C}^{2s+1}$. For a finite subsystem $\Lambda \subset \mathbb{Z}$, the total state space is given by the tensor product of the on-site Hilbert spaces, namely

$$\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathcal{H}_x.$$

The *algebra of observables* $\mathcal{A}_{\{x\}}$ at a site $x \in \mathbb{Z}$ is the set of all $(2s+1)$-dimensional complex matrices, $\mathcal{A}_{\{x\}} = M_{2s+1}(\mathbb{C})$. The algebra of observables for a finite subsystem $\Lambda \subset \mathbb{Z}$ is then given by $\mathcal{A}_\Lambda = \otimes_{x \in \Lambda} \mathcal{A}_{\{x\}}$. All observables corresponding to a measurable quantity in a physical system are Hermitian; the possible values of a measurement are exactly the eigenvalues. One example of an observable is the *Hamiltonian* H, a Hermitian matrix representing the total energy of a system. The smallest eigenvalue of the Hamiltonian is the *ground state energy*, and the others are the *excited state energies*. The gap between the ground state energy and the first excited state energy is called the *spectral gap*.

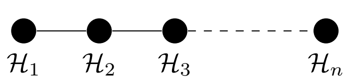
In this thesis, we will calculate the spectral gap of a particular nearest neighbor quantum spin system, called the *ferromagnetic Heisenberg spin-½ model*. After introducing this model, we will calculate its spectral gap in two steps; first, by explicitly calculating an upper bound on the gap, followed by proving a lower bound using a technique called the martingale method. By showing that these bounds are of order $\mathcal{O}(n^{-2})$, we prove the gap must close at exactly this rate, by the squeeze theorem.

2. The Ferromagnetic Heisenberg Spin-½ Model

In this section, we introduce the ferromagnetic Heisenberg spin-½ model. After describing the basic mathematical construction, we give an expression for the Hamiltonian of the system in terms of an operator which transposes the particles on the lattice. This expression is then used to characterize the ground state space of the system as the set of all states which are symmetric under permutations.

2.1. **The Hamiltonian.**

The ferromagnetic Heisenberg spin-½ model (abbreviated from now on as the *Heisenberg-½ model*) describes a one-dimensional lattice of spin-½ particles which interact with their nearest neighbors.



Each particle $x \in \mathbb{Z}$ is described by a vector in $\mathcal{H}_{\{x\}} = \mathbb{C}^2$. A system of n particles is then described by

$$\mathcal{H}_{[1,n]} = \bigotimes_{x=1}^{n} \mathbb{C}^2 = \mathbb{C}^{2^n}.$$

Let $S^i = \frac{1}{2}\sigma^i$, where σ^i is the i^{th} Pauli spin matrix, given by

$$\sigma^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{2.1}$$

The 4×4 interaction of the ferromagnetic Heisenberg-½ model between with two neighboring particles is given by

$$\begin{aligned} h &= -\sum_{x=1}^{3} S^i \otimes S^i + \frac{1}{4}\mathbb{1} \\ &= -\frac{1}{4}\left(\sum_{x=1}^{3} \sigma^i \otimes \sigma^i + \mathbb{1}\right) \\ &= \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{aligned} \tag{2.2}$$

where we have shifted by $-\frac{1}{4}\mathbb{1}$ so that the minimum energy is zero.

In an n particle system, the interaction between particles x and $x+1$ is given by

$$h_{x,x+1} = \underbrace{\mathbb{1} \otimes \dots}_{x-1} \otimes h \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{n-x}.$$

The Hamiltonian of the entire system is then given by

$$H_{[1,n]} = \sum_{x=1}^{n-1} h_{x,x+1}.$$

Theorem 2.1. *The Hamiltonian of the ferromagnetic Heisenberg-½ model is gapless in the thermodynamic limit (i.e., $n \to \infty$). The gap closes at a rate of $\mathcal{O}(n^{-2})$ where n is the number of sites of our lattice. More specifically,*

$$\frac{1}{4n^2} \leq \operatorname{gap}\left(H_{[1,n]}\right) \leq \frac{\pi^2 n}{4(n-1)^2(n+1)}.$$

In the rest of this section, we will demonstrate a useful construction of the Hamiltonian and the ground state space using transposition operators. In Section 3, we will provide useful background information on the group $SU(2)$ and show that our model is $SU(2)$-invariant. In Section 4, we will prove an upper bound on the gap by using the variational principle (see Theorem 4.2). Finally, in Section 5, we will introduce the martingale method and apply it to our model to prove a lower bound on the gap (see Theorem 5.6).

2.2. **The ground state space.** In order to calculate the ground state space, we will rewrite the Hamiltonian in terms of a transposition operator and utilize properties of frustration-freeness, defined below.

Definition 2.2. *A nearest-neighbor quantum spin chain is frustration-free if*

(a) $h_{x,x+1} \geq 0 \ \forall x = 1, \dots, n-1$, *and*
(b) $\ker(H_{[1,n]}) \neq \{0\}$ *for all n.*

For a frustration-free model, the ground state space is given by the kernel of the Hamiltonian. As a consequence, $\operatorname{gap}(H_{[1,n]}) = \lambda_1$, where λ_1 is the first excited energy of the Hamiltonian. We will show that the ferromagnetic Heisenberg-½ model is frustration-free. To this end, the following lemma will be useful.

Lemma 2.3. *In a frustration-free model,* $\ker(H_{[1,n]}) = \bigcap_{x=1}^{n-1} \ker(h_{x,x+1})$.

Proof. Assume that $\psi \in \bigcap_{x=1}^{n-1} \ker(h_{x,x+1})$. Then,

$$\begin{aligned} H_{[1,n]}\psi &= \left(\sum_{x=1}^{n-1} h_{x,x+1}\right)\psi \\ &= \sum_{x=1}^{n-1} (h_{x,x+1}\psi) \\ &= 0. \end{aligned}$$

Therefore, $\ker(H_{[1,n]}) \supseteq \bigcap_{x=1}^{n-1} \ker(h_{x,x+1})$.

Now assume $\psi \in \ker(H_{[1,n]})$ and consider,

$$0 = \left\langle \psi \middle| H_{[1,n]} \middle| \psi \right\rangle = \left\langle \psi \middle| \sum_{x=1}^{n-1} h_{x,x+1} \middle| \psi \right\rangle = \sum_{x=1}^{n-1} \langle \psi | h_{x,x+1} | \psi \rangle .$$

Let $1 \le x \le n-1$ be arbitrary. By Definition 2.2(a), $\langle \psi | h_{x,x+1} | \psi \rangle = 0$. Since $h_{x,x+1}$ is self-adjoint, by the spectral theorem [3, Chapter 8.6] it has a basis of eigenvectors $e_1, \ldots, e_{2^n}$ with corresponding non-negative eigenvalues $\lambda_1, \ldots, \lambda_{2^n}$. Let $\psi = \sum_{i=1}^{2^n} c_i e_i$. Then,

$$\begin{aligned} 0 &= \langle \psi | h_{x,x+1} | \psi \rangle \\ &= \left\langle \sum_{i=1}^{2^n} c_i e_i \middle| h_{x,x+1} \middle| \sum_{i=1}^{2^n} c_i e_i \right\rangle \\ &= \left\langle \sum_{i=1}^{2^n} c_i e_i \middle| \sum_{i=1}^{2^n} c_i \lambda_i e_i \right\rangle \\ &= \sum_{i=1}^{2^n} \lambda_i |c_i|^2. \end{aligned}$$

Therefore, either $\lambda_i = 0$ or $c_i = 0$ for all i, and so

$$\psi = \sum_{\substack{i \text{ s.t.} \\ \lambda_i = 0}} c_i e_i \in \ker\left(h_{x,x+1}\right).$$

This holds for every x, so $\psi \in \bigcap_{x=1}^{n-1} \ker(h_{x,x+1})$. ■

In order to show that the ferromagnetic Heisenberg-½ model is frustration-free, we must now show that its kernel is non-empty. This is equivalent to the ground state space being the kernel because $h_{x,x+1} \ge 0$ by 2.2(a). We will do so by showing that the kernel is the set of all symmetric vectors, which we define next.

A permutation $\sigma \in S_n$ induces a permutation operator $\tau_\sigma : \mathbb{C}^{2^n} \to \mathbb{C}^{2^n}$ given by

$$\tau_\sigma \left(\bigotimes_{x=1}^{n} \psi_x \right) = \bigotimes_{x=1}^{n} \psi_{\sigma(x)}. \tag{2.3}$$

We extend this definition to $\mathcal{H}_{[1,n]}$ linearly. Note that the τ operators form a group under composition, where

$$\tau_{\sigma_1} \circ \tau_{\sigma_2} = \tau_{\sigma_1 \circ \sigma_2}, \quad \tau_\sigma^{-1} = \tau_{\sigma^{-1}}. \tag{2.4}$$

We say that a vector ψ is *symmetric* if $\tau_\sigma(\psi) = \psi$ for every $\sigma \in S_n$.

For a transposition $\sigma = (x\ x+1)$, we write $\tau_\sigma = \tau_{x,x+1} = \mathbb{1} \otimes \cdots \otimes \tau \otimes \cdots \otimes \mathbb{1}$ where

$$\tau = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Now, we may rewrite h in terms of τ, using our prior calculation in (2.2):

$$\begin{aligned} h &= \frac{1}{4}\left(\begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & -2 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} + \mathbb{1} \right) \\ &= \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \\ &= \frac{1}{2}(\mathbb{1} - \tau). \end{aligned}$$

Therefore, the Hamiltonian for a lattice with n sites is given by

$$H_{[1,n]} = \frac{1}{2} \sum_{x=1}^{n-1} (\mathbb{1} - \tau_{x,x+1}).$$

We are now ready to calculate the ground state space. This lemma not only completes our justification for $H_{[1,n]}$ being frustration-free, but will also provide an easy characterization for vectors in the ground state space, which we will need to use throughout our proofs for the upper and lower bounds of the spectral gap.

Lemma 2.4. *The ground state space of $H_{[1,n]}$, denoted $\mathcal{G}_{[1,n]}$, is the set of symmetric vectors.*

Proof. Assume ψ is symmetric. Then, $\psi - \tau_{x,x+1}\psi = 0$ for all $1 \le x < n$. Therefore,

$$H_{[1,n]}\psi = \frac{1}{2} \sum_{x=1}^{n-1} (\mathbb{1} - \tau_{x,x+1})\, \psi = 0,$$

and the set of symmetric vectors is a subset of $\ker(H_{[1,n]})$. Thus, our model is frustration-free.

Assume $\psi \in \ker(H_{[1,n]})$. By Lemma 2.3 and the previous step of this proof, $H_{[1,n]}$ is frustration-free, so $\psi \in \ker(h_{x,x+1})$ for all $1 \le x < n$. Therefore, $\psi = \tau_{x,x+1}\psi$. Since $\{(1\ 2), \ldots, (n-1\ n)\}$ is a generating set for S_n, by (2.4), $\psi = \tau_\sigma \psi$ for all $\sigma \in S_n$, so ψ is symmetric. ∎

3. Representations of $SU(2)$

In this section, we introduce the group of special unitary matrices of dimension 2, $SU(2)$, and its associated Lie algebra $\mathfrak{su}(2)$. We characterize the representations of $\mathfrak{su}(2)$ and show that a unique representation (up to isomorphism) exists for each half-integer spin value. We then apply this to our Heisenberg-½ model, demonstrating that it is $SU(2)$ symmetric. Schur's Lemma then gives a characterization of the ground state space in terms of the representations of $\mathfrak{su}(2)$, which will be used in Section 5 to prove a lower bound on the spectral gap by determining in which irreducible representation the ground state space lies.

3.1. **Irreducible representations.** The group $SU(2)$ is the set of all special unitary matrices of dimension two [3, Chapter 9.6]:

$$SU(2) = \{A \in \mathrm{GL}_2(\mathbb{C}) \mid A^* = A^{-1}\}.$$

The corresponding Lie algebra $\mathfrak{su}(2)$ (over $\mathbb{R}$) is the space of all traceless, self-adjoint matrices

$$\mathfrak{su}(2) = \{A \in \mathrm{GL}_2(\mathbb{C}) \mid A^* = A, \mathrm{Tr}(A) = 0\},$$

where the Lie algebra bracket is given by the usual commutator: $[A, B] = AB - BA$.

To find a basis of $\mathfrak{su}(2)$, we start with the requirement that $a_{11} = -a_{22}$, and then impose self-adjointness:

$$\begin{aligned} A^* = A \implies \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & -a_{11} \end{bmatrix} &= \begin{bmatrix} \overline{a_{11}} & \overline{a_{21}} \\ \overline{a_{12}} & -\overline{a_{11}} \end{bmatrix} \\ \implies A &= \begin{bmatrix} a & c + di \\ c - di & -a \end{bmatrix} \end{aligned}$$

for $a, c, d \in \mathbb{R}$. Therefore, $\mathfrak{su}(2) = \mathrm{span}\{S^1, S^2, S^3\}$ over $\mathbb{R}$ where S^1, S^2, S^3 are given by (2.1).

We consider complex $\mathfrak{su}(2)$, for which a second basis is given by $\{S^3, S^+, S^-\}$ (where $S^+ = S^1 + iS^2$, and $S^- = S^1 - iS^2$), which satisfies the relations

$$[S^3, S^+] = S^+, \quad [S^3, S^-] = -S^-, \quad [S^+, S^-] = 2S^3. \tag{3.1}$$

Lemma 3.1. *If v is an eigenvector of S^3 with eigenvalue λ, then S^+v and S^-v are either zero or eigenvectors of S^3 with eigenvalues $\lambda + 1$ and $\lambda - 1$, respectively.*

Proof. Let v be an eigenvector of S^3 with eigenvalue λ. Then,

$$\begin{aligned} S^3 S^+ v &= S^+ S^3 v + [S^3, S^+]v \\ &= \lambda S^+ v + S^+ v \\ &= (\lambda + 1) S^+ v. \end{aligned}$$

∎

A finite-dimensional *group representation* of a group G is a group homomorphism $\rho : G \to \mathrm{GL}_n(\mathbb{C})$. The value n is the *dimension* of the representation. An *invariant subspace* is a subspace $W \subset V$ such that, for all $g \in G$, $\rho_g W \subset W$. If ρ is a representation on V, and W has no invariant subspace, then ρ is called an *irreducible representation*. Otherwise, the representation is *reducible*, and there are invariant subspaces $V_1, \ldots, V_n$ with corresponding irreducible representations $\rho_i = \rho|_{V_i}$ such that $V = V_1 \oplus \cdots \oplus V_n$, and $\rho = \rho_1 \oplus \cdots \oplus \rho_n$. A map $\rho : A \to GL(V)$ is a representation of the Lie algebra A if $\rho([C, B]) = [\rho(C), \rho(B)]$ for all $B, C \in A$. Similar to group representations, a reducible Lie algebra representation can be decomposed into a sum of irreducible representations acting on invariant subspaces.

Lemma 3.2. *There is a unique (up to isomorphism) n-dimensional representation of $\mathfrak{su}(2)$ for each non-negative integer n.*

We denote the n-dimensional irreducible representations of $\mathfrak{su}(2)$ as $D^{(s)}$ for $1/2$-integers $s = 0, 1/2, \ldots$, where $D^{(s)}$ has dimension $2s + 1$. We denote the associated $n = 2s + 1$ dimensional vector space on which $D^{(s)}$ acts by $V^{(s)}$.

Proof of Lemma 3.2. First, a zero dimensional representation is the trivial representation which maps all elements of $\mathfrak{su}(2)$ to the identity. We will now show a representation exists for all positive integers n. Let $s = \frac{1}{2}(n - 1)$, and let $v_1, \ldots, v_n$ be the standard basis for $\mathbb{C}^n$. Relative to this basis, let

$$S^3 = \begin{bmatrix} s & & & & \\ & s-1 & & & \\ & & \ddots & & \\ & & & 1-s & \\ & & & & -s \end{bmatrix}$$

$$S^+ = \begin{bmatrix} 0 & a_1 & & & \\ & 0 & a_2 & & \\ & & \ddots & & \\ & & & 0 & a_{n-1} \\ & & & & 0 \end{bmatrix}$$

$$S^- = \begin{bmatrix} 0 & & & & \\ a_1 & 0 & & & \\ & a_2 & 0 & & \\ & & \ddots & & \\ & & & a_{n-1} & 0 \end{bmatrix}$$

where $a_m = \sqrt{s(s+1)-(s-m)(s-m+1)}$. These matrices then satisfy the commutation relationships for $\mathfrak{su}(2)$ given by (3.1). Therefore, they generate a representation for each integer dimension.

Furthermore, this representation must be irreducible because the basis can be obtained by repeated applications of S^+ and S^- to an arbitrary (non-zero) vector: Let $v = a_1 v_1 + \cdots + a_n v_n \neq 0$. Let a_k be the last non-zero coefficient (i.e., $a_i = 0$ for all $k < i \leq n$). Now, ${}^1\!/_{a_1'}(S^+)^k v = v_1$ for some $a' \neq 0$. Finally, the remaining basis vectors $v_2, \ldots, v_n$ may be obtained by $v_i = {}^1\!/_{a_i'}(S^-)^{i-1} v_1$ for some $a_i' \neq 0$. Obtaining the basis vectors from any non-zero vector in this way is only possible in an irreducible representation.

We now show that any two irreducible representations of $\mathfrak{su}(2)$ of the same dimension must be isomorphic. Each irreducible representation must have the same n distinct eigenvalues of S^3. A choice of representation then corresponds to a choice of basis, each basis vector being an eigenvalue of S^3. Let V and V' be two such bases, corresponding to representations ρ and ρ'. Then, let $T : V \to V'$ represent a change of basis such that, for each eigenvector $v \in V$ of S^3, $T(v)$ is an eigenvector of S^3 with the same eigenvalue. Now, $T^{-1}\rho T = \rho'$, so the representations are isomorphic. ■

Importantly, the tensor product of two irreducible representations may be rewritten relatively simply as the direct product of irreducible representations.

Theorem 3.3 (Clebsch-Gordon Series)**.** *For two irreducible representations $D^{(s)}, D^{(t)}$ of $\mathfrak{su}(2)$,*

$$D^{(s)} \otimes D^{(t)} = D^{(s+t)} \oplus D^{(s+1-1)} \oplus \cdots \oplus D^{(|s-t|)}.$$

The next theorem demonstrates the usefulness of considering the Hamiltonian in terms of the irreducible representations of $\mathfrak{su}(2)$.

Theorem 3.4 (Schur's Lemma [3, Theorem 10.7.6])**.**

(a) Let ρ and ρ' be irreducible representations of G on vector spaces V and V', respectively, and let $T : V' \to V$ be a G-invariant transformation. Then, either T is an isomorphism, or $T = 0$.

(b) Let ρ be an irreducible representation of G on a vector space V, and let $T : V \to V$ be a G-invariant linear operator (i.e., $\forall g \in G$, $T \circ \rho_g' = \rho_g \circ T$). Then T is multiplication by a scalar: $T = cI$.

There is an equivalent theorem for Lie algebra representations.

On an $SU(2)$-invariant Hamiltonian, the second part of Schur's Lemma guarantees that any vector lying entirely inside an irreducible representation is an eigenvector for the Hamiltonian. Therefore, the decomposition of V into the $\mathfrak{su}(2)$-invariant subspaces simultaneously diagonalizes an $SU(2)$-invariant Hamiltonian.

3.2. **Application to the ferromagnetic Heisenberg-½ model.** We will now consider how $SU(2)$ may be applied to the ferromagnetic Heisenberg-½ model. These results will be particularly useful in Section 5, where we will construct a state which bounds the spectral gap from above by considering states which must lie inside a particular irreducible representation. We now show that the Hamiltonian in the ferromagnetic Heisenberg-½ model is $SU(2)$-invariant, and that Schur's Lemma may therefore be applied.

Proposition 3.5. *The Hamiltonian of the ferromagnetic Heisenberg-½ model is $SU(2)$ symmetric.*

Proof. Let $\{\sigma^1, \sigma^2, \sigma^3\}$ be the basis for $SU(2)$ given in (2.1), and let h be as given in (2.2). Then, $[h, \sigma^i \otimes \sigma^i] = 0$ and $[h, \sigma^i \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^i] = 0$ for each of $i = 1, 2, 3$. Therefore, h is $SU(2)$ and $\mathfrak{su}(2)$ symmetric. ■

The following lemma characterizes one of the irreducible representations, and therefore one of the eigenspaces. We will later see that this eigenspace corresponds to the first excited state.

Lemma 3.6. *The highest weight irreducible representation of $(V^{(\frac{1}{2})})^{\otimes n}$ is the space of symmetric vectors.*

Proof. We generate a basis for the highest weight irreducible representation as in Lemma 3.2. The vector corresponding to the largest eigenvector of S^3 will be in the highest weight irreducible representation; in this case, $\psi_0 = |\uparrow \dots \uparrow\rangle$. This vector is symmetric. In the representation $(D^{(\frac{1}{2})})^{\otimes n}$,

$$S^- = \sum_{k=0}^{n} (\mathbb{1}_2)^{\otimes k} \otimes S^-_{1/2} \otimes (\mathbb{1}_2)^{\otimes (n-k-1)}$$

where

$$S^-_{1/2} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

Let $\sigma \in S_n$. Then,

$$\begin{aligned} \tau_\sigma(S^-) &= \sum_{k=0}^{n} \tau_\sigma \left((\mathbb{1}_2)^{\otimes k} \otimes S^-_{1/2} \otimes (\mathbb{1}_2)^{\otimes (n-k-1)} \right) \\ &= \sum_{k=0}^{n} (\mathbb{1}_2)^{\otimes \sigma(k)} \otimes S^-_{1/2} \otimes (\mathbb{1}_2)^{\otimes (n-\sigma(k)-1)} \\ &= S^-. \end{aligned}$$

Therefore, S^- is symmetric. A symmetric operator applied to a symmetric vector will yield a symmetric vector; therefore, $\psi_{i+1} = S^-\psi_i$ is symmetric, so $V^{(n/2)} \subseteq \mathcal{G}_{[1,n]}$.

By induction, all of the basis vectors are symmetric and therefore in the kernel; therefore, the highest weight irreducible representation is in the kernel. All that remains to show is that every symmetric vector is in the highest weight irreducible representation. Note that there are $n+1$ linearly independent symmetric vectors on n sites. This is the same as the dimension of the highest weight irreducible representation, $V^{(n/2)}$, so $V^{(n/2)} = \mathcal{G}_{[1,n]}$. ■

4. Upper Bound on the Spectral Gap

In this section, we prove an upper bound on the spectral gap of $\mathcal{O}(n^{-2})$ for the ferromagnetic Heisenberg-½ model. We first introduce the variational principle, a technique for calculating energies, and then apply this technique to our model.

4.1. **The variational principle.** The variational principle can be used to establish an upper bound on the lowest non-zero eigenvalue of linear operators. When applied to a frustration-free quantum system, it gives an upper bound for the spectral gap above the ground state.

Theorem 4.1 (Variational Principle)**.** *Let $H \in M_n(\mathbb{C})$ be an $n \times n$ Hermitian matrix with spectrum $\lambda_0 < \lambda_1 \leq \ldots \leq \lambda_m$. Denote the ground state of H by $\mathcal{G} = \ker(H - \lambda_0 I)$. Then,*

$$\lambda_1 = \inf_{\substack{\psi \in \mathbb{C}^n \\ \psi \perp \mathcal{G}}} \frac{\langle \psi | H | \psi \rangle}{\|\psi\|^2}$$

where λ_1 is the second smallest (distinct) eigenvalue of H.

Proof. By the spectral theorem, let $\{e_1, \ldots, e_n\}$ be an orthonormal basis for $\mathbb{C}^n$. By relabeling, let $e_1, \ldots, e_m$, $e_{m+1}, \ldots, e_n$ have eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_m, 0, \ldots, 0$. Then, for any $\psi \in \mathcal{G}^\perp$,

$$\psi = \langle e_1 | \psi_1 \rangle |e_1\rangle + \cdots + \langle e_m | \psi_m \rangle |e_m\rangle .$$

When applied to H,

$$H |\psi\rangle = \lambda_1 \langle e_1 | \psi_1 \rangle |e_1\rangle + \cdots + \lambda_m \langle e_m | \psi_m \rangle |e_m\rangle .$$

Left-multiplying by $\langle \psi | = \langle e_1 | \langle e_1 | \psi_1 \rangle + \cdots + \langle e_m | \langle e_m | \psi_m \rangle$ yields

$$\begin{aligned}
\langle \psi | H | \psi \rangle &= \lambda_1 |\langle e_1 | \psi \rangle|^2 + \cdots + \lambda_m |\langle e_m | \psi \rangle|^2 \\
&\geq \lambda_1 \left(|\langle e_1 | \psi \rangle|^2 + \cdots + |\langle e_m | \psi \rangle|^2 \right) \\
&= \lambda_1 \|\psi\|^2 .
\end{aligned}$$

Therefore,

$$\lambda_1 \leq \inf_{\substack{\psi \perp \mathcal{G} \\ \psi \neq 0}} \frac{\langle \psi | H | \psi \rangle}{\|\psi\|^2}.$$

Let ψ be in the eigenspace corresponding to eigenvalue λ_1. Since H is Hermitian, $\psi \perp \mathcal{G}$. Then,

$$\frac{\langle \psi | H | \psi \rangle}{\|\psi\|^2} = \frac{\lambda_1 \langle \psi | \psi \rangle}{\|\psi\|^2} = \lambda_1.$$

Therefore, λ_1 is the infimum. ■

4.2. **Application to the ferromagnetic Heisenberg-½ model.** In this section, we apply the variational principle we introduced in Section 4.1 to prove an upper bound on the first excited energy of the ferromagnetic Heisenberg-½ model. To apply this method, we need to consider vectors that are orthogonal to the ground state space. We will begin by establishing a criterion using the permutation operators introduced in (2.3) for determining if a vector ψ belongs to the orthogonal complement of the ground state space. We will define a variational vector that satisfies this criterion, which belongs to the class of so-called *one-particle states*, defined below. In Lemma 4.5 we will prove an upper bound on the expected energy of any one particle state, that we will apply to our variational vector to prove the main result, which we now state.

Theorem 4.2 (Upper bound on spectral gap)**.** *Let λ_1 be the first excited energy of $H_{[1,n]}$. Then,*

$$\lambda_1 \leq \frac{\pi^2 n}{4(n-1)^2(n+1)}.$$

In Lemma 4.4 we establish a criteria for determining if a vector is orthogonal to the ground state space. To state this result, recall our definition of a permutation operator given by (2.3),

$$\tau_\sigma \left(\bigotimes_{i=1}^{n} \psi_i \right) = \bigotimes_{i=1}^{n} \psi_{\sigma(i)}.$$

The next proposition demonstrates that the permutation operators are unitary.

Proposition 4.3. *For all $\sigma \in S_n$, $\tau_{\sigma^{-1}} = \tau_\sigma^*$. Namely, τ_σ is unitary.*

Proof. Let $\sigma \in S_n$. Since τ_σ only permutes the vectors of the standard orthonormal basis of $\mathbb{C}^{2^n}$ without changing the magnitude of a vector, $\langle \tau_\sigma \psi | \tau_\sigma \psi \rangle = \langle \psi | \psi \rangle$ for all $\psi \in \mathbb{C}^{2^n}$. But, by the definition of an adjoint, we also have that $\langle \psi | \psi \rangle = \langle \psi | \tau_\sigma^* \tau_\sigma \psi \rangle$. Therefore, $\tau_\sigma^* \circ \tau_\sigma = \mathbb{1}$. A similar calculation shows that $\tau_\sigma \circ \tau_\sigma^* = \mathbb{1}$. So, $\tau_\sigma^* = \tau_\sigma^{-1} = \tau_{\sigma^{-1}}$ by (2.4). Therefore, τ_σ is unitary. ∎

We can now state a sufficient condition for being in an excited state of the Hamiltonian in terms of the permutation operator.

Lemma 4.4. *Let $\psi \in \mathbb{C}^{2^n}$. If there is a $\sigma \in S_n$ such that $\tau_\sigma \psi = -\psi$, then $\psi \perp \mathcal{G}$.*

Proof. Let $\psi \in \mathbb{C}^{2^n}$ and $\varphi \in \mathcal{G}$. Assume that there is a $\sigma \in S_n$ such that $\tau_\sigma \psi = -\psi$. Then, by Lemma 4.3,

$$\begin{aligned}
\langle \psi | \varphi \rangle &= \langle \psi | \tau_{\sigma^{-1}} \varphi \rangle \\
&= \langle \tau_\sigma \psi | \varphi \rangle \\
&= \langle -\psi | \varphi \rangle \\
&= - \langle \psi | \varphi \rangle .
\end{aligned}$$

Therefore, $\langle \psi | \varphi \rangle = - \langle \psi | \varphi \rangle = 0$. Since ψ and φ are orthogonal, $\psi \perp \mathcal{G}$. ∎

We define a *one particle state* to be a linear combination of vectors of the form $|x\rangle = |\uparrow \ldots \uparrow\downarrow\uparrow \ldots \uparrow\rangle$ with the down spin in the x^{th} position. We will begin by deriving a general expression for $\langle \psi | H_{[1,n]} | \psi \rangle$ for one particle states by using the permutation operator. Then, we will choose an excited state, apply Lemma 4.4 to show that it is perpendicular to the ground state, and apply the variational principle to establish an upper bound on the spectral gap.

For a general one-particle state, the expected energy can be calculated exactly. This is the content of the next lemma.

Lemma 4.5. *Let $\psi = \sum_{x=1}^n c_x |x\rangle$ be a one-particle state. Then,*

$$\langle \psi | H_{[1,n]} | \psi \rangle = \sum_{x=1}^n |c_x - c_{x+1}|^2.$$

Proof. Let $\psi = \sum_{x=1}^n c_x |x\rangle$. Consider the energy of a one-particle state,

$$\begin{aligned}
\langle \psi | H_{[1,n]} | \psi \rangle &= \left\langle \psi \middle| \sum_{x=1}^{n-1} (\mathbb{1} - \tau_{x,x+1}) \middle| \psi \right\rangle \\
&= (n-1) \|\psi\|^2 - \sum_{x=1}^{n-1} \langle \psi | \tau_{x,x+1} \psi \rangle .
\end{aligned}$$

When $|\psi\rangle$ is a one-particle state, we may expand $|\psi\rangle = \sum_{x=1}^n c_x |x\rangle$,

$$\sum_{x=1}^{n-1} \langle \psi | \tau_{x,x+1} \psi \rangle = \sum_{x=1}^{n-1} \sum_{y=1}^{n} \sum_{z=1}^{n} \overline{c_y} c_z \langle y | \tau_{x,x+1} z \rangle .$$

Now, $\langle y | \tau_{x,x+1} z \rangle = \delta_{y,\tau_x z}$ where $\delta_{\cdot,\cdot}$ is the Kronecker delta. Note that $y = \tau_{x,x+1} z$ for all possible x, y, z if and only if one of the following is true:

(1) $y = x + 1$, $z = x$,
(2) $y = x$, $z = x + 1$,
(3) $y = z$ and $y \neq x, x + 1$.

Therefore, for any fixed $1 \leq x \leq n-1$ and $1 \leq y \leq n$,

$$\sum_{z=1}^{n} \overline{c_y} c_z \langle y | \tau_{x,x+1} z \rangle = |c_y|^2 (1 - \delta_{y,x+1} - \delta_{x,y}) + \overline{c_y} c_{y-1} \delta_{y,x+1} + \overline{c_y} c_{y+1} \delta_{x,y}.$$

We will now sum over x and y for each term. Taking into account that $\sum_{y=1}^{n} |c_y|^2 = \|\psi\|^2$,

$$\begin{aligned}\sum_{x=1}^{n-1}\sum_{y=1}^{n} |c_y|^2(1-\delta_{y,x+1}-\delta_{x,y}) &= \sum_{x=1}^{n-1}\left[\left(\sum_{y=1}^{n}|c_y|^2\right) - |c_x|^2 - |c_{x+1}|^2\right] \\ &= (n-1)\|\psi\|^2 - \sum_{x=1}^{n-1}\left(|c_x|^2 + |c_{x+1}^2|\right).\end{aligned}$$

Additionally,

$$\begin{aligned}\sum_{x=1}^{n-1}\sum_{y=1}^{n}\overline{c_y}c_{y-1}\delta_{y,x+1} &= \sum_{x=1}^{n-1}\overline{c_{x+1}}c_x, \\ \sum_{x=1}^{n-1}\sum_{y=1}^{n}\overline{c_y}c_{y+1}\delta_{x,y} &= \sum_{x=1}^{n-1}\overline{c_x}c_{x+1}.\end{aligned}$$

Combining these summations, we obtain

$$\begin{aligned}\langle\psi|H_{[1,n]}|\psi\rangle &= (n-1)\|\psi\|^2 + \sum_{x=1}^{n-1}\left(|c_x|^2 + |c_{x+1}|^2 - \|\psi\|^2 - \overline{c_x}c_{x+1} - c_x\overline{c_{x+1}}\right) \\ &= \sum_{x=1}^{n-1}\left(|c_x|^2 - \overline{c_x}c_{x+1} - c_x\overline{c_{x+1}} + |c_{x+1}|^2\right) \\ &= \sum_{x=1}^{n-1}|c_x - c_{x+1}|^2.\end{aligned}$$

■

Proof of Theorem 4.2. We will now prove this section's main theorem by constructing a one-particle state perpendicular to the ground state with energy decaying at a rate of n^{-2}. We make the ansatz

$$c_x = \cos\left(\frac{(x-1)\pi}{n-1}\right).$$

We first show that this vector is perpendicular to the ground states using Lemma 4.4. From our definition of c_x, $c_x = -c_{x-n+1}$. Let

$$\sigma = \prod_{x=1}^{\lfloor n/2\rfloor}(x \quad (n-x+1))$$

where there is no ambiguity because the above transpositions mutually commute. By this construction, $\tau_\sigma|x\rangle = |n-x+1\rangle$ for all $1 \le x \le n$, so

$$\begin{aligned}\tau_\sigma\psi &= \sum_{x=1}^{n} c_x|x\rangle \\ &= -\sum_{x=1}^{n} -c_{x-n+1}|n-x+1\rangle \\ &= -\psi.\end{aligned}$$

Thus, by Lemma 4.4, $\psi \perp \mathcal{G}$. So, by the variational principle,

$$\lambda_1 \le \frac{\langle\psi_1|H_{[1,n]}|\psi_1\rangle}{\|\psi_1\|^2}.$$

We first calculate the magnitude of ψ, namely,

$$\begin{aligned}
\|\psi\|^2 &= \sum_{x=1}^{n} \cos^2\left(\frac{(x-1)\pi}{n-1}\right) \\
&= \sum_{x=1}^{n} \left[\frac{1}{2} + \frac{1}{2}\cos\left(\frac{2(x-1)\pi}{n-1}\right)\right] \\
&= \frac{n}{2} + \frac{1}{2}\left[1 + \sum_{x=1}^{n-1} \cos\left(\frac{2x\pi}{n-1}\right)\right].
\end{aligned}$$

Using the trigonometric identity

$$\sum_{k=1}^{N} \cos(k\theta) = -\frac{1}{2} + \frac{\sin\big((N+\frac{1}{2})\theta\big)}{2\sin\big(\frac{\theta}{2}\big)}$$

we can simplify $\|\psi\|^2$ as

$$\begin{aligned}
\|\psi\|^2 &= \frac{n}{2} + \frac{1}{2}\left[1 - \frac{1}{2} + \frac{\sin\left(\frac{(n-\frac{1}{2})2\pi}{n-1}\right)}{2\sin\left(\frac{\pi}{n-1}\right)}\right] \\
&= \frac{n}{2} + \frac{1}{2}\left[\frac{1}{2} + \frac{\sin\left(2\pi + \frac{\pi}{n-1}\right)}{2\sin\left(\frac{\pi}{n-1}\right)}\right] \\
&= \frac{n}{2} + \frac{1}{2}.
\end{aligned}$$

Finally, we calculate the energy of this ansatz. Using $\sin\theta < \theta$ for $\theta > 0$ and the trigonometric identity

$$\cos\theta - \cos\phi = -2\sin\left(\frac{\theta+\phi}{2}\right)\sin\left(\frac{\theta-\phi}{2}\right),$$

Lemma 4.5 shows

$$\begin{aligned}
\big\langle\psi\big|H_{[1,n]}\big|\psi\big\rangle = \sum_{x=1}^{n} |c_x - c_{x+1}|^2 &= \sum_{x=1}^{n} \left|\cos\left(\frac{(x-1)\pi}{n-1}\right) - \cos\left(\frac{x\pi}{n-1}\right)\right|^2 \\
&= \sum_{x=1}^{n} \left|2\sin\left(\frac{(2x-1)\pi}{2(n-1)}\right)\sin\left(\frac{\pi}{2(n-1)}\right)\right|^2 \\
&= 4\sin^2\left(\frac{\pi}{2(n-1)}\right)\sum_{x=1}^{n}\sin^2\left(\frac{(2x-1)}{2(n-1)\pi}\right) \\
&\le 4\sin^2\left(\frac{\pi}{2(n-1)}\right) n \\
&< 4\left(\frac{\pi}{2(n-1)}\right)^2 n \\
&= \frac{\pi^2 n}{(n-1)^2}.
\end{aligned}$$

Therefore, by Theorem 4.1,

$$\begin{aligned}\lambda_1 &\leq \frac{\langle\psi|H_{[1,n]}|\psi\rangle}{\|\psi\|^2} \\ &\leq \frac{\pi^2 n}{4(n-1)^2(n+1)}.\end{aligned}$$ ■

5. Lower Bound on the Spectral Gap

In this section, we calculate a lower bound on the spectral gap of the Heisenberg-½ model of order $\mathcal{O}(n^{-2})$, which is the same order as found in Section 4. To do this, we begin by introducing the martingale method in general, and then applying this method to our model specifically.

5.1. **The martingale method.** We consider a frustration-free, translational invariant (i.e., shifting the lattice does not change the observables) quantum spin system with Hamiltonian acting on $\mathcal{H}_{[1,L]} = \mathbb{C}^{2^n}$ given by

$$H_{[1,L]} = \sum_{x=1}^{L-1} h_{x,x+1}.$$

Recall that by Lemma 2.3,

$$\ker(H_{[1,L]}) = \bigcap_{x=1}^{L-1} \ker(h_{x,x+1}).$$

For any $\Lambda \subset [1, L]$, define G_Λ to be the orthogonal projection onto $\mathcal{G}_\Lambda := \ker(H_\Lambda)$, where we use the convention $G_{\{x\}} = \mathbb{1}$. A consequence of frustration-freeness is the following:

Proposition 5.1.

(a) If $\Lambda_1 \subset \Lambda_2$, then $G_{\Lambda_1}G_{\Lambda_2} = G_{\Lambda_2}G_{\Lambda_1} = G_{\Lambda_2}$.
(b) If $\Lambda_1 \cap \Lambda_2 = \emptyset$, then $G_{\Lambda_1}G_{\Lambda_2} = G_{\Lambda_2}G_{\Lambda_1}$.

Proof. By Lemma 2.3,

$$\begin{aligned}\mathrm{Im}(G_{\Lambda_1}) &= \bigcap_{\{x,x+1\}\subseteq\Lambda_1} \ker(h_{x,x+1}), \\ \mathrm{Im}(G_{\Lambda_2}) &= \bigcap_{\{x,x+1\}\subseteq\Lambda_2} \ker(h_{x,x+1}).\end{aligned}$$

Assume $\Lambda_1 \subset \Lambda_2$. Then, $\bigcap_{\{x,x+1\}\subseteq\Lambda_2} \ker(h_{x,x+1}) \subseteq \bigcap_{\{x,x+1\}\subseteq\Lambda_1} \ker(h_{x,x+1})$, so that, by definition, $\mathrm{Im}(G_{\Lambda_2}) \subseteq \mathrm{Im}(G_{\Lambda_1})$.

Let $\{e_1, \ldots, e_m\}$ be an orthogonal basis for $\mathrm{Im}(G_{\Lambda_2})$, and by the basis extension theorem, extend this to orthogonal bases $\{e_1, \ldots, e_n\}$ and $\{e_1, \ldots, e_p\}$ for $\mathrm{Im}(G_{\Lambda_1})$ and $\mathcal{H}_{[1,L]}$, respectively $(p \geq n \geq m)$. Let $|\psi\rangle = \sum_{i=1}^p c_i e_i$ be arbitrary, and consider

$$\begin{aligned}G_{\Lambda_2}G_{\Lambda_1}|\psi\rangle &= G_{\Lambda_2}\left|\sum_{i=1}^n c_i e_i\right\rangle \\ &= \sum_{i=1}^m c_i e_i \\ &= G_{\Lambda_2}|\psi\rangle.\end{aligned}$$

Similarly,

$$\begin{aligned}
G_{\Lambda_1}G_{\Lambda_2}\left|\psi\right\rangle &= G_{\Lambda_1}\left|\sum_{i=1}^{n} c_i e_i\right\rangle \\
&= \sum_{i=1}^{m} c_i e_i \\
&= G_{\Lambda_2}\left|\psi\right\rangle .
\end{aligned}$$

Therefore, $G_{\Lambda_1}G_{\Lambda_2} = G_{\Lambda_2}G_{\Lambda_1}$ as claimed.

Assume that $\Lambda_1 \cap \Lambda_2 = \emptyset$. Further assume, without loss of generality, that Λ_1 precedes Λ_2. Then, for some orthonormal projections $P \in \mathcal{A}_{\Lambda_1}$ and $Q \in \mathcal{A}_{\Lambda_2}$, we may write

$$\begin{aligned}
G_{\Lambda_1} &= P \otimes \mathbb{1}_{\Lambda_2} \otimes \mathbb{1}_{\Lambda\setminus(\Lambda_1\cup\Lambda_2)}, \\
G_{\Lambda_2} &= \mathbb{1}_{\Lambda_1} \otimes Q \otimes \mathbb{1}_{\Lambda\setminus(\Lambda_1\cup\Lambda_2)}, \\
G_{\Lambda_1}G_{\Lambda_2} = G_{\Lambda_2}G_{\Lambda_1} &= P \otimes Q \otimes \mathbb{1}_{\Lambda\setminus(\Lambda_1\cup\Lambda_2)}.
\end{aligned}$$

■

Next, we define operators E_n $(1 \leq n \leq L)$ on $\mathcal{H}_{[1,L]}$ as

$$E_n = \begin{cases} \mathbb{1} - G_{[1,2]} & n = 1 \\ G_{[1,n]} - G_{[1,n+1]} & 1 < n < L \\ G_{[1,L]} & n = L. \end{cases} \tag{5.1}$$

Immediately from this definition, E_n forms a resolution of the identity:

$$\sum_{n=1}^{L} E_n = \mathbb{1}. \tag{5.2}$$

We show that the set $\{E_n \mid 1 \leq n \leq L\}$ is a mutually orthogonal family of orthogonal projections, that is,

$$E_n^* = E_n, \quad E_n E_m = \delta_{n,m} E_m. \tag{5.3}$$

First, note that E_n is the sum of orthogonal projections. Orthogonal projections are self-adjoint, so E_n is also self-adjoint, i.e., $E_n^* = E_n$. Consider $E_n E_m$ for $1 \leq n, m \leq L$. Without loss of generality, assume $n \leq m$. Then, by Proposition 5.1(a), we have

$$\begin{aligned}
E_n E_m &= \left(G_{[1,n]} - G_{[1,n+1]}\right)\left(G_{[1,m]} - G_{[1,m+1]}\right) \\
&= G_{[1,n]}G_{[1,m]} - G_{[1,n]}G_{[1,m+1]} - G_{[1,n+1]}G_{[1,m]} + G_{[1,n+1]}G_{[1,m+1]} \\
&= G_{[1,m]} - G_{[1,m+1]} - (1 - \delta_{n,m})G_{[1,m]} + G_{[1,m+1]} \\
&= \delta_{n,m} E_m.
\end{aligned}$$

A similar calculation shows that (5.3) holds if $m < n$.

For the martingale method, we will need a bound of the spectral gap of a single interaction term $h_{x,x+1}$.

Proposition 5.2. *Let γ be the smallest non-zero eigenvalue of $h_{x,x+1}$. Then,*

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

Proof. Recall that $h_{x,x+1} \geq 0$ because our model is frustration-free. Since the image of a map is orthogonal to the kernel of the map,

$$\operatorname{Im}(h_{x,x+1})^{\perp} = \operatorname{Im}(G_{[x,x+1]}).$$

Therefore, $\mathbb{1} - G_{[x,x+1]}$ is the orthogonal projection onto the image of $h_{x,x+1}$.

By the spectral theorem, there exists non-negative eigenvalues $\lambda_1, \ldots, \lambda_n$ and an orthonormal basis $\{e_1, \ldots, e_n\}$ such that

$$h_{x,x+1} |\psi\rangle = \sum_{i=1}^{n} \lambda_i \langle e_i|\psi\rangle e_i.$$

Furthermore, the elements e_i corresponding to non-negative eigenvalues form an orthogonal basis for the image of $h_{[x,x+1]}$, and thus for the image of $\mathbb{1} - G_{[x,x+1]}$. Therefore,

$$\begin{aligned} \langle\psi|h_{x,x+1}|\psi\rangle &= \sum_{i=1}^{n} \lambda_i \langle e_i|\psi\rangle \\ &\geq \gamma \sum_{\substack{i=1 \\ \lambda_i \neq 0}}^{n} \langle e_i|\psi\rangle \\ &= \gamma \left\langle \psi \middle| \mathbb{1} - G_{[x,x+1]} \middle| \psi \right\rangle . \end{aligned}$$

Therefore, $h_{x,x+1} \geq \gamma(\mathbb{1} - G_{[x,x+1]})$. ■

The next assumption is key for the martingale method. We will show that it is satisfied by the ferromagnetic Heisenberg-½ model.

Assumption 5.3. *There exists a constant ϵ, $0 \leq \epsilon < \frac{1}{\sqrt{2}}$, such that, for all $1 \leq n \leq L-1$,*

$$E_n G_{[n,n+1]} E_n \leq \epsilon^2 E_n. \tag{5.4}$$

Equivalently,

$$\left\|G_{[n,n+1]} E_n\right\| \leq \epsilon. \tag{5.5}$$

That the above two expressions are equivalent can be seen by the following equivalences:

$$\begin{aligned} \left\|G_{[n,n+1]} E_n\right\| \leq \epsilon &\iff \left\|G_{[n,n+1]} E_n \psi\right\|^2 \leq \epsilon^2 \left\|\psi\right\|^2 \\ &\iff \left\langle \psi \middle| E_n G_{[n,n+1]}^2 E_n \psi \right\rangle \leq \epsilon^2 \langle\psi|\psi\rangle \\ &\iff E_n G_{[n,n+1]} E_n \leq \epsilon^2 E_n, \end{aligned}$$

where the final equivalence follows from (5.3).

Given Assumption 5.3 holds, we can prove a lower bound for the spectral gap of $H_{[1,L]}$.

Theorem 5.4 (Martingale method)**.** *Let λ_1 be the lowest non-zero eigenvalue of the translation invariant, frustration-free Hamiltonian $H_{[1,L]}$. Then, the following estimate holds under Assumption 5.3:*

$$\lambda_1 \geq \gamma(1 - \sqrt{2}\epsilon)^2.$$

The proof of this theorem will rely on the following inequality.

Proposition 5.5. *For any $\phi_1, \phi_2 \in \mathbb{C}^n$ and $c > 0$,*

$$|\langle\phi_1|\phi_2\rangle| \leq \frac{c}{2} \|\phi_1\| + \frac{1}{2c} \|\phi_2\| .$$

Proof. Consider,

$$\begin{aligned} 0 &\leq \left(\sqrt{c}\,\|\phi_1\| - \frac{1}{\sqrt{c}\,\|\phi_2\|}\right)^2 \\ &= c\,\|\phi_1\|^2 - 2\,\|\phi_1\|\,\|\phi_2\| + \frac{1}{c}\,\|\phi_2\|^2 \\ &= \frac{c}{2}\,\|\phi_1\|^2 - \|\phi_1\|\,\|\phi_2\| + \frac{1}{2c}\,\|\phi_2\|^2 . \end{aligned}$$

So, $\|\phi_1\|\,\|\phi_2\| \le \frac{c}{2}\|\phi_1\|^2 + \frac{1}{2c}\|\phi_2\|^2$. Invoking the Cauchy-Swartz inequality $|\langle\phi_1|\phi_2\rangle| \le \|\phi_1\|\,\|\phi_2\|$ gives

$$|\langle\phi_1|\phi_2\rangle| \le \frac{c}{2}\|\phi_1\| + \frac{1}{2c}\|\phi_2\|\,. \qquad \blacksquare$$

Proof of Theorem 5.4. Let $\psi \perp \mathcal{G}_{[1,L]}$. Then, $G_{[1,L]}\psi = E_L\psi = 0$; by plugging in the resolution of the identity (5.2) and using the mutual orthogonality of E_n (5.1) and (5.3) we find

$$\begin{aligned}\|\psi\|^2 &= \left\langle \psi \middle| \sum_{n=1}^{L} E_n \middle| \psi \right\rangle \\ &= \sum_{n=1}^{L-1} \langle\psi|E_n|\psi\rangle\,. \end{aligned} \tag{5.6}$$

Moreover,

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

By introducing another resolution of the identity and using Proposition 5.1,

$$\begin{aligned}\big\langle\psi\big|G_{[n,n+1]}E_n\big|\psi\big\rangle &= \left\langle \psi \middle| \sum_{m=1}^{L-1} E_m G_{[n,n+1]}E_n\psi \right\rangle \\ &= \big\langle\psi\big|(E_{n-1}+E_n)G_{[n,n+1]}E_n\psi\big\rangle\,, \end{aligned} \tag{5.7}$$

where E_{n-1} is absent for $n = 1$. The final line follows by observing that, if $m \le n-2$, then E_m and $G_{[n,n+1]}$ commute by Proposition 5.1(a), and if $m \ge n+1$, then they commute by Proposition 5.1(b). In either case, $E_m G_{[n,n+1]}E_n = G_{[n,n+1]}E_m E_n = 0$ by (5.3).

Invoking Proposition 5.5, for any constants $c_1, c_2 > 0$, (5.7) becomes

$$\begin{aligned}\|E_n\psi\|^2 \le{}& \frac{1}{2c_1}\big\langle\psi\big|\left(\mathbb{1} - G_{[n,n+1]}\right)\psi\big\rangle + \frac{c_1}{2}\langle\psi|E_n\psi\rangle \\ &+ \frac{1}{2c_2}\big\langle\psi\big|E_nG_{[n,n+1]}E_n\psi\big\rangle + \frac{c_2}{2}\big\langle\psi\big|(E_{n-1}+E_n)^2\psi\big\rangle\,. \end{aligned} \tag{5.8}$$

By Proposition 5.2, the first term of (5.8) can be estimated by

$$\big\langle\psi\big|\left(\mathbb{1} - G_{[n,n+1]}\right)\psi\big\rangle \le \frac{1}{\gamma}\langle\psi|h_{n,n+1}\psi\rangle\,,$$

and by (5.2), the third term of (5.8) can be estimated by

$$\big\langle\psi\big|E_nG_{[n,n+1]}E_n\psi\big\rangle \le \epsilon^2 E_n.$$

Plugging these estimates back into (5.8),

$$\left(2 - c_1 - \frac{\epsilon^2}{c_2}\right)\|E_n\psi\|^2 - c_2\,\|(E_{n-1}+E_n)\psi\|^2 \le \frac{1}{c_1\gamma}\langle\psi|h_{n,n+1}\psi\rangle\,. \tag{5.9}$$

Note that $\|(E_{n-1}+E_n)\psi\|^2 = \|E_{n-1}\psi\|^2 + \|E_n\psi\|^2$ since E_{n-1}, E_n are mutually orthogonal. Now, by (5.6),

$$\sum_{n=1}^{L-1}\left(2 - c_1 - \frac{\epsilon^2}{c_2}\right)\|E_n\psi\|^2 = \left(2 - c_1 - \frac{\epsilon^2}{c_2}\right)\|\psi\|^2$$

and

$$\sum_{n=1}^{L-1} c_2 \left\|(E_{n-1}+E_n)\psi\right\|^2 = c_2 \sum_{n=1}^{L-1} (\|E_{n-1}\psi\|^2 + \|E_n\psi\|^2)$$
$$= c_2 \left(\|\psi\|^2 + \sum_{n=1}^{L-2} \|E_n\psi\|^2 \right)$$
$$\leq 2c_2 \|\psi\|^2 .$$

Therefore, summing (5.9) over n yields

$$(2 - c_1 - \frac{\epsilon^2}{c_2} - 2c_2) \|\psi\|^2 \leq \frac{1}{c_1\gamma} \left\langle \psi \middle| H_{[1,L]}\psi \right\rangle .$$

Recall that ψ was chosen to be in the eigenspace corresponding to the eigenvalue λ_1. Therefore, $\lambda_1 \|\psi\|^2 = \left\langle \psi \middle| H_{[1,L]}\psi \right\rangle$, and we obtain the inequality

$$\lambda_1 \|\psi\|^2 \geq \gamma c_1 \left(2 - c_1 - \frac{\epsilon^2}{c_2} - 2c_2 \right) \|\psi\|^2 .$$

We are interested in optimizing the lower bound λ_1. To do so, we must maximize

$$f(c_1, c_2) = c_1 \left(2 - c_1 - \frac{\epsilon^2}{c_2} - 2c_2 \right).$$

Solving $f_{c_1}(c_1, c_2) = f_{c_2}(c_1, c_2) = 0$ produces $c_1 = 1 - \sqrt{2}\epsilon$ and $c_2 = \epsilon/\sqrt{2}$.

Finally, by plugging in these values of c_1 and c_2, we find

$$c_1 \left(2 - c_1 - \frac{\epsilon^2}{c_2} - 2c_2 \right) = (1 - \sqrt{2}\epsilon)^2.$$

Therefore,

$$\lambda_1 \geq \gamma(1 - \sqrt{2}\epsilon)^2. \qquad \blacksquare$$

5.2. **Application to the ferromagnetic Heisenberg-½ model.** We are now ready to apply the martingale method to the ferromagnetic Heisenberg-½ model to obtain a lower bound on the spectral gap.

Theorem 5.6. *The spectral gap of the Heisenberg-½ Hamiltonian $H_{[1,L]}$ closes at a rate bounded below by $\mathcal{O}(n^{-2})$. Specifically,*

$$\mathrm{gap}(H_{[1,n]}) \geq \frac{1}{4n^2}.$$

In order to invoke Theorem 5.4, we must show that the Heisenberg-½ model satisfies Assumption 5.3. In order to do so, we must calculate the value

$$\epsilon = \sup_{\psi \neq 0} \frac{\left\| G_{[n,n+1]} E_n \right\|}{\|\psi\|}. \tag{5.10}$$

To do so, we will use the following lemma.

Lemma 5.7. *Let $A \in M_{2^{n+1}}(\mathbb{C})$. Then,*

$$\sup_{\psi \neq 0} \frac{\|AE_n\psi\|^2}{\|\psi\|^2} = \sup_{\substack{\psi \in \mathcal{G}_{[1,n]} \cap \mathcal{G}_{[1,n+1]}^{\perp} \\ \psi \neq 0}} \frac{\|A\psi\|^2}{\|\psi\|^2}.$$

Proof. Note that $E_n = G_{[1,n]} - G_{[1,n+1]} = G_{[1,n]}(\mathbb{1} - G_{[1,n+1]})$ by Proposition 5.1(a). We will rely on the fact that $E_n\psi = \psi$ if and only if $\psi \in \mathcal{G}_{[1,n]} \cap \mathcal{G}_{[1,n+1]}^{\perp}$. To demonstrate this, first assume that $E_n\psi = \psi$. Then, since $G_{[1,n]} = G_{[1,n]}^2$,

$$\begin{aligned} G_{[1,n]}\psi &= G_{[1,n]}E_n\psi \\ &= E_n\psi \\ &= \psi. \end{aligned}$$

Therefore, $\psi \in \mathcal{G}_{[1,n]}$. Now, by Proposition 5.1(a),

$$\begin{aligned} \psi &= G_{[1,n]}\left(\mathbb{1} - G_{[1,n+1]}\right)\psi \\ &= \left(\mathbb{1} - G_{[1,n+1]}\right)G_{[1,n]}\psi \\ &= \left(\mathbb{1} - G_{[1,n+1]}\right)\psi. \end{aligned}$$

Therefore, $(\mathbb{1} - G_{[1,n+1]})\psi = \psi$, or equivalently, $G_{[1,n+1]}\psi = 0$. Therefore, $\psi \in \mathcal{G}_{[1,n]} \cap \mathcal{G}_{[1,n+1]}^{\perp}$.

Next, assume that $\psi \in \mathcal{G}_{[1,n]} \cap \mathcal{G}_{[1,n+1]}^{\perp}$. Then, $(\mathbb{1} - G_{[1,n+1]})\psi = \psi$ and $G_{[1,n]}\psi = \psi$, so

$$E_n\psi = G_{[1,n]}\left(\mathbb{1} - G_{[1,n+1]}\right)\psi = \psi.$$

This finishes establishing that $E_n\psi = \psi$ if and only if $\psi \in \mathcal{G}_{[1,n]} \cap \mathcal{G}_{[1,n+1]}^{\perp}$.

We now prove our lemma. Let $\phi \notin G_{[1,n]} \cap G_{[1,n+1]}^{\perp}$, and let $\phi' = E_n\phi$. Then, $E_n\phi' = \phi'$, and

$$\|AE_n\phi'\| = \|A\phi'\| = \|AE_n\phi\|.$$

Note that $\phi = \phi' + (\mathbb{1} - E_n)\phi$. By the mutual orthogonality of E_n, $\|\phi\|^2 = \|\phi'\|^2 + \|(\mathbb{1} - E_n)\phi\|^2$, and so $\|\phi\| > \|\phi'\|$. Therefore,

$$\frac{\|AE_n\phi\|}{\|\phi\|} < \frac{\|AE_n\phi'\|}{\|\phi'\|},$$

so the supremum could not have been achieved at ϕ, and the supremum of $\frac{\|AE_n\phi\|}{\|\phi\|}$ must be achieved on $\mathcal{G}_{[1,n]} \cap \mathcal{G}_{[1,n+1]}^{\perp}$.

Therefore,

$$\sup_{\psi \neq 0} \frac{\|AE_n\psi\|^2}{\|\psi\|^2} = \sup_{\substack{\psi \in \mathcal{G}_{[1,n]} \cap \mathcal{G}_{[1,n+1]}^{\perp} \\ \psi \neq 0}} \frac{\|A\psi\|^2}{\|\psi\|^2}. \qquad \blacksquare$$

Proof of Theorem 5.6. By Lemma 5.7, we are interested in vectors $\psi \in \mathcal{G}_{[1,n]} \cap \mathcal{G}_{[1,n+1]}^{\perp}$. Since $\mathcal{G}_{[1,n]} \approx V^{(n/2)}$ is the space of symmetric vectors on the first n sites, ψ will be of the form

$$\psi = \sum_{\substack{p = -\frac{n}{2}, \ldots, \frac{n}{2} \\ k = \uparrow, \downarrow}} c_{k,p}\psi_p \otimes |k\rangle, \quad c_{k,p} \in \mathbb{C}$$

where ψ_p is the normalized, symmetric state with spin p, and $c_{k,p} \in \mathbb{C}$.

Recall the definition of $V^{(n/2)}$ introduced in Section 3.1, and see the comment following the statement of Lemma 3.2. Since $\psi_p \in G_{[1,n]} \approx V^{(n/2)}$ it must be that $\psi \in V^{(n/2)} \otimes V^{(1/2)} \approx V^{(n+1/2)} \oplus V^{(n-1/2)}$ where we are applying Theorem 3.3. By Lemmas 2.4 and 3.6, we know that $V^{(n+1/2)} = \mathcal{G}_{[1,n+1]}$. Therefore, $\psi \in \mathcal{G}_{[1,n]} \cap \mathcal{G}_{[1,n+1]}^{\perp} = V^{(n-1/2)}$.

It can be shown that $[G_{[n,n+1]}, \sigma_{[1,L]}^i] = 0$ for all $i = 1, 2, 3$; therefore, $G_{[n,n+1]}$ is $SU(2)$-invariant. Along with $V^{((n-1)/2)}$ being an irreducible representation of $SU(2)$, by Schur's Lemma [3, Chapter 10.7], $G_{[n,n+1]}$ is multiplication by a scalar on $V^{((n-1)/2)}$. Therefore, $\left\|G_{[n,n+1]}\psi\right\|$ is a constant scalar, regardless of the choice of ψ, and so we need only construct a single $\psi \in V^{(n-1/2)}$

Let $\psi_1, \psi_2 \in \mathcal{G}_{[1,n]}$ be $\psi_1 = \psi_{n/2} \otimes |{\downarrow}\rangle$, $\psi_2 = \psi_{n/2-1} \otimes |{\uparrow}\rangle$, and $\psi = -n\psi_1 + \psi_2$. Let $|i\rangle \in \mathbb{C}^{2^n}$ refer to a spin-up particle being in only the i^{th} position. Note that $\psi_1 = |{\uparrow} \dots {\uparrow}{\downarrow}\rangle = |n+1\rangle$ and $\psi_2 = \sum_{i=1}^{n} |i\rangle$. Note that $\psi \perp \mathcal{G}_{[1,n+1]}$ as

$$\begin{aligned} \langle \psi | \psi_1 + \psi_2 \rangle &= -n \left\| \psi_1 \right\|^2 + \left\| \psi_2 \right\|^2 \\ &= -n + n \\ &= 0. \end{aligned}$$

We can now show that Assumption 5.3 is satisfied by 5.10. By Lemma 5.7,

$$\begin{aligned} G_{[n,n+1]} E_n \psi &= G_{[n,n+1]} \psi \\ &= G_{[n,n+1]} \psi_2 - n G_{[n,n+1]} \psi_1 \\ &= |1\rangle + \cdots + |n-1\rangle + \frac{1}{2}(|n\rangle + |n+1\rangle) - \frac{n}{2}(|n\rangle + |n+1\rangle) \\ &= |1\rangle + \cdots + |n-1\rangle - \frac{n-1}{2}(|n\rangle + |n+1\rangle). \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{\left\| G_{[n,n+1]} \psi \right\|}{\left\| \psi \right\|} &= \frac{\sqrt{n - 1 + 2(\frac{n-1}{2})^2}}{\sqrt{n + n^2}} \\ &= \frac{1}{\sqrt{2}} \sqrt{\frac{n^2 - 1}{n^2 + n}}. \end{aligned} \tag{5.11}$$

Our value of ϵ is given by (5.11). Note that this is less than $1/\sqrt{2}$, satisfying Assumption 5.3. Finally, we may invoke Theorem 5.4 to show that the rate at which the spectral gap closes is bounded from below by $\mathcal{O}(n^{-2})$. By plugging ϵ into Theorem 5.4 and using the value of $\gamma = 1$ (corresponding to the smallest non-zero eigenvalue of $h_{x,x+1}$, see (2.2)) gives

$$\begin{aligned} \lambda_1 &\geq \gamma(1 - \sqrt{2}\epsilon)^2 \\ &= \left(1 - \sqrt{\frac{n^2 - 1}{n^2 + n}}\right)^2 \\ &= \left(1 - \sqrt{\frac{(n-1)(n+1)}{n(n+1)}}\right)^2 \\ &= \left(1 - \sqrt{1 - \frac{1}{n}}\right)^2. \end{aligned}$$

To see that this is $\mathcal{O}(n^{-2})$, we now take the Taylor expansion of $\sqrt{1 - \frac{1}{n}}$ with respect to $\frac{1}{n}$:

$$\begin{aligned} \sqrt{1 - \frac{1}{n}} &= 1 - \frac{1}{2n} - \frac{1}{8n^2} - \dots \\ &\leq 1 - \frac{1}{2n}. \end{aligned}$$

This converges for all $n > 1$. Therefore,

$$\begin{aligned} \lambda_1 &\geq \left(1 - 1 + \frac{1}{2n}\right)^2 \\ &= \frac{1}{4n^2}. \end{aligned}$$

■

6. Conclusion

In this thesis, we applied two broad techniques, the variational principle and the martingale method, to prove both an upper and lower bound on the spectral gap of the ferromagnetic ferromagnetic Heisenberg-½ model in the thermodynamic limit. The variational principle is a general principle applicable to a wide variety of quantum systems, and we utilized a specific representation of our Hamiltonian in order to apply it. The martingale method is applicable to more general systems than demonstrated here, including to multi-dimensional lattices.

However, the techniques demonstrated here will are not applicable to the *antiferromagnetic* Heisenberg-½ quantum spin chain (in which the negative sign of (2.2) is dropped) as this model is not frustration free. A technique called the *Bethe ansatz* provides an exact expression for the spectral gap in this model [7, 8, 9].

This thesis also focused specifically on particles with spin value ½. A famous conjecture by Haldane [4, 5] states that integer-spin Heisenberg ferromagnets are gapped, while the half-integer Heisenberg ferromagnets are gapless. In 1988, Affleck, Kennedy, Lieb and Tasaki introduce a variation of the spin-1 Heisenberg ferromagnetic chain (known as the AKLT model) that satisfied Haldane's conjectured [1, 2].

Proving that the upper bound closes at a rate of $\mathcal{O}(n^{-2})$ is sufficient to prove that the ferromagnetic ferromagnetic Heisenberg-½ model is gapless. By proving that this is also a lower bound, we have proven that the spectral gap closes at *exactly* this rate by the squeeze theorem.

References

[1] I. Affleck, T. Kennedy, E. H. Lieb, H. Tasaki. *Rigorous results on valence-bond ground states in antiferromagnets.* Phys. Rev. Lett. **59** (1987).

[2] I. Affleck, T. Kennedy, E. H. Lieb, H. Tasaki. *Valence bond ground states in isotropic quantum antiferromagnets.* Comm. Math. Phys. **115** (1988).

[3] M. Artin. *Algebra (Second Edition).* Prentice Hall, 2011.

[4] F.D.M. Haldane. *Continuum dynamics of the 1-d Heisenberg antiferromagnet: identification with the $O(3)$ nonlinear sigma model.* Phys. Lett. **93** (1983).

[5] F.D.M. Haldane. *Nonlinear field theory of large-spin Heisenberg antiferromagnets: semiclassically quantized solutions of the one-dimensional easy-axis Neel state.* Phys. Rev. Lett. **50** (1983).

[6] M. Hastings, T. Koma. *Spectral gap and exponential decay of correlations.* Comm. Math. Physics. **265** (2006), no. 3, 781-804.

[7] M. Karbach, Gerhard Muller. *Introduction to the Bethe Ansatz I.* `arXiv:cond-mat/9809162 [cond-mat.stat-mech]` (1998).

[8] M. Karbach, Gerhard Muller. *Introduction to the Bethe Ansatz II.* `arXiv:cond-mat/9809163 [cond-mat.stat-mech]` (1998).

[9] M. Karbach, Gerhard Muller. *Introduction to the Bethe Ansatz III.* `arXiv:cond-mat/0008018 [cond-mat.stat-mech]` (2000).

[10] B. Nachtergaele. *Quantum Spin Systems.* `arXiv:0409006 [math.ph]` (2004).

[11] B. Nachtergaele, R. Sims. *Lieb-Robinson bounds and the exponential clustering theorems.* Comm. Math. Phys. **265** (2006), no. 1, 119-130