Universiteit Utrecht

Faculteit Bètawetenschappen

The Bethe Ansatz in the Heisenberg model and the Square Ice model

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A thesis submitted to the Department of Mathematics at Utrecht University in partial fulfillment of the requirements for the degrees of

Bachelor in Physics and Astronomy
and
Bachelor in Mathematics.

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9th June 2019

Universiteit Utrecht

Abstract

Two physical models are discussed. We start out with the Heisenberg spin chain, which consists of a number of atoms in a circular configuration, each with spin up or down. We set up a Hamiltonian of this system considering only nearest-neighbour interactions, and determine the energy of the spin chain. The mathematical description of the state in which these atoms will be, i.e. the wave functions of these atoms, satisfies a certain template, which is called the Bethe Ansatz. Using this Ansatz, we can solve the eigenvalue equation of the Hamiltonian and thus calculate the energy of the system. What follows is a discussion on a model for water ice, of which we want to determine the entropy at absolute zero. This leads to a set of equations that is very similar to that encountered in the Heisenberg model, and it turns out that the Bethe Ansatz is useful in this model as well: it enables us to explicitly calculate the entropy of an infinitely big system.

Contents

Notation

In this thesis, we will use some consistency in our notation for clarity purposes.
We will indicate the end of definitions with a $\triangleleft$, the end of remarks and examples with a $\diamond$ and the end of proofs with a $\square$.
We will underline any definitions we introduce.
If there can exist any doubt about the summands of a summation sign $\sum$, we will put square brackets $[\dots]$ around the summands. For example,

$$\sum_{j=1}^{2}[j] + 1 = 1 + 2 + 1 = 4.$$

1 Introduction

In the early 1930's, the physicist Hans Bethe found, using his great intuition, the template that the wave functions of the atoms of a 1-dimensional spin chain have to fit. Using this template, he was able to calculate the energies of this system. This template has since been used by people from various fields, including higher-dimensional spin systems, Kondo effect problems and the entropy of crystals. Not surprisingly, this template, or *assumption* on the form of functions, was called the Bethe Ansatz. The goal of this thesis is to present two models from two different fields (to wit: the original Heisenberg spin model and the Square Ice model) and show how this Ansatz finds its way into two seemingly different problems, to solve two completely different questions. In chapter 2, we will introduce the problem that Hans Bethe tackled himself, namely the 1-dimensional spin chain, and look at some special cases before handling the general case in chapter 3. We will see that the Bethe Ansatz indeed solves the problem, i.e. that all wave functions fit his template and that this enables us to solve our equations. In chapter 4, we will introduce a 2-dimensional model for 3-dimensional water ice, and we will employ the Bethe Ansatz trying to find the entropy of this system. We will see that the configurations that our system can take on fit Bethe's template, and if we let the size of our system (i.e. our block of water ice) go to infinity, we will be able to calculate its entropy exactly. We end by summarizing our results and discussing the similarities of the methods that we employed to solve the problems in the two models.

At the end of each chapter, we will make clear what parts are my work and what parts are others' work. Everything in the Appendices is my work.

2 Introduction to the Heisenberg model and some special cases

The goal is to find the energies of the physical system discussed below. With these energies, one can find a partition function, which allows us to calculate many interesting physical quantities such as the entropy S, the Helmholtz free energy F and the heat capacity C_v. For more on this, please consult a textbook on Statistical Mechanics. We will not explicitly calculated these thermodynamical quantities in this thesis: we will only be concerned with finding the energies, and the main focus will be on *how* to find them.

We will use terminology about spins of particles. For an elaborate discussion about spin, please consult a textbook on Quantum Mechanics. However, the only required knowledge about spin is that the spin of spin-$\frac{1}{2}$ particles can be in a state of up, down, or a superposition (i.e. a linear combination) of these two linearly independent states. We see the state of such particles as a vector in a 2-dimensional space with basis vectors up and down. Consequently, the state of the particles in a spin chain will be a superposition of all the possible configurations of spins in that spin chain, so it will be a vector in a 2^N-dimensional space. The energy of our system will depend on the state of the particles, because each state, seen as an eigenvector of the Hamiltonian, has a certain energy (eigenvalue) associated with it.

2.1 Introduction to the mathematics of the model

We consider a one-dimensional grid of N equally spaced points with periodic boundary conditions, in the sense that point $N+k$ corresponds to point k for all points $k \in \{1, \dots, N\}$. At each point, there is a particle with spin-$\frac{1}{2}$. We call this situation a spin chain. Measured in the z-direction, one spin can be either up or down, which we will indicate with $|\uparrow\rangle$ or $|\downarrow\rangle$, respectively. These two states are actually orthonormal vectors in a spin Hilbert space $\mathscr{H}_s$ of a particle, and the set $\{|\uparrow\rangle, |\downarrow\rangle\}$ is a basis for $\mathscr{H}_s$ over the complex field $\mathbb{C}$ ([16] p. 79). We get a spin Hilbert space of the total system by a tensor product of the individual particles ([16] p. 158 et seq.):

$$\mathscr{H} = \bigotimes_{k=1}^{N} \mathscr{H}_s. \tag{1}$$

We introduce the notation for the tensor product of basis vectors of $\mathscr{H}_s$ by writing

$$|\, \sigma_1 \dots \sigma_N \,\rangle := \bigotimes_{k=1}^{N} |\, \sigma_k \,\rangle\,, \tag{2}$$

where $\sigma_k \in \{\uparrow, \downarrow\}$ for $k \in \{1, \dots, N\}$.
We want to choose a basis for the spin Hilbert space $\mathscr{H}$ of our spin chain, because the discussion on the Bethe Ansatz relies on working in a basis. In fact, we want to construct the Hamiltonian, but to actually calculate the energies, we need our Hamiltonian to be formulated in a certain basis. Before we can do this, however, let us introduce some more concepts.

Definition 2.1. Let X and Y be two sets and let $B(X, Y)$ denote all the bounded linear operators $X \to Y$. Then the dual space of the space X is defined to be $X' := B(X, \mathbb{C})$. Elements of a dual space are called bounded linear functionals, but we will refer to them as just functionals. ◁

Remark 2.2. Let H be a Hilbert space and denote its inner product by $\langle\, .\, ,\, .\,\rangle$. By the Riesz Representation Theorem ([12]), every functional $\phi \in H'$ can be written as $\phi = \langle\, \psi\, ,\, .\,\rangle$, with $\psi \in H$.
In fact, the theorem states that there is a one-to-one correspondence between the $\psi \in H$ and the $\phi \in H'$. In other words, for every $\phi \in H'$, there exists a unique $\psi \in H$ such that $\phi = \langle\, \psi\, ,\, .\,\rangle$, and vice versa. ◇

Using this one-to-one correspondence, we introduce the following notation.

Definition 2.3. We denote the unique $\phi \in H'$ corresponding to $\psi \in H$ as $\langle\, \psi \,|\, \in H'$, and we denote $\psi \in H$ as $|\, \psi \,\rangle$[1]. This gives us a quick way of telling if a vector lives in a space or its dual space.

[1] Following the bra-ket notation introduced by Paul Dirac.

We write the standard inner product of two vectors $|\psi\rangle, |\phi\rangle$ in a Hilbert space H as $\langle\psi|\phi\rangle$. This notation is meant to remind you of the fact that, in principle, we are replacing the inner product function with a functional in H' working on a vector in H. ◁

Lastly, let us define the inner product on a tensor product space.

Definition 2.4. The standard inner product on a tensor product space, notated $\mathscr{H} = \bigotimes_{k=1}^{N} \mathscr{H}_s$ with basis vector elements $|\sigma_1 \dots \sigma_N\rangle, |\delta_1 \dots \delta_N\rangle \in \mathscr{H}$, is defined on these basis vectors as

$$\langle \sigma_1 \dots \sigma_N | \delta_1 \dots \delta_N \rangle := \prod_{k=1}^{N} \langle \sigma_k | \delta_k \rangle.$$

One can easily check that this is still an inner product. We define the inner product for all elements $|\psi\rangle \in \mathscr{H}$ by writing them as a linear combination of basis vectors. ◁

Now we are ready to define a basis of $\mathscr{H}$. As always with bases, it is desirable to have an orthogonal one, so we will construct an orthogonal basis.

Lemma 2.5. *The set* $\mathcal{B} := \left\{ \ |\sigma_1 \dots \sigma_N\rangle \ \middle| \ \forall k \in \{1, \dots, N\} : \sigma_k \in \{\uparrow, \downarrow\} \ \right\}$ *is an orthonormal basis of* $\mathscr{H}$.

Proof. We remind ourselves that the set $\{|\uparrow\rangle, |\downarrow\rangle\}$ is an orthonormal basis for $\mathscr{H}_s$. This means that $\langle\uparrow | \downarrow\rangle = 0$, so if two vectors in $\mathcal{B}$ have a different arrow in at least one place, the inner product between the two vanishes. This means that $\mathcal{B}$ is an orthogonal system, i.e. that all vectors in the set are orthogonal to each other.
Furthermore, using $\langle\uparrow | \uparrow\rangle = \langle\downarrow | \downarrow\rangle = 1$, it is clear that the elements of $\mathcal{B}$ are normalized as well.
To prove that $\mathcal{B}$ actually spans $\mathscr{H}$, we argue that a tensor product of all vectors that span a space will span the new tensor product space as well, as a consequence of the properties of the tensor product space. □

We will use this basis of $\mathscr{H}$ in our discussion on the Bethe Ansatz, which will be highly dependent on the independence of the basis vectors.

Remark 2.6. In the remainder of this thesis, we will not be concerned with normalizing any vectors, as this is not of interest for the material discussed. As we will only be dealing with finite linear combinations of our normalized basis vectors, everything will be normalizable. However, please note that we will be using the normalization of the basis vectors. ◇

In $\mathscr{H}$, we will be using several operators.

Definition 2.7. For the purpose of this definition, let us choose a basis of the two-dimensional spin space $\mathscr{H}_s$ such that

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ , \ |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{3}$$

Then we define the operators $\mathrm{id}, S^x, S^y, S^z, S^\pm : \mathscr{H}_s \to \mathscr{H}_s$ and $\vec{S} : \mathscr{H}_s \to \mathscr{H}_s^3$ as follows:

$$S^x := \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^y := \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^z := \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$
$$\mathrm{id} := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad S^\pm := S^x \pm i S^y, \quad \vec{S} := \begin{pmatrix} S^x \\ S^y \\ S^z \end{pmatrix}.$$

◁

Remark 2.8. We can easily see that the operators work on the basis vectors as follows:

$$S^z |\uparrow\rangle = \frac{1}{2}|\uparrow\rangle, \quad S^+|\uparrow\rangle = 0, \quad S^-|\uparrow\rangle = |\downarrow\rangle, \quad S^z|\downarrow\rangle = -\frac{1}{2}|\downarrow\rangle, \quad S^+|\downarrow\rangle = |\uparrow\rangle, \quad S^-|\downarrow\rangle = 0.$$

◇

For this reason, $S^{\pm}$ are called the spin flip operators.
All of the introduced operators can work on one of the spins in our spin chain. To make things rigorous, we define new operators that work on the Hilbert space of the whole spin chain, as follows.

Definition 2.9. We define $S_n^z : \mathscr{H} \to \mathscr{H}$ as

$$S_n^z := \left(\bigotimes_{k=1}^{n-1} \mathrm{id} \right) \otimes S^z \otimes \left(\bigotimes_{l=n+1}^{N} \mathrm{id} \right).$$

We define S_n^x, S_n^y, $S_n^{\pm}$ and $\vec{S}_n$ similarly. Furthermore, we define the total spin in the z-direction $S_{\mathrm{tot}}^z : \mathscr{H} \to \mathscr{H}$ as

$$S_{\mathrm{tot}}^z := \sum_{n=1}^{N} S_n^z.$$

◁

We see that S_n^z is the spin operator acting only on the nth spin with S^z, and leaving the other spins alone.

Lemma 2.10. *The spin operators S_n^z commute for different n (and trivially for same n):*

$$[S_n^z, S_m^z] = 0 \text{ for } n, m \in \{1, \ldots, N\}. \tag{4}$$

Proof. If $n = m$, then the operators commute trivially.
If $n \neq m$, then without loss of generality, we assume $n < m$, and we can check the following:

$$\begin{aligned}
S_n^z \circ S_m^z &= \left[\left(\bigotimes_{k=1}^{n-1} \mathrm{id} \right) \otimes S^z \otimes \left(\bigotimes_{l=n+1}^{N} \mathrm{id} \right) \right] \circ \left[\left(\bigotimes_{k=1}^{m-1} \mathrm{id} \right) \otimes S^z \otimes \left(\bigotimes_{l=m+1}^{N} \mathrm{id} \right) \right] \\
&= \left(\bigotimes_{k=1}^{n-1} (\mathrm{id} \circ \mathrm{id}) \right) \otimes (S^z \circ \mathrm{id}) \otimes \left(\bigotimes_{k=n+1}^{m-1} (\mathrm{id} \circ \mathrm{id}) \right) \otimes (\mathrm{id} \circ S^z) \otimes \left(\bigotimes_{k=m+1}^{N} (\mathrm{id} \circ \mathrm{id}) \right) \\
&= \left(\bigotimes_{k=1}^{n-1} (\mathrm{id} \circ \mathrm{id}) \right) \otimes (\mathrm{id} \circ S^z) \otimes \left(\bigotimes_{k=n+1}^{m-1} (\mathrm{id} \circ \mathrm{id}) \right) \otimes (S^z \circ \mathrm{id}) \otimes \left(\bigotimes_{k=m+1}^{N} (\mathrm{id} \circ \mathrm{id}) \right) \\
&= \left[\left(\bigotimes_{k=1}^{m-1} \mathrm{id} \right) \otimes S^z \otimes \left(\bigotimes_{l=m+1}^{N} \mathrm{id} \right) \right] \circ \left[\left(\bigotimes_{k=1}^{n-1} \mathrm{id} \right) \otimes S^z \otimes \left(\bigotimes_{l=n+1}^{N} \mathrm{id} \right) \right] = S_m^z \circ S_n^z.
\end{aligned}$$

□

Remark 2.11. Because the z-direction is not a preferred direction in any way, and by the linearity of the commutator brackets, we now also know that

$$[S_n^+, S_m^+] = [S_n^-, S_m^-] = [S_l^+, S_m^-] = 0 \text{ for } l \neq m, n \in \{1, \ldots, N\}.$$

This means that, for $m \neq n$, we can place the S_n^+ and S_m^- operators in front of the vectors $|\,\sigma_1 \ldots \sigma_N\,\rangle$ in any order we want. ◇

We are now ready to define the model we will be studying in this thesis, thereby introducing the Hamiltonian of which we want to find the eigenvalues.

2.2 The specifics of the model

Definition 2.12. The Heisenberg model of spins is defined by the situation described above, i.e. a one-dimensional spin chain of N spins with periodic boundary conditions $\vec{S}_n = \vec{S}_{n+N}$, together with the Hamiltonian $\mathcal{H}$ of the system that is given by

$$\mathcal{H} = -J \sum_{n=1}^{N} \vec{S}_n \cdot \vec{S}_{n+1},$$

where $J \in \mathbb{R}$ is a constant that describes the type and strength of the interaction between neighbouring particles. $\triangleleft$

Qualitatively, we see that this Hamiltonian only depends on the relative spin direction of neighbouring particles, and that there is no external field. We also see that if J is positive, then the energy will be minimal if every spin is pointed in the same direction, which will lead to ferromagnetism. In addition, if J is negative, spins will tend to alternate directions, which we call antiferromagnetism. Lastly, $|J|$ determines the strength of the interaction. We can rewrite the Hamiltonian as follows:

$$\begin{aligned}\mathcal{H} &= -J\sum_{n=1}^{N}\left[S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z\right] \\ &= -J\sum_{n=1}^{N}\left[\frac{1}{2}\left((S_n^x + iS_n^y)(S_{n+1}^x - iS_{n+1}^y) + (S_n^x - iS_n^y)(S_{n+1}^x + iS_{n+1}^y)\right) + S_n^z S_{n+1}^z\right] \\ &= -J\sum_{n=1}^{N}\left[\frac{1}{2}\left(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+\right) + S_n^z S_{n+1}^z\right]. \end{aligned} \tag{5}$$

Now, we want to get started diagonalizing our Hamiltonian already. We notice that the Hamiltonian's dependency on operators is $\mathcal{H} = \mathcal{H}(S_n^+ S_{n+1}^-, S_n^- S_{n+1}^+, S_n^z S_{n+1}^z)$. From Remark 2.8, we see that $\mathcal{H}$ will leave the total spin S_{tot}^z the same, i.e.

$$\forall \,|\, \sigma_1 \dots \sigma_N \,\rangle \in \mathscr{H} : \mathcal{H} S_{tot}^z \,|\, \sigma_1 \dots \sigma_N \,\rangle = S_{tot}^z \mathcal{H} \,|\, \sigma_1 \dots \sigma_N \,\rangle\,.$$

Remark 2.13. This means that the total spin operator commutes with the Hamiltonian: $[\mathcal{H}, S_{tot}^z] = 0$. In turn, given that $\mathcal{H}$ is independent of time, this means ([16], p. 229) that the total spin S_{tot}^z is a conserved quantity. $\diamond$

The fact that $\mathcal{H}$ working on a state of total spin S_{tot}^z will give a linear combination of states of the same total spin S_{tot}^z means that, if we order our basis $\mathcal{B}$ such that the basis vectors are sorted to decreasing S_{tot}^z, then the Hamiltonian will be of block-diagonal form. This is a first step in diagonalizing the Hamiltonian, but we are not quite there yet. Let us introduce some short-hand notation for the vectors in $\mathscr{H}$.

Definition 2.14. We define the following states in $\mathscr{H}$: $|\, F \,\rangle$ as the state with all spins up, and $|\, n \,\rangle$ as the state with all spins up but one spin down at position n.

$$\begin{aligned}&|\, F \,\rangle := |\uparrow \dots \uparrow\rangle \\ &\forall n \in \{1, \dots, N\},\ |\, n \,\rangle := S_n^- \,|\, F \,\rangle\end{aligned}$$

We can generalize this notational idea to multiple spins down at sites $n_1, \dots, n_r \in \mathbb{N}$:

$$\forall\ r \in \{1, \dots, N\},\ \forall n_1 < n_2 < \dots < n_r,\ |\, n_1, n_2, \dots, n_r \,\rangle := S_{n_1}^- S_{n_2}^- \dots S_{n_r}^- \,|\, F \,\rangle\,.$$

We will refer to the number of spins down as r. $\triangleleft$

As an example, for $N = 4$: $|\, 1, 2, 4 \,\rangle = |\downarrow\downarrow\uparrow\downarrow\rangle$. Remember that we are busy finding ways to diagonalize our Hamiltonian: we want to find eigenvectors of $\mathscr{H}$. Let us separate this task into increasingly difficult parts by considering finding eigenvectors per value of r. At some point, we will see a pattern of how to find them, and this pattern will be the Bethe Ansatz. Let us start things off with the trivial case of $r = 0$. We will use the following notation for the subspaces of the total Hilbert space $\mathscr{H}$ that we will be considering:

$$\forall r \in \{1, \dots, N\},\ \mathscr{H}_r := \operatorname{span}\left(\left\{|\, \sigma_1 \dots \sigma_N \,\rangle \in \mathscr{H} \;\middle|\; S_{tot}^z \,|\, \sigma_1, \dots, \sigma_N \,\rangle = \left(\frac{N}{2} - r\right) |\, \sigma_1, \dots, \sigma_N \,\rangle\right\}\right).$$

In other words, $\mathscr{H}_r$ is the subspace spanned by all basis vectors with r spins down.

Lemma 2.15. *For every $r \in \{1, \dots, N\}$, $\mathscr{H}_r$ is a Hilbert space.*

Proof. We recall that a Hilbert space $\mathscr{H}$ is a complete inner product space. We will denote by $|\,\psi_r\,\rangle$ elements of $\mathscr{H}_r$.
$\mathscr{H}_r$ is a vector (sub)space, because it is defined as the span of vectors in $\mathscr{H}$.
The inner product $\langle\,.\,|\,.\,\rangle_r$ on $\mathscr{H}_r$ is the same as the inner product $\langle\,.\,|\,.\,\rangle$ on $\mathscr{H}$, i.e. $\langle\,\psi_r\,|\,\phi_r\,\rangle_r = \langle\,\psi_r\,|\,\phi_r\,\rangle$. Therefore, $\mathscr{H}_r$ is an inner product space.
We remark that $\dim(\mathscr{H}) = 2^N < \infty$, so $\dim(\mathscr{H}_r) < \infty$. Because $\mathscr{H}_r$ is a finite-dimensional vector subspace, it is closed. Now, closed subsets of complete metric spaces are complete, so $\mathscr{H}_r$ is complete. Thus, $\mathscr{H}_r$ is a complete inner product space, i.e. a Hilbert space. □

This means that it is, at least technically, possible for a state to be a vector that lies completely in $\mathscr{H}_r$. In fact, we can prove that all vectors lie in a single $\mathscr{H}_r$.

Lemma 2.16. *For all eigenvectors $|\,\psi\,\rangle$ of the Hamiltonian $\mathcal{H}$, there is an $r \in \{1, \ldots, N\}$ such that $|\,\psi\,\rangle \in \mathscr{H}_r$.*

Proof. We know from Remark 2.13 that $|\,\psi\,\rangle$ will also be an eigenvector of the total spin operator S^z_{tot}, of which the eigenvalue will give us the total spin. This total spin will thus be well-defined, and every measurement will provide the same total spin, which corresponds to a certain $r \in \{1, \ldots, N\}$. This means that the amplitude of the wave function outside $\mathscr{H}_r$ is 0, so $|\,\psi\,\rangle$ lies completely in $\mathscr{H}_r$. □

Based on this lemma, we will look for the eigenvectors of $\mathcal{H}$ in order of r.

2.3 The case $r = 0$

For $r = 0$, we know that $\mathscr{H}_0 = \text{span}\left(\{|\,F\,\rangle\}\right)$, so we calculate:

$$\begin{aligned}\mathcal{H}\,|\,F\,\rangle &= -J\sum_{n=1}^{N}\left[\frac{1}{2}\left(S_n^+S_{n+1}^- + S_n^-S_{n+1}^+\right) + S_n^zS_{n+1}^z\right]|\uparrow\ldots\uparrow\rangle \quad (6)\\ &= -J\sum_{n=1}^{N}S_n^zS_{n+1}^z\,|\uparrow\ldots\uparrow\rangle = -J\sum_{n=1}^{N}\frac{1}{2}\cdot\frac{1}{2}\,|\uparrow\ldots\uparrow\rangle = -\frac{JN}{4}\,|\,F\,\rangle\,. \quad (7)\end{aligned}$$

Thus we see that $|\,F\,\rangle$ is an eigenvector of the Hamiltonian, and it is the only vector with total spin $S^z_{\text{tot}} = \frac{N}{2}$, so we have found all the eigenvectors of the Hamiltonian for $r = 0$. The eigenvalues of the Hamiltonian are the energies of the system, which justifies the symbol E_0 that we will give to the eigenvalue of $|\,F\,\rangle$:

$$E_0 = -\frac{JN}{4}. \tag{8}$$

We have now found all the eigenvectors of $r = 0$ and the corresponding eigenvalues of the Hamiltonian.

2.4 The case $r = 1$

For $r = 1$, we know that the set $\{|\,n\,\rangle \ \mid n \in \{1, \ldots, N\}\}$ forms a basis of the subspace $\mathscr{H}_1$, because $\mathscr{H}_1$ is constructed to be the span of this set, and the set is orthogonal. We can write our eigenvectors as linear combinations of these basis vectors. We want to find N eigenvectors, because $\mathscr{H}_1$ is N-dimensional and $\mathcal{H}$ works on this whole space, so $\mathcal{H}$ can be represented by an $N \times N$ matrix. We will thus label our eigenvectors $|\,\psi\,\rangle$ with an $m \in \{1, \ldots, N\}$. We write

$$|\,\psi_m\,\rangle = \sum_{n=0}^{N} a_m(n)\,|\,n\,\rangle\,, \tag{9}$$

where $a_m(n) : \{1, \ldots, N\} \to \mathbb{C}$. Our goal is to find $a_m(n)$. We want our vectors $|\,\psi_m\,\rangle$ to satisfy the eigenvalue equation $\mathcal{H}\,|\,\psi_m\,\rangle = E\,|\,\psi_m\,\rangle$, so we calculate:

$$\mathcal{H}\,|\,\psi_m\,\rangle = -J\sum_{l=1}^{N}\left[\frac{1}{2}\left(S_l^+S_{l+1}^- + S_l^-S_{l+1}^+\right) + S_l^zS_{l+1}^z\right]\sum_{n=0}^{N} a_m(n)\,|\,n\,\rangle\,.$$

Both of these sums are finite, so we can switch them. Also, $[S_l^+, S_j^-] = 0$ if $l \neq j$ because they act on different parts of the Hilbert space:

$$\begin{aligned}
\mathcal{H}\,|\,\psi_m\,\rangle &= -J\sum_{n=0}^{N} a_m(n) \sum_{l=1}^{N}\left[\frac{1}{2}\left(S_{l+1}^- S_l^+\,|\,n\,\rangle + S_l^- S_{l+1}^+\,|\,n\,\rangle\right) + S_l^z S_{l+1}^z\,|\,n\,\rangle\right] \\
&= -\frac{J}{4}\sum_{n=0}^{N} a_m(n)\left[2\left(|\,n+1\,\rangle + |\,n-1\,\rangle\right) + (N-4)\,|\,n\,\rangle\right] \\
&= \sum_{n=0}^{N}\left[-\frac{J}{4}a_m(n)\left[2\left(|\,n+1\,\rangle + |\,n-1\,\rangle\right) - 4\,|\,n\,\rangle\right] + E_0 a_m(n)\,|\,n\,\rangle\right] \overset{!}{=} E\,|\,\psi_m\,\rangle = E\sum_{n=0}^{N} a_m(n)\,|\,n\,\rangle\,.
\end{aligned}$$

Here we have used the result for E_0 from the previous discussion on $r = 0$. We can rewrite this equation as

$$\sum_{n=0}^{N} a_m(n)\Big[J\left(2\,|\,n\,\rangle - |\,n+1\,\rangle - |\,n-1\,\rangle\right) + 2(E_0 - E)\,|\,n\,\rangle\Big] = 0.$$

Because $|\,n\,\rangle$ are all linearly independent, we get the following equation for every $n \in \{1, \ldots, N\}$.

$$a_m(n)(2J\,|\,n\,\rangle + 2(E_0 - E)\,|\,n\,\rangle) - Ja_m(n+1)\,|\,n\,\rangle - Ja_m(n-1)\,|\,n\,\rangle = 0$$

We can let the functional $\langle\,n\,| \in \mathscr{H}'$ work on this equation and we will be left with

$$\begin{aligned}
&\langle\,n\,|\,\big(a_m(n)(2J + 2(E_0 - E)) - Ja_m(n+1) - Ja_m(n-1)\big)\,|\,n\,\rangle = 0 \\
\iff &\big(a_m(n)(2J + 2(E_0 - E)) - Ja_m(n+1) - Ja_m(n-1)\big)\langle\,n\,|\,n\,\rangle = 0.
\end{aligned}$$

We know that $\langle\,n\,|\,n\,\rangle = 1$, so we conclude that $|\,\psi\,\rangle$ is an eigenvector of $\mathcal{H}$ if the coefficients $a_m(n)$ satisfy

$$2(E - E_0)a_m(n) = J\big[2a_m(n) - a_m(n-1) - a_m(n+1)\big]. \tag{10}$$

To find the solutions, we take another route at this point, which we will not be able to take for $r \geq 2$. This route is enabled by the fact that our Hamiltonian is translationally invariant, and we can formulate eigenvectors of the translation operator to help us find the solutions. Let us start by defining the translation operator and deriving a few of its properties.

Definition 2.17. The translation operator $T : \mathscr{H} \to \mathscr{H}$ is defined by its operation on the basis vectors:

$$T\,|\,\sigma_1 \ldots \sigma_N\,\rangle := |\,\sigma_2 \ldots \sigma_N \sigma_1\,\rangle\,. \tag{11}$$

◁

Now, we suspect that the energy of our spin chain does not change if we perform a pure translation to the system, but in principle we do not know this (yet). We do expect to find this, though, so we expect $[T, \mathcal{H}] = 0$, therefore we also expect the spectrum of T to be the same as the spectrum of the Hamiltonian, which we want to find. Thus, our strategy will be to find the spectrum of T and see if the eigenvectors we find are also eigenvectors of $\mathcal{H}$.

To find eigenvectors $|\,\psi\,\rangle$ of T, we want that $T\,|\,\psi\,\rangle = C\,|\,\psi\,\rangle$ with $C \in \mathbb{C}$. In other words, looking at particle n in particular, and denoting the value of the wavefunction ψ in the location of particle n as $\psi(n)$, we want: $\psi(n) = C\psi(n+1)$. But this has to be true for all $n \in \{1, \ldots, N\}$, so

$$\psi(1) = C\psi(2) = C^2\psi(3) = \cdots = C^N\psi(1),$$

so $C = \sqrt[N]{1} = \mathrm{e}^{\mathrm{i}k}$ where

$$k = k(m) := \frac{2\pi m}{N} \text{ with } m \in \{1, \ldots, N\}. \tag{12}$$

Let us look at a solution for the equation that we now have: $T \mid \psi \rangle = \mathrm{e}^{\mathrm{i}k} \mid \psi \rangle$. We want the phase of our wave function ψ to differ by k when looking at neighbours. This inspires us to define

$$\mid \psi_m \rangle := \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}kn} \mid n \rangle \, . \tag{13}$$

We can check:

$$T \mid \psi_m \rangle = \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}kn} T \mid n \rangle = \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}kn} \mid n-1 \rangle = \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}k(n+1)} \mid n \rangle = \mathrm{e}^{\mathrm{i}k} \mid \psi_m \rangle \, .$$

As we see, k acts as a generator of the translation operator T. For this reason, we will call k the wave number of a solution $\mid \psi_m \rangle$. Because T can be represented by an $N \times N$ matrix[2] , and we found N eigenvectors, we have found all the eigenvectors of T with corresponding eigenvalues. Now, we suspect that these eigenvectors are also eigenvectors of $\mathcal{H}$, so we want to check if this is the case. If it is true, then we have found the eigenvectors of $\mathcal{H}$ by giving an argument about translational invariance in combination with the periodic boundary conditions of our system. We try:

$$\begin{aligned}
\mathcal{H} \mid \psi_m \rangle &= \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}kn} \mathcal{H} \mid n \rangle \\
&= -J \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}kn} \sum_{j=1}^{N} \left[S_j^z S_{j+1}^z + \frac{1}{2} S_j^+ S_{j+1}^- + \frac{1}{2} S_{j-1}^- S_j^+ \right] \mid n \rangle \\
&= -J \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}kn} \left[\left(\frac{N}{4} - 1 \right) \mid n \rangle + \frac{1}{2} \mid n+1 \rangle + \frac{1}{2} \mid n-1 \rangle \right] \\
&= -J \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}kn} \left[\left(\frac{N}{4} - 1 \right) + \frac{1}{2} \mathrm{e}^{-\mathrm{i}k} + \frac{1}{2} \mathrm{e}^{\mathrm{i}k} \right] \mid n \rangle \\
&= -J \left[\left(\frac{N}{4} - 1 \right) + \cos(k) \right] \mid \psi_m \rangle \, .
\end{aligned}$$

As we expected, $\mid \psi_m \rangle$ are eigenvectors of our Hamiltonian with eigenvalues

$$E = -J \left[\left(\frac{N}{4} - 1 \right) + \cos(k) \right] = E_0 + J(1 - \cos(k)),$$

so for the energy difference between the $\mid F \rangle$ state and an $\mid n \rangle$ state, we have now

$$\boxed{E_1 - E_0 = J(1 - \cos(k))} \tag{14}$$

where we have called the energy E of the $r = 1$ system E_1. Note that for $J > 0$, i.e. the ferromagnetic case, the energy of the system with one spin down will be higher than that of the system with all spins up in all cases but one, which reflects the fact that a ferromagnetic material wants all of its spins to be the same.

To conclude, we did *not* solve Eq. 10 directly. Instead, we looked at an easier operator T of which we suspected that it commuted with the Hamiltonian, resulting in the same spectrum between the two. We succeeded, and we know the solutions to Eq. 10, namely:

$$a_m(n) = \mathrm{e}^{\mathrm{i}kn} \ , \ k = \frac{2\pi m}{N}. \tag{15}$$

[2] To know:

$$T = \begin{pmatrix} 0 & 1 & 0 & \dots & \dots \\ 0 & 0 & 1 & 0 & \dots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 1 & 0 & \dots & \dots & \dots \end{pmatrix}$$

We have now found all the eigenvectors of $r = 1$ and corresponding eigenvalues of the Hamiltonian.

As said, we employed a technique that is only possible for $r = 1$. This is so because the basis we are using now does not diagonalize the Hamiltonian in the block of $r = 2$, as will become apparent in the next section about the case of $r = 2$. The technique we *will* be employing is the Bethe Ansatz, which we will first introduce in the $r = 2$ system, before introducing it in a general setting. We do this because it will make the Bethe Ansatz more insightful, and we will see results that we suspect we will be able to generalize in the case of general r, so that we know what results we could expect.

2.5 The case $r = 2$

We will try to follow the same procedure as in the case of $r = 1$, so it will be clear where things begin to fail.

2.5.1 Setting up the equations

For $r = 2$, we need to pick 2 spins out of N to be spins down. For this reason, $\mathscr{H}_2$ is an $\frac{N(N-1)}{2}$-dimensional subspace, so we want to find as many eigenvectors of $\mathcal{H}$ with $S^z_{tot} = \frac{N}{2} - 2$. We let $m \in \left\{1, \ldots, \frac{N(N-1)}{2}\right\}$ and we write our eigenvectors-to-be as

$$|\,\psi_m\,\rangle = \sum_{1\le n_1<n_2\le N} a_m(n_1,n_2)\,|\,n_1,n_2\,\rangle\,, \tag{16}$$

where our goal is again to find the coefficients $a_m(n_1, n_2)$. From now on, we will not include the subscript m anymore, to improve readability. Our starting point is again the eigenvalue equation for our Hamiltonian:

$$\mathcal{H}\,|\,\psi\,\rangle = E\,|\,\psi\,\rangle\,.$$

We calculate

$$\begin{aligned}\mathcal{H}\,|\,\psi\,\rangle &= \sum_{1\le n_1<n_2\le N} a(n_1,n_2)\mathcal{H}\,|\,n_1,n_2\,\rangle\\ &= -J\sum_{1\le n_1<n_2\le N} a(n_1,n_2)\sum_{j=1}^{N}\left[S^z_jS^z_{j+1}+\frac{1}{2}S^+_jS^-_{j+1}+\frac{1}{2}S^-_{j-1}S^+_j\right]|\,n_1,n_2\,\rangle\,.\end{aligned}$$

We notice that, for example, the term $\sum_{j=1}^{N} S^z_jS^z_{j+1}\,|\,n_1,n_2\,\rangle$ depends on the position of the spins down: if the spins are neighbours, then the term will be $N/4-1$, but if they are *not* neighbours, the term will be $N/4-2$. This means we get two different parts in our sum. We proceed as follows:

$$\begin{aligned}\mathcal{H}\,|\,\psi\,\rangle = -J\Bigg[&\sum_{n_1+1=n_2} a(n_1,n_2)\left[\left(\frac{N}{4}-1\right)|\,n_1,n_2\,\rangle+\frac{1}{2}\,|\,n_1,n_2+1\,\rangle+\frac{1}{2}\,|\,n_1-1,n_2\,\rangle\right]\\ &+\sum_{n_1+1<n_2} a(n_1,n_2)\Bigg[\left(\frac{N}{4}-2\right)|\,n_1,n_2\,\rangle\\ &\qquad+\frac{1}{2}\Big(|\,n_1+1,n_2\,\rangle+|\,n_1,n_2+1\,\rangle+|\,n_1-1,n_2\,\rangle+|\,n_1,n_2-1\,\rangle\Big)\Bigg]\Bigg]\\ = -J\Bigg[&\sum_{n_1=1}^{N} a(n_1,n_1+1)\Big[-2\,|\,n_1,n_1+1\,\rangle+|\,n_1,n_1+2\,\rangle+|\,n_1-1,n_1+1\,\rangle\Big]\\ &+\sum_{n_1+1<n_2} a(n_1,n_2)\Big[-4\,|\,n_1,n_2\,\rangle+|\,n_1+1,n_2\,\rangle+|\,n_1,n_2+1\,\rangle+|\,n_1-1,n_2\,\rangle+|\,n_1,n_2-1\,\rangle\Big]\Bigg]\\ &+E_0\,|\,\psi\,\rangle\\ \overset{!}{=}\;&E\,|\,\psi\,\rangle\,.\end{aligned}$$

We are still using basis vectors from our basis $\mathcal{B}$ from Lemma 2.5, so they are all linearly independent. Therefore, the equation we have now,

$$\begin{aligned}2(E-E_0)\sum_{n_1<n_2} a(n_1,n_2)\,|\,n_1,n_2\,\rangle =&J\Bigg[\sum_{n=1}^{N} a(n,n+1)\Big[2\,|\,n,n+1\,\rangle - |\,n,n+2\,\rangle - |\,n-1,n+1\,\rangle\Big] \\ &+\sum_{n_1+1<n_2} a(n_1,n_2)\Big[4\,|\,n_1,n_2\,\rangle - |\,n_1+1,n_2\,\rangle - |\,n_1,n_2+1\,\rangle \\ &- |\,n_1-1,n_2\,\rangle - |\,n_1,n_2-1\,\rangle\Big]\Bigg],\end{aligned}$$

translates into $\frac{N(N-1)}{2}$ equations by grouping the basis vectors and making sure that the equation above is true for every basis vector. This is easily done, and we obtain the following equations for $a(n_1,n_2)$:

$$2(E-E_0)a(n,n+1) = J\left(2a(n,n+1) - a(n-1,n+1) - a(n,n+2)\right), \tag{17}$$

and for $n_2 > n_1+1$:

$$2(E-E_0)a(n_1,n_2) = J\big(4a(n_1,n_2) - a(n_1-1,n_2) - a(n_1,n_2-1) - a(n_1+1,n_2) - a(n_1,n_2+1)\big). \tag{18}$$

Note that we have two different equations: one for $n_2 = n_1+1$ and one for $n_2 > n_1+1$. This, in itself, is nothing to worry about, because what we will show in the following is that the tactic using the translation operator T will no longer be useful.

2.5.2 Using the Bethe Ansatz

Naturally, we want to use the translation operator again, to give us the eigenfunctions. Following the exact same reasoning as in the case of $r=1$, we reach the conclusion that

$$T\,|\,\psi\,\rangle = \mathrm{e}^{\mathrm{i}k}\,|\,\psi\,\rangle \text{ where } k = \frac{2\pi m}{N} \text{ with } m\in\{1,\dots,N\}.$$

But we cannot take the eigenfunctions from Eq. 13, because those are functions with only 1 spin down. Furthermore, we want our k to work on both n_1 and n_2. This leads us to assume the following translationally invariant form of the coefficients $a(n_1,n_2)$, which is called the **Bethe Ansatz** (in this case for $r=2$):

$$a(n_1,n_2) = A\mathrm{e}^{\mathrm{i}(k_1n_1+k_2n_2)} + B\mathrm{e}^{\mathrm{i}(k_1n_2+k_2n_1)}, \tag{19}$$

with $A,B,k_1,k_2\in\mathbb{C}$. The eigenvalue equation for T now reads

$$\begin{aligned}T\,|\,\psi\,\rangle &= \sum_{1\le n_1<n_2\le N} a(n_1,n_2)T\,|\,n_1,n_2\,\rangle = \sum_{2\le n_1<n_2\le N+1} a(n_1,n_2)\,|\,n_1-1,n_2-1\,\rangle \\ &= \sum_{1\le n_1<n_2\le N} a(n_1+1,n_2+1)\,|\,n_1,n_2\,\rangle = \mathrm{e}^{\mathrm{i}(k_1+k_2)}\,|\,\psi\,\rangle\,.\end{aligned}$$

Thus, we call $k := k_1+k_2$ the wave number, and we already know that $k=\frac{2\pi m}{N}$ with $m\in\{1,\dots,N\}$. Later we will encounter conditions on A, B, k_1 and k_2. In the following, we will work from this ansatz, and if we find all the $\frac{N(N-1)}{2}$ solutions, then we are done. If we do not find all the solutions, then the ansatz is wrong. Let us start by finding solutions for coefficients for the basis vectors that do not have neighbouring spins down, namely a solution of Eq. 18.

$$\begin{aligned}&\frac{2}{J}(E-E_0)\left(A\mathrm{e}^{\mathrm{i}(k_1n_1+k_2n_2)} + B\mathrm{e}^{\mathrm{i}(k_1n_2+k_2n_1)}\right) = \frac{2}{J}(E-E_0)a(n_1,n_2) \\ &= 4a(n_1,n_2) - a(n_1-1,n_2) - a(n_1,n_2-1) - a(n_1+1,n_2) - a(n_1,n_2+1) \\ &= 4\left(A\mathrm{e}^{\mathrm{i}(k_1n_1+k_2n_2)} + B\mathrm{e}^{\mathrm{i}(k_1n_2+k_2n_1)}\right) - 2(\cos(k_1)+\cos(k_2))\left(A\mathrm{e}^{\mathrm{i}(k_1n_1+k_2n_2)} + B\mathrm{e}^{\mathrm{i}(k_1n_2+k_2n_1)}\right) \\ &= 4a(n_1,n_2) - 2(\cos(k_1)+\cos(k_2))a(n_1,n_2).\end{aligned}$$

As one can see, this is indeed a solution to the equation, for

$$E - E_0 = J\big[2 - (\cos(k_1) + \cos(k_2))\big] = J \sum_{j=1}^{2} \big[1 - \cos(k_j)\big], \tag{20}$$

where we have written out the summation to indicate the similarity with the result for $r = 1$ (Eq. 14). Let us now find solutions to Eq. 17.

$$\frac{2}{J}(E - E_0)\left(A\mathrm{e}^{\mathrm{i}((k_1+k_2)n+k_2)} + B\mathrm{e}^{\mathrm{i}((k_1+k_2)n+k_1)}\right) = \frac{2}{J}(E - E_0)a(n, n+1)$$
$$= 2a(n, n+1) - a(n-1, n+1) - a(n, n+2)$$
$$= 2\left(A\mathrm{e}^{\mathrm{i}((k_1+k_2)n+k_2)} + B\mathrm{e}^{\mathrm{i}((k_1+k_2)n+k_1)}\right) - A\left(\mathrm{e}^{-\mathrm{i}k_1} + \mathrm{e}^{\mathrm{i}k_2}\right)\mathrm{e}^{\mathrm{i}((k_1+k_2)n+k_2)} - B\left(\mathrm{e}^{-\mathrm{i}k_2} + \mathrm{e}^{\mathrm{i}k_1}\right)\mathrm{e}^{\mathrm{i}((k_1+k_2)n+k_1)}.$$

We see that this is not necessarily a solution to the equation, but hold on.
We proved that the Bethe Ansatz (Eq. 19) without further conditions on A, B, k_1 or k_2 was sufficient to prove Eq. 18 in general, i.e. for every n_1 and n_2. In particular, Eq. 18 holds for $n_2 = n_1 + 1$. Then the equation for $a(n, n+1)$, Eq. 17, is equivalent to the equation we get when we substract Eq. 18 for $n_2 = n_1 + 1$ from Eq. 17. We get the following equivalent condition for $a(n_1, n_2)$:

$$\text{"Eq. 18 - Eq. 17": } 2a(n, n+1) = a(n, n) + a(n+1, n+1). \tag{21}$$

Let's take a step back and look at what we seek to find. We want to know more about the coefficients (A, B, k_1, k_2) in the Bethe Ansatz. Therefore, let us rewrite the last equation with the correct form of the coefficients:

$$2\left(A\mathrm{e}^{\mathrm{i}((k_1+k_2)n+k_2)} + B\mathrm{e}^{\mathrm{i}((k_1+k_2)n+k_1)}\right) = (A + B)(1 + \mathrm{e}^{\mathrm{i}(k_1+k_2)})\mathrm{e}^{\mathrm{i}((k_1+k_2)n)}$$
$$\Longleftrightarrow 2\left(A\mathrm{e}^{\mathrm{i}k_2} + B\mathrm{e}^{\mathrm{i}k_1}\right) = (A + B)(1 + \mathrm{e}^{\mathrm{i}(k_1+k_2)})$$
$$\Longleftrightarrow \frac{A}{B} = -\frac{2\mathrm{e}^{\mathrm{i}k_1} - 1 - \mathrm{e}^{\mathrm{i}(k_1+k_2)}}{2\mathrm{e}^{\mathrm{i}k_2} - 1 - \mathrm{e}^{\mathrm{i}(k_1+k_2)}}.$$

In Appendix A.1 it is shown that $\left|\frac{A}{B}\right| = 1$. This means that we can define a phase angle φ and write

$$\frac{A}{B} =: \mathrm{e}^{\mathrm{i}\varphi}. \tag{22}$$

Because of the normalization of the wave function ψ, the amplitude of A and B is not important, and thus both $|A|$ and $|B|$ can be set to 1. Furthermore, all wave functions that only differ by a phase factor are equivalent, i.e. they produce the same physical system ([16], p. 98), and thus we can multiply both A and B with the same phase factor. Therefore, we can choose to write

$$A = \mathrm{e}^{\mathrm{i}\varphi/2}\ ,\ B = \mathrm{e}^{-\mathrm{i}\varphi/2},$$

where the value of φ is shown in Appendix A.2 to be determined by k_1 and k_2 in the following sense:

$$2\cot\left(\frac{\varphi}{2}\right) = \cot\left(\frac{k_1}{2}\right) - \cot\left(\frac{k_2}{2}\right). \tag{23}$$

A more accurate version of the $r = 2$ Bethe Ansatz is then

$$a(n_1, n_2) = \mathrm{e}^{\mathrm{i}(k_1 n_1 + k_2 n_2 + \frac{1}{2}\varphi)} + \mathrm{e}^{\mathrm{i}(k_1 n_2 + k_2 n_1 - \frac{1}{2}\varphi)}. \tag{24}$$

Now we can look to find the energies $E - E_0$ that are a solution to Eq. 17 by dividing by $B\mathrm{e}^{\mathrm{i}(k_1+k_2)n}$ and using that $\frac{A}{B} = \mathrm{e}^{\mathrm{i}\varphi}$. This is done in Appendix A.3. The result is again $E - E_0 = J\sum_{j=1}^{2}\big[1 - \cos(k_j)\big]$. This means that no matter the positions of the spins down, we have the following relation for the energy of the system with $r = 2$:

$$\boxed{E_2 - E_0 = J\sum_{j=1}^{2}\big[1 - \cos(k_j)\big].} \tag{25}$$

Remember that we want to find solutions for $a(n_1, n_2)$, so what is left to do is to find restrictions for k_1 and k_2. If we find $N(N-1)/2$ combinations for those two parameters, we will have found all the solutions. The first observation that we can make is that the functions $|\,\psi\,\rangle$ will not be affected if we replace n_1 by n_2 and n_2 by n_1+N, by the periodicity of the lattice. In short, we have the condition $a(n_1, n_2) = a(n_2, n_1+N)$. Using our newest version of the Bethe Ansatz, we get for every $n_1 < n_2 \in \{1, \ldots, N\}$:

$$\mathrm{e}^{\mathrm{i}(k_1 n_1 + k_2 n_2 + \frac{1}{2}\varphi)} + \mathrm{e}^{\mathrm{i}(k_1 n_2 + k_2 n_1 - \frac{1}{2}\varphi)} = \mathrm{e}^{\mathrm{i}(k_1 n_2 + k_2 n_1 + N k_2 + \frac{1}{2}\varphi)} + \mathrm{e}^{\mathrm{i}(k_1 n_1 + k_2 n_2 + N k_1 - \frac{1}{2}\varphi)}.$$

Now let us take a look at Eq. 19 again. If $k_1 = k_2$ for all solutions for $a(n_1, n_2)$, then the Bethe Ansatz says that the coefficients only depend on the sum $n_1 + n_2$ of the positions of the spins down. This is not right, as for example (for $N = 5$) two neighbouring spins on positions 2 and 3 will have a different energy than two non-neighbouring spins at positions 1 and 4. A different energy means a different eigenvalue, which means a different eigenfunction, which means that the coefficients $a(n_1, n_2,)$ are not the same. However, the sum $n_1 + n_2 = 5$ *is* the same. Therefore, there is at least one solution with $k_1 \neq k_2$. Looking at this solution, and remembering the equation above is valid for all $n_1 < n_2 \in \{1, \ldots, N\}$, we conclude that

$$\mathrm{e}^{\mathrm{i}(k_1 n_1 + k_2 n_2 + \frac{1}{2}\varphi)} = \mathrm{e}^{\mathrm{i}(k_1 n_1 + k_2 n_2 + N k_1 - \frac{1}{2}\varphi)}\ ,\ \mathrm{e}^{\mathrm{i}(k_1 n_2 + k_2 n_1 - \frac{1}{2}\varphi)} = \mathrm{e}^{\mathrm{i}(k_1 n_2 + k_2 n_1 + N k_2 + \frac{1}{2}\varphi)}.$$

From here, we get the following restrictions on k_1 and k_2:

$$N k_1 - \varphi = 2\pi m_1 \text{ and } N k_2 + \varphi = 2\pi m_2 \text{ where } m_1, m_2 \in \mathbb{Z}. \tag{26}$$

We notice that indeed $k = \frac{2\pi}{N}(m_1 + m_2)$. We will remember this and look for such a form for the wave number in the case of general r later.
The first question we should ask ourselves is if there exists a solution where $k_1 = k_2$ at all. We observe that in this case, $\cot\left(\frac{\varphi}{2}\right) = 0$, so $\varphi = \pi$, so

$$a(n_1, n_2) = \mathrm{e}^{\mathrm{i}(k_1 n_1 + k_1 n_2 + \frac{1}{2}\pi)} + \mathrm{e}^{\mathrm{i}(k_1 n_2 + k_1 n_1 - \frac{1}{2}\pi)} = \mathrm{e}^{\mathrm{i}(k_1 n_1 + k_1 n_2)}\,(\mathrm{i} - \mathrm{i}) = 0.$$

This means that $|\,\psi_{k_1 = k_2}\,\rangle = 0$, which is not a normalizable function, and therefore not a physical solution. We conclude that there exists no solution where $k_1 = k_2$.
Furthermore, we know that we can always add a multiple of $2\pi\mathrm{i}$ in an exponent:

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}(k_1 n_1 + k_2 n_2 + \frac{1}{2}\varphi)} + \mathrm{e}^{\mathrm{i}(k_1 n_2 + k_2 n_1 - \frac{1}{2}\varphi)} &= \mathrm{e}^{\mathrm{i}(k_1 n_1 + 2\pi n_1 + k_2 n_2 + \frac{1}{2}\varphi)} + \mathrm{e}^{\mathrm{i}(k_1 n_2 + k_2 n_1 + 2\pi n_2 - \frac{1}{2}\varphi)} \\
&= \mathrm{e}^{\mathrm{i}((k_1 + 2\pi) n_1 + k_2 n_2 + \frac{1}{2}\varphi)} + \mathrm{e}^{\mathrm{i}((k_1 + 2\pi) n_2 + k_2 n_1 - \frac{1}{2}\varphi)},
\end{aligned}$$

so solutions with $N k_1 = x$ or $N k_1 = x + 2\pi N$ are equivalent. This means that, in Eq. 26, m_1 (and analogously m_2) effectively runs from 0 to $N-1$.
We also see in Eq. 23 that switching k_1 and k_2 changes the sign of φ, because cot is an antisymmetric function. This means, looking at the Bethe Ansatz again, that $a(n_1, n_2)_{k_1, k_2} = a(n_1, n_2)_{k_2, k_1}$: we get equivalent solutions.
At this moment, this symmetry invites us to set $k_1 < k_2$, so as to not get the same solution twice. However, a priori, $k_1, k_2 \in \mathbb{C}$, so we cannot do this. In the following, we will assume $k_1, k_2 \in \mathbb{R}$, so we can continue our discussion and see if there are any real solutions, and if so, how many. If we do not find all the solutions, we need to find the rest of the solutions in $\mathbb{C} - \mathbb{R}$.

2.5.3 Assuming $k_1, k_2 \in \mathbb{R}$

We can set $k_1 < k_2$, so we require $N(k_1 - k_2) < 0$. Looking at Eq. 26 again, we see that this means $\varphi < \pi(m_2 - m_1)$. This is trivially the case if $m_2 - m_1 \geq 2$, but we need to look at the case $m_2 = m_1 + 1$ separately to see if this is a solution after all.

We do this by observing that if $\pi < \varphi < 2\pi$, then $\cot\left(\frac{\varphi}{2}\right) < 0$, so then $\cot\left(\frac{k_1}{2}\right) < \cot\left(\frac{k_2}{2}\right)$, or $\cot\left(\frac{\pi m_1}{N} + \frac{\varphi}{2N}\right) < \cot\left(\frac{\pi m_2}{N} - \frac{\varphi}{2N}\right)$. But $m_1 \leq N-2$ and $m_2 \geq 1$, so both of the arguments of the cot are between 0 and π. In this domain, cot is a strictly decreasing function, so this would mean that $k_1 > k_2$, which is a contradiction. From this short discussion, it follows that $\varphi \leq \pi$ if $m_2 = m_1 + 1$ is a solution. We

now want to check whether or not $\varphi < \pi$ is a solution.[3]
In Appendix A.4 it is shown that φ is strictly increasing in k_1 for $k_1 \notin 2\pi\mathbb{Z}$ and strictly decreasing in k_2 for $k_2 \notin 2\pi\mathbb{Z}$. Looking at Eq. 26, this means that a given pair m_1, m_2 uniquely defines a pair k_1, k_2, only if N is big enough for $Nk_1 - \varphi$ to be a strictly increasing function in k_1 and similarly for the other equation.

2.5.4 Assuming a bijection $(m_1, m_2) \to (k_1, k_2)$

In this section, we will assume that a given pair m_1, m_2 uniquely defines a pair k_1, k_2.
If $k_1 = k_2$, then $\varphi = \pi$, so from Eq. 26 it follows that $m_2 = m_1 + 1$. The one-to-one correspondence between the m_i and the k_i tells us that if $m_2 = m_1 + 1$, then $\varphi = \pi$ and this does *not* meet our requirement. Thus, m_2 runs from 2 to $N-1$, and m_1 runs from 0 to $m_2 - 2$. This gives us $m_2 - 1$ solutions per m_2, so

$$\sum_{m_2=2}^{N-1} [m_2 - 1] = \frac{(N-1)N}{2} - 1 - \big[(N-1) - 1\big] = \frac{(N-2)(N-1)}{2}$$

solutions in total.

What we have found, are $(N-1)(N-2)/2$ solutions for (m_1, m_2), i.e. for (k_1, k_2). These solutions can be substituted in Eq. 24, where we remind the reader that φ is a function of k_1 and k_2. In turn, we substitute our solutions for Eq. 24 into Eq. 16, and we get $(N-1)(N-2)/2$ eigenfunctions with their corresponding eigenvalues given by Eq. 25, which was our original intention.

Example. As an example, let us calculate the energy of a system where $N = 8$, $m_1 = 0$ and $m_2 = 2$. Then $Nk = 2\pi(m_1 + m_2) = 4\pi$, and according to Eq. 26,

$$\frac{\varphi}{2} = 4k_1.$$

Plugging this result, and $k_2 = k - k_1$, into Eq. 23 gives us a numerical answer of

$$k_1 \simeq 2.54, \;\; k_2 \simeq 0.97,$$

and using Eq. 25, we find out that the energy of our system is given by

$$E_2 - E_0 \simeq 2.26J.$$

◇

However, we have too few solutions, because we wanted to have $\dim(\mathscr{H}_2) = N(N-1)/2$ solutions! There must be a missing

$$\frac{N(N-1)}{2} - \frac{(N-2)(N-1)}{2} = N - 1$$

solutions that do not meet our two assumptions. It turns out that throwing away the assumption of the bijection $(m_1, m_2) \to (k_1, k_2)$ gives us one extra solution, and that the remaining $N-2$ solutions are given by taking $k_1, k_2 \in \mathbb{C} - \mathbb{R}$. We will look for these solutions in the remainder of this chapter, which can be skipped without loss of continuity.

2.5.5 Looking for the missing solutions in $\mathbb{C} - \mathbb{R}$

Unfortunately, we can only find exact solutions if we let $N \to \infty$. Thus, in this section, we will **assume** that $N \to \infty$. This assumption will not give us any less solutions: it will only make sure that the solutions are exactly computable.

[3] Note that we proved that $\varphi \neq \pi$ already, because it gave us a non-normalizable wave function.

The first thing we notice is that we still require $k_1 + k_2 = k \in \mathbb{R}$, so we want to find complex conjugate pairs: $k_1 = \overline{k_2}$. We write

$$k_1 = u + \mathrm{i}v, \quad k_2 = u - \mathrm{i}v,$$

with $u, v \in \mathbb{R}$. Let us first find out what restrictions hold for u and v. From Eq. 26 and the equation above, it follows that

$$\begin{aligned} 2N\mathrm{i}v = N(k_1 - k_2) = 2\pi(m_1 - m_2) + 2\varphi \\ \iff \varphi = \pi(m_2 - m_1) + \mathrm{i}Nv \to \mathrm{i}Nv. \end{aligned}$$

Now we know an expression for φ in terms of v and an expression for k_1 and k_2 in terms of u and v, we can use Eq. 23 to get an equation for u and v:

$$\begin{aligned} &2\cot\left(\frac{\varphi}{2}\right) = 2\cot\left(\frac{\mathrm{i}Nv}{2}\right) = 2i\frac{\mathrm{e}^{-Nv} + \mathrm{e}^{Nv}}{\mathrm{e}^{-Nv} - \mathrm{e}^{Nv}} \to -2\mathrm{i} \\ &\cot\left(\frac{k_1}{2}\right) - \cot\left(\frac{k_2}{2}\right) = i\frac{\mathrm{e}^{\mathrm{i}(u+iv)/2} + \mathrm{e}^{-\mathrm{i}(u+iv)/2}}{\mathrm{e}^{\mathrm{i}(u+iv)/2} - \mathrm{e}^{-\mathrm{i}(u+iv)/2}} - i\frac{\mathrm{e}^{\mathrm{i}(u-iv)/2} + \mathrm{e}^{-\mathrm{i}(u-iv)/2}}{\mathrm{e}^{\mathrm{i}(u-iv)/2} - \mathrm{e}^{-\mathrm{i}(u-iv)/2}} = 2i\frac{\sinh(v)}{\cos(u) - \cosh(v)} \\ &\implies \cos(u) = \cosh(v) - \sinh(v) = \mathrm{e}^{-v}. \end{aligned} \tag{27}$$

This means in particular that $-\pi/2 \le u < \pi/2$. We recall that $k = \frac{2\pi}{N}(m_1 + m_2)$, so $0 \le k < 2\pi$. For a given k, then, we get, using that k only needs to be defined modulo 2π, and $k = k_1 + k_2 = 2u$:

$$u = \begin{cases} \frac{k}{2} & \text{if } 0 \le k < \pi, \\ \frac{k}{2} - \pi & \text{if } \pi \le k < 2\pi, \end{cases}$$

or

$$u = \begin{cases} \frac{\pi(m_1+m_2)}{N} & \text{if } 0 \le k < \pi, \\ \frac{\pi(m_1+m_2-N)}{N} & \text{if } \pi \le k < 2\pi. \end{cases} \tag{28}$$

The fact that $-\pi/2 \le u < \pi/2$ now fixes

$$-N/2 \le m_1 + m_2 < N/2. \tag{29}$$

Now we have to be very careful. Remember that if $m_2 - m_1 \ge 2$, then $\varphi < \pi(m_2 - m_1)$ and from Eq. 26 it follows that $N(k_1 - k_2) < 0$ and so $k_1 < k_2$, so then $k_1, k_2 \in \mathbb{R}$. If we take the negation of this statement, we conclude that in our case of $k_1, k_2 \in \mathbb{C} - \mathbb{R}$, either $m_2 = m_1 + 1$ or $m_1 = m_2$. If we count all the possible pairs (m_1, m_2) in the range of Eq. 29, we get

$$|\{(m_1, m_2)\}| = |\{(m_1, m_2) \mid m_1 = m_2\}| + |\{(m_1, m_2) \mid m_2 = m_1 + 1\}| = \left\lfloor \frac{N-1}{2} \right\rfloor + \left\lfloor \frac{N-2}{2} \right\rfloor = N - 2.$$

We know that u only depends on $m_1 + m_2$, and that v only depends on u according to Eq. 27, so a pair $(u, v) \in \mathbb{R}^2$ - and thus a pair $(k_1, k_2) \in \mathbb{C}^2$ - depends on $m_1 + m_2$ only, of which there are $N - 2$ configurations. Using $\varphi \to iNv$ and the Bethe Ansatz (Eq. 24), we compute

$$a(n_1, n_2) = \mathrm{e}^{\mathrm{i}u(n_1+n_2)}\left(\mathrm{e}^{v(n_1-n_2+N/2)} \pm \mathrm{e}^{-v(n_1-n_2+N/2)}\right), \tag{30}$$

where we choose the $\pm$ sign depending on if $0 \le k < \pi$ or not.

We can also compute the energy of the system in terms of u and v using Eq. 25 and Eq. 27:

$$\begin{aligned} E_2 - E_0 &= 2 - \cos(k_1) - \cos(k_2) = 2 - \cos(u + iv) - \cos(u - iv) \\ &= 2 - 2\cos(u)\cos(-iv) = 2 - \cos(u)\left[\mathrm{e}^{-v} + \frac{1}{\mathrm{e}^{-v}}\right] \\ &= 2 - \cos(u)\left[\cos(u) + \frac{1}{\cos(u)}\right] = \sin^2(u). \end{aligned} \tag{31}$$

We notice that this energy is always smaller than or equal to one, so we are interested to see if this is indeed smaller than the real solutions. In fact, we can prove the following lemma.

Lemma 2.18. *If $J > 0$, then the energy of any complex solution $k_1, k_2 \in \mathbb{C} - \mathbb{R}$ is smaller than the energy of any real solution $k_1, k_2 \in \mathbb{R}$.*

Proof. For real solutions, we have

$$E_2 - E_0 = J\big(2 - \cos(k_1) - \cos(k - k_1)\big).$$

We can determine the minimal energy by differentiating this expression to k_1 and setting it equal to zero to get[4]:

$$\sin(k_1) = \sin(k - k_1)$$
$$\iff k_1 = \frac{k}{2}, \quad k_1 = \frac{k}{2} + \pi,$$

where we choose to add π depending on if $0 \leq k < \pi$ or not. The 'solution'[5] with minimal energy is thus $k_1 = k_2 = u$ and we compute

$$\big(E_2 - E_0\big)_{\text{real}} = 2\big(1 - \cos(u)\big) = 2\left(\frac{1 - \cos^2(u)}{1 + \cos(u)}\right) = \frac{2}{1 + \cos(u)}\big(E_2 - E_0\big)_{\text{complex}} > \big(E_2 - E_0\big)_{\text{complex}},$$

where the strict $>$-sign comes from the fact that $u = 0$ (and thus $v = 0$, i.e. $k_1 = k_2 = 0$) is not an actual solution of our problem. □

We have now found $N - 2$ solutions $(k_1, k_2) \in \mathbb{C} - \mathbb{R}$. This means that there is still one solution left to be found. We only have one non-corrected assumption left, so we will encounter the remaining solution if we investigate this assumption further.

2.5.6 Looking for the last solution

In this section, we will throw away our assumption that there exists a bijection $(m_1, m_2) \to (k_2, k_2)$. We can compute the derivative of the left-most term in Eq. 26 to k_1 using Appendix A.4, and we will see that this is *not* always positive, as we assumed earlier.

$$\begin{aligned}\frac{\mathrm{d}\,(Nk_1 - \varphi)}{\mathrm{d}k_1} &= N - \frac{\partial\varphi}{\partial k_1} - \frac{\partial\varphi}{\partial k_2}\frac{\partial k_2}{\partial k_1} \\ &= N - \frac{1}{2}\frac{1}{1 + \left(\frac{1}{2}\left[\cot\left(\frac{k_1}{2}\right) - \cot\left(\frac{k_2}{2}\right)\right]\right)^2}\frac{1}{\sin^2\left(\frac{k_1}{2}\right)} - \frac{1}{2}\frac{1}{1 + \left(\frac{1}{2}\left[\cot\left(\frac{k_1}{2}\right) - \cot\left(\frac{k_2}{2}\right)\right]\right)^2}\frac{1}{\sin^2\left(\frac{k_2}{2}\right)}.\end{aligned}$$

We want to try to make this negative, so we want to minimize $\cot\left(\frac{k_1}{2}\right) - \cot\left(\frac{k_2}{2}\right)$. We do this by setting $k_2 = k_1 + \varepsilon$, with $\varepsilon \ll 1$. We get

$$\lim_{\varepsilon 7to0} \cot\left(\frac{k_1}{2}\right) - \cot\left(\frac{k_1 + \varepsilon}{2}\right) = \frac{\varepsilon}{2\sin^2\left(\frac{k_1}{2}\right)},$$

so

$$\begin{aligned}\lim_{\varepsilon\to 0}\frac{\mathrm{d}\,(Nk_1 - \varphi)}{\mathrm{d}k_1} &= \lim_{\varepsilon\to 0} N - \frac{1}{2}\frac{1}{1 + \left(\frac{\varepsilon}{4\sin^2\left(\frac{k_1}{2}\right)}\right)^2}\frac{1}{\sin^2\left(\frac{k_1}{2}\right)} - \frac{1}{2}\frac{1}{1 + \left(\frac{\varepsilon}{4\sin^2\left(\frac{k_1}{2}\right)}\right)^2}\frac{1}{\sin^2\left(\frac{k_1+\varepsilon}{2}\right)} \\ &= \lim_{\varepsilon\to 0} N - \frac{1}{2\sin^2\left(\frac{k_1}{2}\right)} - \frac{1}{2\sin^2\left(\frac{k_1+\varepsilon}{2}\right)} = N - \frac{1}{\sin^2\left(\frac{k_1}{2}\right)}.\end{aligned}$$

[4]We should check that this is a minimum by differentiating another time, but it is easy to check that this is the case if we notice that $0 \leq k_1 < \pi/2$

[5]This is not an actual solution to the problem, because $k_1 = k_2$, but the energy of any solution is higher than the energy that we get if we compute the energy of this 'solution', so it is still a lower bound.

If $k < 4\arcsin\left(\frac{1}{\sqrt{N}}\right)$, then $k_1 = \frac{k}{2+\varepsilon} < \frac{k}{2} < 2\arcsin\left(\frac{1}{\sqrt{N}}\right)$, so the derivative of $Nk_1 - \varphi$ becomes negative. Note that we want ε to be very small, so we require $m_2 = m_1 + 1$, so by $m_1 + m_2 = \frac{Nk}{2\pi}$, we require $\frac{Nk}{2\pi}$ to be odd. Furthermore, $k \ll 1$ implies that also $k_1, k_2 \ll 1$, so we can write $\cot(k_j/2)$ as $2/k_j$ and we get the following:

$$2\cot\left(\frac{\varphi}{2}\right) = \lim_{\varepsilon\to 0}\cot\left(\frac{k_1}{2}\right) - \cot\left(\frac{k_1+\varepsilon}{2}\right) = \lim_{\varepsilon\to 0}\frac{2}{k_1} - \frac{2}{k_1+\varepsilon} = \lim_{\varepsilon\to 0}\frac{2\varepsilon}{k_1(k_1+\varepsilon)} \to \frac{2\varepsilon}{k_1^2}. \tag{32}$$

However, from Eq. 26, we also get

$$\begin{aligned} &2\varphi = -N(k_2 - k_1) + 2\pi(m_2 - m_1) = -N\varepsilon + 2\pi \\ \implies &\frac{\varphi}{2} = \frac{\pi}{2} - \frac{N\varepsilon}{4} \\ \implies &2\cot\left(\frac{\varphi}{2}\right) = 2\cot\left(\frac{\pi}{2} - \frac{N\varepsilon}{4}\right) = 2\tan\left(\frac{N\varepsilon}{4}\right). \end{aligned} \tag{33}$$

Combining the two expressions for $2\cot(\varphi/2)$, we end up with

$$\frac{\varepsilon}{k_1^2} = \tan\left(\frac{N\varepsilon}{4}\right).$$

This equation is not exactly solvable, but there are two solutions: one is $\varepsilon = 0$, the case in which we are not interested, and for the other solution, $0 < \varepsilon < \pi/2$ holds. With ε, you can compute φ using Eq. 33, and you can find the solution (k_1, k_2) using Eq. 32 and $k_2 = k_1 + \varepsilon$.
This is the last solution that was to be found: we have found all the solutions to the $r = 2$ problem, of which $N - 2$ complex conjugate solutions and $\frac{1}{2}(N-1)(N-2) + 1$ real solutions. The complex solutions have the lowest energy.

The outline and order of explanation in this chapter are largely based on [13] and [2]. The mathematically formal definitions and remarks are mostly my work. The methods used in the special cases in Sections 2.4 and 2.5 are based on both [13] and [2], while all the proofs in this chapter are mine.

3 The general Bethe Ansatz in the Heisenberg model

In this section, we will uncover the general procedure to find the eigenfunctions and their eigenvalues of the Hamiltonian $\mathcal{H}$ of the Heisenberg model using the Bethe Ansatz. We will be inspired by the procedures and observations of the special case for $r = 2$ discussed previously.

3.1 Setting up the equations

We begin by remarking that $\mathscr{H}_r$ is a $\binom{N}{r}$-dimensional subspace of $\mathscr{H}$, which means we are looking for $\binom{N}{r}$ eigenfunctions of $\mathcal{H}$. We will call the eigenfunctions $|\,\psi\,\rangle$ (again without an index m for clarity), and we will write them as

$$|\,\psi\,\rangle = \sum_{1\leq n_1<\cdots<n_r\leq N} a(n_1,\ldots,n_r)\,|\,n_1,\ldots,n_r\,\rangle\,. \tag{34}$$

We want to have expressions for $a(n_1,\ldots,n_r)$. Let us start by writing down the eigenvalue equation for the Hamiltonian again:

$$\begin{aligned}\mathcal{H}\,|\,\psi\,\rangle &= \sum_{1\leq n_1<\cdots<n_r\leq N} a(n_1,\ldots,n_r)\mathcal{H}\,|\,n_1,\ldots,n_r\,\rangle \\ &= -J\sum_{1\leq n_1<\cdots<n_r\leq N} a(n_1,\ldots,n_r)\sum_{j=1}^{N}\left[S_j^zS_{j+1}^z+\frac{1}{2}S_j^+S_{j+1}^-+\frac{1}{2}S_j^-S_{j+1}^+\right]|\,n_1,\ldots,n_r\,\rangle\,.\end{aligned} \tag{35}$$

As before, we have to split this sum into parts with the different possible amounts of neighbours. It is, however, highly unfeasible to identify all these states for a random r and a random N. What we can do, is introduce notation so we are at least able to formulate the equation for the coefficients. We will do this by looking at the matrix form of our Hamiltonian, in the basis of the elements $|\,n_1,\ldots,n_r\,\rangle$. Before we do this, we notice that the Hamiltonian depends on how many transitions there are from spins down to spins up and vice versa, so we want to define the following quantity.

Definition 3.1. Given a basis state $|\,n_1,\ldots,n_r\,\rangle \in \mathcal{B}$, we define

$$M_{|\,n_1,\ldots,n_r\,\rangle} := \frac{N}{4} - \sum_{n=1}^{N}\langle\,n_1,\ldots,n_r\,|\,S_n^zS_{n+1}^z\,|\,n_1,\ldots,n_r\,\rangle\,. \tag{36}$$

We define a group of spins down as a set of spins down $(n_l,\ldots,n_{l+s-1})$ for which $n_{j+1} = n_j + 1$ for every $j \in \{l, l+s-2\}$ and $n_{j+1} \geq n_j + 2$ for $j \in \{l-1, l+s-1\}$. We call s the size of the group.
Intuitively, $M_{|\,n_1,\ldots,n_r\,\rangle}$ is the number of groups of spins down in a configuration $(n_1,\ldots,n_r)$, and s is the number of spins down in a group. As an example for $N = 4$:

$$M_{|\,1,2\,\rangle} = 1\ ,\ M_{|\,1,3\,\rangle} = 2.$$

If it is clear in which configuration we are working, we will often omit the subscript and just write M. ◁

Now we have a manner to write down how many neighbouring spins down there are, we can go on with our discussion on the form of $\mathcal{H}$. First of all, we know that $\mathcal{H}$ can be represented by a $\binom{N}{r}\times\binom{N}{r}$-matrix. In our basis, we call the representation matrix A. Looking at Eq. 35, we see that the diagonal elements of A are

$$A_{|\,n_1,\ldots,n_r\,\rangle,|\,n_1,\ldots,n_r\,\rangle} = -\frac{JN}{4} + M_{|\,n_1,\ldots,n_r\,\rangle}J = E_0 + M_{|\,n_r,\ldots,n_r\,\rangle}J. \tag{37}$$

We also see that there are exchange terms due to the $S_n^+S_{n+1}^-$ and $S_n^-S_{n+1}^+$ terms. These terms switch a spin down with a neighbouring spin up. This means that the non-zero terms only appear in row $|\,n_1,\ldots,n_r\,\rangle$, column $|\,n_1',\ldots,n_r'\,\rangle$ for which there is an $n \in \{1,\ldots,N\}$ such that $S_n^+S_{n+1}^-\,|\,n_1',\ldots,n_r'\,\rangle = |\,n_1,\ldots,n_r\,\rangle$ or

$S_n^- S_{n+1}^+ \,|\, n_1', \ldots, n_r' \,\rangle = |\, n_1, \ldots, n_r \,\rangle$, i.e. for which it holds that you can switch exactly one spin up with a neighbouring spin down in one of the states and get the other state as a result. For these $|\, n_1', \ldots, n_r' \,\rangle$, we see that those elements are

$$A_{|\, n_1, \ldots, n_r \,\rangle, |\, n_1', \ldots, n_r' \,\rangle} = -\frac{J}{2}. \tag{38}$$

To make this relation extra clear, let us get back to our example of $N = 4$. First, we consider the states $|\downarrow\uparrow\downarrow\uparrow\rangle$ and $|\downarrow\downarrow\uparrow\uparrow\rangle$. Clearly, exactly one spin up is switched with a spin down. We see that

$$\left[\sum_{n=1}^{4} S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+\right] |\downarrow\uparrow\downarrow\uparrow\rangle = |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle,$$

so indeed the matrix A gets the elements $-J/2$ if there is exactly one switch-up.
Second, we consider the states $|\downarrow\uparrow\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\uparrow\downarrow\rangle$. Clearly, two spins up are switched with spins down. We see that $|\uparrow\downarrow\uparrow\downarrow\rangle$ does not show up in the equation above, so the corresponding matrix element in A will be 0.

Definition 3.2. In the following, we will notate by $|\, n_1', \ldots, n_r' \,\rangle$ a vector for which there exists an $n \in \{1, \ldots, N\}$ such that $|\, n_1', \ldots, n_r' \,\rangle \in \left\{S_n^+ S_{n+1}^- \,|\, n_1, \ldots, n_r \,\rangle, S_n^- S_{n+1}^+ \,|\, n_1, \ldots, n_r \,\rangle\right\}$. ◁

Let us also use a notation for the basis we will be using.

Definition 3.3. We define

$$\mathcal{B}_r := \mathscr{H}_r \cap \mathcal{B}, \tag{39}$$

as the basis for our subspace $\mathscr{H}_r$ we will be working in. It consists of the basis vectors which have r spins down. ◁

We can now write our eigenfunction $|\, \psi \,\rangle$ as a $\binom{N}{r}$-vector in the basis $\mathcal{B}_r$, where the components will be our coefficients $a(n_1, \ldots, n_r)$, as easily seen from Eq. 34. Our eigenvalue equation in this basis then becomes

$$(A - E) \,|\, \psi \,\rangle = 0. \tag{40}$$

Here we have our $\binom{N}{r}$ equations for the coefficients $a(n_1, \ldots, n_r)$. Looking at one of the rows in the above, we see that

$$\begin{aligned} &\left(E_0 - E + M_{|\, n_1, \ldots, n_r \,\rangle} J\right) a(n_1, \ldots, n_r) - \frac{J}{2} \sum_{|\, n_1', \ldots, n_r' \,\rangle} a(n_1', \ldots, n_r') = 0 \\ \iff &2\,(E - E_0)\, a(n_1, \ldots, n_r) - 2M_{|\, n_1, \ldots, n_r \,\rangle} J a(n_1, \ldots, n_r) + J \sum_{|\, n_1', \ldots, n_r' \,\rangle} a(n_1', \ldots, n_r') = 0 \end{aligned}$$

But our M indicates how many groups of spins down there are, so $2M$ indicates how many opportunities there are for spins down to switch with a neighbouring spin up, as this is possible at both 'borders' of the spin down group. Thus, $2M = |\{|\, n_1', \ldots, n_r' \,\rangle\}|$ and we get the equations for our coefficients:

$$\boxed{\begin{aligned} &2\,(E - E_0)\, a(n_1, \ldots, n_r) + J \sum_{|\, n_1', \ldots, n_r' \,\rangle} \left[a(n_1', \ldots, n_r') - a(n_1, \ldots, n_r)\right] = 0, \\ &\forall j \in \{1, \ldots, r\} \;:\; a(n_1, \ldots, n_j, \ldots, n_r) = a(n_1, \ldots, n_j + N, \ldots, n_r), \end{aligned}} \tag{41}$$

where we added the periodic boundary conditions that we require from the spin chain. We like to stress the peculiar domain of the summation, namely only the states that meet the requirement in Definition 3.2.
Let us now check if this equation indeed reduces to the equations we already derived for the cases $r = 0, 1, 2$.

3.2 Reduction to $r = 0, 1, 2$

For $r = 0$, we see that

$$2(E - E_0)a = 0 \iff E = E_0,$$

as expected.
For $r = 1$, we can see that

$$\begin{aligned} &2(E - E_0)a(n) + J\left[(a(n-1) - a(n)) + (a(n+1) - a(n))\right] = 0 \\ \iff &2(E - E_0)a(n) = J(2a(n) - a(n-1) - a(n+1)), \end{aligned}$$

which corresponds to Eq. 10.
For $r = 2$, we check for neighbouring spins down:

$$\begin{aligned} &2(E - E_0)a(n, n+1) + J\big[(a(n, n+2) - a(n, n+1)) + (a(n-1, n+1) - a(n, n+1))\big] \\ \iff &2(E - E_0)a(n, n+1) = J\left(2a(n, n+1) - a(n-1, n+1) - a(n, n+2)\right), \end{aligned}$$

which corresponds to Eq. 17. We can also check for non-neighbouring spins down, so for $n_2 > n_1 + 1$:

$$\begin{aligned} 2(E - E_0)a(n_1, n_2) + J\Big[&(a(n_1 - 1, n_2) - a(n_1, n_2)) + (a(n_1 + 1, n_2) - a(n_1, n_2)) \\ &+ (a(n_1, n_2 - 1) - a(n_1, n_2)) + (a(n_1, n_2 + 1) - a(n_1, n_2))\Big] = 0 \\ \iff 2(E - E_0)a(n_1, n_2) = J\big(&4a(n_1, n_2) - a(n_1 - 1, n_2) - a(n_1, n_2 - 1) - a(n_1 + 1, n_2) - a(n_1, n_2 + 1)\big), \end{aligned}$$

which corresponds to Eq. 18. Indeed, the general equation (Eq. 41) reduces to the familiar equations in the special cases we discussed in the previous chapter.

3.3 Solving the equation

To solve Eq. 41, we need some more notation.

Definition 3.4. We define

$$\mathcal{P} := \big\{P \ : \ \{1, \dots, r\} \to \{1, \dots, r\} \ \big| \ P \text{ is a bijection}\big\} \tag{42}$$

as the set of permutations of the numbers 1 through r. For $j \in \{1, \dots, r\}$, we will use the short-hand notation $Pj := P(j)$. ◁

Note that $|\mathcal{P}| = r!$. It is time again to employ the Bethe Ansatz for the form of the coefficients $a(n_1, \dots, n_r)$.
The **Bethe Ansatz** for general r and N now reads

Bethe Ansatz

$$a(n_1, \dots, n_r) = \sum_{P \in \mathcal{P}} \exp\left[\mathrm{i}\sum_{j=1}^{r} k_{Pj} n_j + \frac{1}{2}\mathrm{i}\sum_{j<q} \varphi_{Pj,Pq}\right] \tag{43}$$

where $\varphi_{j,l}$ is a priori just a real function of j and l of which we will derive the properties later. We will use this Ansatz to calculate the energies of our spin chain for a general $r \in \{1, \dots, N\}$.

Hypothesis 1. *Looking at the cases for $r = 0, 1, 2$, we expect to find*

$$E_r - E_0 = J\sum_{j=1}^{r}\big[1 - \cos(k_j)\big].$$

Please note that we do not know this yet. As we did in the case of $r = 2$, let us begin by considering a system without any neighbouring spins down. We can always do this, because $r \leq N/2$ by construction, because systems with $r > N/2$ are equivalent to turning all the spins around, which gives us $r < N/2$ again. Because $[\mathcal{H}, \vec{S}] = 0$, it is impossible to find this system in a state *with* neighbouring spins down, so the amplitudes of these states must be zero. Therefore, all the coefficients a will have arguments $n_1, \ldots, n_r$ for which $n_{j+1} - n_j \geq 2$ for all $j \in \{1, \ldots, r\}$. Looking at Eq. 41, the summation in this system will be relatively simple, and the equation reads

$$2(E_r - E_0)a(n_1, \ldots, n_r) = J\sum_{j=1}^{r}\left[2a(n_1, \ldots, n_r) - a(n_1, \ldots, n_j - 1, \ldots, n_r) - a(n_1, \ldots, n_j + 1, \ldots, n_r)\right]. \tag{44}$$

We will now substitute the Bethe Ansatz (Eq. 43) into this equation to solve it explicitly.

$$\begin{aligned}
2(E_r - E_0)a(n_1, \ldots, n_r) &= 2(E_r - E_0)\sum_{P\in\mathcal{P}}\exp\left[\mathrm{i}\sum_{j=1}^{r}k_{Pj}n_j + \frac{1}{2}\mathrm{i}\sum_{j<q}\varphi_{Pj,Pq}\right] \\
&= J\sum_{l=1}^{r}\left(2\sum_{P\in\mathcal{P}}\exp\left[\mathrm{i}\sum_{j=1}^{r}k_{Pj}n_j + \frac{1}{2}\mathrm{i}\sum_{j<q}\varphi_{Pj,Pq}\right]\right. \\
&\qquad - \sum_{P\in\mathcal{P}}\exp\left[-\mathrm{i}k_{P_l} + \mathrm{i}\sum_{j=1}^{r}k_{Pj}n_j + \frac{1}{2}\mathrm{i}\sum_{j<q}\varphi_{Pj,Pq}\right] \\
&\qquad \left. - \sum_{P\in\mathcal{P}}\exp\left[\mathrm{i}k_{P_l} + \mathrm{i}\sum_{j=1}^{r}k_{Pj}n_j + \frac{1}{2}\mathrm{i}\sum_{j<q}\varphi_{Pj,Pq}\right]\right) \\
&= J\sum_{P\in\mathcal{P}}\exp\left[\mathrm{i}\sum_{j=1}^{r}k_{Pj}n_j + \frac{1}{2}\mathrm{i}\sum_{j<q}\varphi_{Pj,Pq}\right]\sum_{l=1}^{r}\left(2 - \mathrm{e}^{-\mathrm{i}k_{Pl}} - \mathrm{e}^{\mathrm{i}k_{Pl}}\right) \\
&= 2Ja(n_1, \ldots, n_r)\sum_{l=1}^{r}\left[1 - \cos\left(k_{Pl}\right)\right]
\end{aligned}$$

We see that the statement below is true.

Lemma 3.5. *Disregarding the physical interpretation of the coefficients, the Bethe Ansatz (Eq. 43) without further conditions on k_l or $\varphi_{j,l}$ is sufficient to satisfy Eq. 44 in general, i.e. for every pair $(n_1, \ldots, n_r)$.*

We will use this fact later.
We mention that $P : \{1, \ldots, r\} \to \{1, \ldots, r\}$ is a bijection, so the summation of Pl from 1 to r is the same as the summation of l from 1 to r, so we can simplify the result above to:

$$(E_r - E_0)a(n_1, \ldots, n_r) = Ja(n_1, \ldots, n_r)\sum_{l=1}^{r}\left[1 - \cos\left(k_l\right)\right].$$

This must hold for every $a(n_1, \ldots, n_r)$ for which $n_{j+1} - n_j \geq 2$. Because $|\psi\rangle \neq 0$, there is at least one coefficient $a(n_1, \ldots, n_r)$ that is not zero, so the equation above implies that

$$E_r - E_0 = J\sum_{l=1}^{r}\left[1 - \cos\left(k_l\right)\right] \quad \text{(no neighbouring spins down)}, \tag{45}$$

as we expected already. Although the result for the energy E_r is only proven for this no-neighbours system, we still expect to find the same result for all the other systems based on our discussions on the special case of $r = 2$.
We have found solutions for the system without neighbouring spins down, but now we want to find solutions for all pairs $(n_1, \ldots, n_r)$. We start off by looking at what we did in the case $r = 2$ again, and there we found Eq. 21. This motivates the statement of the following hypothesis.

Hypothesis 2. *Eq. 41 will be satisfied by the Bethe Ansatz (Eq. 43) for all states* $|\, n_1, \ldots, n_r \,\rangle$ *if we require that*

$$2a(n_1, \ldots, n_r) = a(n_1, \ldots, n_j, n_j, n_{l+2}, \ldots, n_r) + a(n_1, \ldots, n_{j-1}, n_j + 1, n_j + 1, n_{j+2}, \ldots, n_r)$$

for all $j \in \{1, \ldots, r\}$ *for which* $n_{j+1} = n_j + 1$.

To prove this, we need an auxiliary lemma.

Lemma 3.6. *Let* $|\, n_1, \ldots, n_r \,\rangle$ *have* M *groups of spins down. We will indicate the size of group* m *(*$m \in \{1, \ldots, M\}$*) by* s_m*. The spin down in group* m *that has a left-neighbour with spin up will be numbered* n_{l_m}*, i.e.* l_m *is the number of the left-most spin down in group* m*. Suppose that the coefficents* $a(n_1, \ldots, n_r)$ *satisfy the Bethe Ansatz. Then the coefficients* $a(n_1, \ldots, n_r)$ *satisfy Eq. 41 if and only if these coefficients satisfy*

$$2 \sum_{m=1}^{M} [s_m - 1]\, a(n_1, \ldots, n_r) = \sum_{m=1}^{M} \sum_{j=l_m}^{l_m+s_m-2} \big[a(n_1, \ldots, n_j, n_j, \ldots, n_r) + a(n_1, \ldots, n_{j+1}, n_{j+1}, \ldots, n_r)\big]. \quad (46)$$

Proof. We begin by expressing the right term in Eq. 41 explicitly:

$$\sum_{|\, n'_1, \ldots, n'_r \,\rangle} \big[a(n'_1, \ldots, n'_r) - a(n_1, \ldots, n_r)\big] = \sum_{m=1}^{M} \Big[a(n_1, \ldots, n_{l_m} - 1, \ldots, n_r) + a(n_1, \ldots, n_{l_m+s_m-1} + 1, \ldots, n_r) - 2a(n_1, \ldots, n_r)\Big].$$

Let $|\, n_1, \ldots, n_r \,\rangle$ be a given state. We proved that the Bethe Ansatz (Eq. 43) without further conditions on k_l or $\varphi_{j,l}$ is sufficient to satisfy Eq. 44 for every pair $(n_1, \ldots, n_r)$ (Lemma 3.5). If we subtract Eq. 44 from Eq. 41, we get

$$\sum_{m=1}^{M} \big[a(n_1, \ldots, n_{l_m} - 1, \ldots, n_r) + a(n_1, \ldots, n_{l_m+s_m-1} + 1, \ldots, n_r) - 2a(n_1, \ldots, n_r)\big]$$
$$= \sum_{j=1}^{r} \big[a(n_1, \ldots, n_j - 1, \ldots, n_r) + a(n_1, \ldots, n_j + 1, \ldots, n_r) - 2a(n_1, \ldots, n_r)\big].$$

Note that we used the requirement of the coefficients satisfying the Bethe Ansatz here, by taking Eq. 44 to be true. We can rewrite this as follows:

$$
\begin{aligned}
2(r-M)a(n_1,\ldots,n_r) &= \sum_{j=1}^{r}\big[a(n_1,\ldots,n_j-1,\ldots,n_r)+a(n_1,\ldots,n_j+1,\ldots,n_r)\big] \\
&\quad -\sum_{m=1}^{M}\big[a(n_1,\ldots,n_{l_m}-1,\ldots,n_r)+a(n_1,\ldots,n_{l_m+s_m-1}+1,\ldots,n_r)\big] \\
&= \sum_{m=1}^{M}\Bigg[\sum_{j=l_m}^{l_m+s_m-1}\big[a(n_1,\ldots,n_j-1,\ldots,n_r)+a(n_1,\ldots,n_j+1,\ldots,n_r)\big] \\
&\qquad -\big[a(n_1,\ldots,n_{l_m}-1,\ldots,n_r)+a(n_1,\ldots,n_{l_m+s_m-1}+1,\ldots,n_r)\big]\Bigg] \\
&= \sum_{m=1}^{M}\Bigg[\sum_{j=l_m}^{l_m+s_m-1}\big[a(n_1,\ldots,n_j-1,\ldots,n_r)\big]-a(n_1,\ldots,n_{l_m}-1,\ldots,n_r) \\
&\qquad +\sum_{j=l_m}^{l_m+s_m-1}\big[a(n_1,\ldots,n_j+1,\ldots,n_r)\big]-a(n_1,\ldots,n_{l_m+s_m-1}+1,\ldots,n_r)\Bigg] \\
&= \sum_{m=1}^{M}\Bigg[\sum_{j=l_m+1}^{l_m+s_m-1}\big[a(n_1,\ldots,n_j-1,\ldots,n_r)\big]+\sum_{j=l_m}^{l_m+s_m-2}\big[a(n_1,\ldots,n_j+1,\ldots,n_r)\big]\Bigg] \\
&= \sum_{m=1}^{M}\sum_{j=l_m}^{l_m+s_m-2}\big[a(n_1,\ldots,n_{j+1}-1,\ldots,n_r)+a(n_1,\ldots,n_j+1,\ldots,n_r)\big] \\
&= \sum_{m=1}^{M}\sum_{j=l_m}^{l_m+s_m-2}\big[a(n_1,\ldots,n_j,n_j,\ldots,n_r)+a(n_1,\ldots,n_{j+1},n_{j+1},\ldots,n_r)\big].
\end{aligned}
$$

Furthermore, because the sum of the lengths of all the groups must be r, we calculate

$$
r-M=\sum_{m=1}^{M}[s_m]-M=\sum_{m=1}^{M}[s_m-1]\,.
$$

Inserting this result in the derivation above concludes our proof. □

We see that in the case of $r=2$ with neighbouring spins down (i.e. $M=1$ and $s_1=2$), Eq. 46 reduces nicely to Eq. 21 we found earlier. We are now ready to prove Hypothesis 2.

Theorem 3.7. *Eq. 41 will be satisfied by the Bethe Ansatz (Eq. 43) for all configurations $(n_1,\ldots,n_r)$ if we require that*

$$
2a(n_1,\ldots,n_r)=a(n_1,\ldots,n_j,n_j,n_{j+2},\ldots,n_r)+a(n_1,\ldots,n_{j-1},n_{j+1},n_{j+1},n_{j+2},\ldots,n_r) \tag{47}
$$

for all $j\in\{1,\ldots,r\}$ for which $n_{j+1}=n_j+1$.

Proof. Suppose we are in a given configuration $|\,n_1,\ldots,n_r\,\rangle$. Let us begin by introducing some notation we've used before: $|\,n_1,\ldots,n_r\,\rangle$ has $M:=M_{|\,n_1,\ldots,n_r\,\rangle}$ groups of spins down, and $m\in\{1,\ldots,M\}$ denotes the number of the group we are talking about. We let $s_m\in\{1,\ldots,r\}$ denote the size of group m. We denote by n_{l_m} the number of the left-most spin down of group m. The if-statement in this theorem contains conditions for all $j\in\{1,\ldots,r\}$ for which $n_{j+1}=n_j+1$. This means that we have conditions for $j\in\{l_1,\ldots,l_1+s_1-2,l_2,\ldots,l_M+s_M-2\}$. We can add all of these conditions together, so we will use

$$
\sum_{j\in\{l_1,\ldots,l_1+s_1-2,l_2,\ldots,l_M+s_M-2\}}=\sum_{m=1}^{M}\sum_{j=l_m}^{l_m+s_m-2}
$$

and get

$$\sum_{m=1}^{M}\sum_{j=l_m}^{l_m+s_m-2} 2a(n_1,\dots,n_r) = \sum_{m=1}^{M}\sum_{j=l_m}^{l_m+s_m-2}\Big[a(n_1,\dots,n_j,n_j,n_{j+2},\dots,n_r) + a(n_1,\dots,n_{j-1},n_j+1,n_j+1,n_{j+2},\dots,n_r)\Big]$$

$$\iff 2\sum_{m=1}^{M}\left[s_m-1\right]a(n_1,\dots,n_r) = \sum_{m=1}^{M}\sum_{j=l_m}^{l_m+s_m-2}\big[a(n_1,\dots,n_j,n_j,\dots,n_r) + a(n_1,\dots,n_{j+1},n_{j+1},\dots,n_r)\big].$$

According to Lemma 3.6, this is equivalent to the fact that the coefficients $a(n_1,\dots,n_r)$ satisfy Eq. 41, which proves the theorem. □

This theorem states that if there are groups of size ≥ 2 in $|\,n_1,\dots,n_r\,\rangle$, then by requiring Eq. 47 to be true, we ensure that the Bethe Ansatz satisfies Eq. 41. We stress here that the requirement of Eq. 47 is stronger than it needs to be. The only actual requirement we have is Eq. 46.
In the following, we will assume that Eq. 47 is true. If we find all the solutions, we are done. If we do not find all the solutions, we have to abandon this assumption and work with Eq. 46.

3.3.1 Assuming the strong requirement

From here, we will assume that Eq. 47 is true.

Let us first determine the energies of the system. Please remember that we already found the energy of a system without any neighbouring spins down in Eq. 45. According to Theorem 3.7, the Bethe Ansatz always satisfies Eq. 44 for an energy given by Eq. 45. Therefore, all the energies are given by

$$\boxed{E_r - E_0 = J\sum_{l=1}^{r}\left[1-\cos\left(k_l\right)\right],} \tag{48}$$

which proves Hypothesis 1. What remains to do, is find all possible $\{k_l\}$. As we have seen in the case of $r=2$, we need to find an expression for $\varphi_{j,l}$. We can take a good guess of what its form will be, and we will be able to prove this analogously to the case of $r=2$.

Lemma 3.8. *If*

$$2\cot\left(\frac{\varphi_{j,l}}{2}\right) = \cot\left(\frac{k_j}{2}\right) - \cot\left(\frac{k_l}{2}\right), \tag{49}$$

then, writing our coefficients in the form of the Bethe Ansatz (Eq. 43), Eq. 47 holds for all $j \in \{1,\dots,r\}$ *for which* $n_{j+1} = n_j + 1$.

Proof. We begin by stating the equation that we want to prove, namely Eq. 47, and substituting the Bethe Ansatz. For every $l \in \{1,\dots,r\}$ such that $n_{l+1} = n_l + 1$, we must have

$$2\sum_{P\in\mathcal{P}}\exp\left[i\sum_{j=1}^{r}k_{Pj}n_j + \frac{1}{2}i\sum_{j<q}\varphi_{Pj,Pq}\right] = \sum_{P\in\mathcal{P}}\exp\left[i\sum_{j=1}^{r}k_{Pj}n_j + ik_{P(l+1)}(n_l-n_{l+1}) + \frac{1}{2}i\sum_{j<q}\varphi_{Pj,Pq}\right] + \sum_{P\in\mathcal{P}}\exp\left[i\sum_{j=1}^{r}k_{Pj}n_j + ik_{Pl}(n_{l+1}-n_l) + \frac{1}{2}i\sum_{j<q}\varphi_{Pj,Pq}\right].$$

As this is only true for $l \in \{1,\dots,r\}$ such that $n_{l+1} = n_l + 1$, we can rewrite this to

$$\text{To prove:}\quad t(l) := \sum_{P\in\mathcal{P}}\left[2-\left(\mathrm{e}^{-\mathrm{i}k_{P(l+1)}} + \mathrm{e}^{\mathrm{i}k_{Pl}}\right)\right]\exp\left[i\sum_{j=1}^{r}k_{Pj}n_j + \frac{1}{2}i\sum_{j<q}\varphi_{Pj,Pq}\right] = 0. \tag{50}$$

Now it is clear what equation we want to prove, we can begin our proof.
We begin by 'defining' our square root sign as follows. Let $r \in \mathbb{R}$, $r \geq 0$ and $\theta \in [0, 2\pi)$. Denote by ${}_R\sqrt{\ldots}$ the positive real root of r. Then we define

$$\sqrt{r\mathrm{e}^{\mathrm{i}\theta}} :={}_R \sqrt{r}\mathrm{e}^{\mathrm{i}\theta/2}.$$

Note that if $\theta \in [-\pi, \pi)$, then we get a $-$-sign before the square root if $\theta < 0$. Please remember this, because we will be taking square roots of $\varphi \in [-\pi, \pi)$.
We can state, for some $P \in \mathcal{P}$:

$$\begin{aligned}\exp\left[i\sum_{j=1}^{r} k_{Pj}n_j + \frac{1}{2}i\sum_{j<q}\varphi_{Pj,Pq}\right] &= \exp\left(i\sum_{j=1}^{r} k_{Pj}n_j\right)\prod_{j<q}\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}/2} \\ &= \exp\left(i\sum_{j=1}^{r} k_{Pj}n_j\right)\prod_{j<q}\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}},\end{aligned}$$

where we choose the $+$-sign if $\varphi_{Pj,Pq} > 0$ and the $-$-sign if $\varphi_{Pj,Pq} < 0$, because of the way e^{φ} changes into $\mathrm{e}^{\varphi/2}$ via a rotation in $\mathbb{C}$ that's opposite of the rotation involved in the change from $\mathrm{e}^{-\varphi}$ to $\mathrm{e}^{-\varphi/2}$. This is already discussed in the definition of our square root sign. We can now compute t in Eq. 50 and see if it becomes zero. If it does, our proof is complete. We calculate:

$$\begin{aligned}t(l) &= \sum_{P\in\mathcal{P}}\left[2-\left(\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}+\mathrm{e}^{\mathrm{i}k_{Pl}}\right)\right]\exp\left[i\sum_{j=1}^{r}k_{Pj}n_j+\frac{1}{2}i\sum_{j<q}\varphi_{Pj,Pq}\right] \\ &= \sum_{P\in\mathcal{P}}\left[2-\left(\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}+\mathrm{e}^{\mathrm{i}k_{Pl}}\right)\right]\exp\left(i\sum_{j=1}^{r}k_{Pj}n_j\right)\prod_{j<q}\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}} \\ &= \sum_{P\in\mathcal{P}}\mathrm{e}^{\mathrm{i}(k_{Pl}+k_{P(l+1)})n_l}\exp\left[i\left(\sum_{j=1}^{l-1}k_{Pj}n_j+\sum_{j=l+2}^{r}k_{Pj}n_j\right)\right] \\ &\qquad\times\mathrm{e}^{\mathrm{i}k_{P(l+1)}}\left[2-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}\right]\prod_{j<q}\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}} \\ &= \frac{1}{2}\left[\sum_{P\in\mathcal{P}}\mathrm{e}^{\mathrm{i}(k_{Pl}+k_{P(l+1)})n_l}\exp\left[i\left(\sum_{j=1}^{l-1}k_{Pj}n_j+\sum_{j=l+2}^{r}k_{Pj}n_j\right)\right]\right. \\ &\qquad\times\mathrm{e}^{\mathrm{i}k_{P(l+1)}}\left[2-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}\right]\prod_{j<q}\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}} \\ &\qquad+\sum_{P\circ(l,l+1)\in\mathcal{P}}\mathrm{e}^{\mathrm{i}(k_{Pl}+k_{P(l+1)})n_l}\exp\left[i\left(\sum_{j=1}^{l-1}k_{Pj}n_j+\sum_{j=l+2}^{r}k_{Pj}n_j\right)\right] \\ &\qquad\left.\times\mathrm{e}^{\mathrm{i}k_{P(l+1)}}\left[2-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}\right]\prod_{j<q}\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}}\right].\end{aligned}$$

To be clear, $P \circ (l, l+1)$ is the permutation we get when we switch l and $l+1$ and then apply P. We can now continue rewriting this expression by splitting the product so that we can perform our permutation of l

and $l+1$:

$$
\begin{aligned}
t(l) = \frac{1}{2} \Bigg[& \sum_{P \in \mathcal{P}} \mathrm{e}^{\mathrm{i}(k_{Pl}+k_{P(l+1)})n_l} \exp\left[i \left(\sum_{j=1}^{l-1} k_{Pj} n_j + \sum_{j=l+2}^{r} k_{Pj} n_j \right) \right] \mathrm{e}^{\mathrm{i}k_{P(l+1)}} \left[2 - \mathrm{e}^{-\mathrm{i}k_{P(l+1)}} - \mathrm{e}^{\mathrm{i}k_{Pl}} \right] \left(\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pl,P(l+1)}}} \right) \\
& \times \left(\prod_{q=1}^{l-1} \prod_{j=1}^{q-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}} \right) \left(\prod_{j=1}^{l-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,P(l+1)}}} \right) \left(\prod_{q=l+2}^{r} \prod_{j=1}^{q-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}} \right) \left(\prod_{j=1}^{l-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pl}}} \right) \\
& + \sum_{P\circ(l,l+1) \in \mathcal{P}} \mathrm{e}^{\mathrm{i}(k_{Pl}+k_{P(l+1)})n_l} \exp\left[i \left(\sum_{j=1}^{l-1} k_{Pj} n_j + \sum_{j=l+2}^{r} k_{Pj} n_j \right) \right] \mathrm{e}^{\mathrm{i}k_{P(l+1)}} \left[2 - \mathrm{e}^{-\mathrm{i}k_{P(l+1)}} - \mathrm{e}^{\mathrm{i}k_{Pl}} \right] \left(\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pl,P(l+1)}}} \right) \\
& \times \left(\prod_{q=1}^{l-1} \prod_{j=1}^{q-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}} \right) \left(\prod_{j=1}^{l-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,P(l+1)}}} \right) \left(\prod_{q=l+2}^{r} \prod_{j=1}^{q-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}} \right) \left(\prod_{j=1}^{l-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pl}}} \right) \Bigg] \\
= \frac{1}{2} & \sum_{P \in \mathcal{P}} \mathrm{e}^{\mathrm{i}(k_{Pl}+k_{P(l+1)})n_l} \exp\left[i \left(\sum_{j=1}^{l-1} k_{Pj} n_j + \sum_{j=l+2}^{r} k_{Pj} n_j \right) \right] \\
& \times \left(\prod_{q=1}^{l-1} \prod_{j=1}^{q-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}} \right) \left(\prod_{q=l+2}^{r} \prod_{j=1}^{q-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pq}}} \right) \left(\prod_{j=1}^{l-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,P(l+1)}}} \right) \left(\prod_{j=1}^{l-1} \pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pj,Pl}}} \right) \\
& \times \left[\mathrm{e}^{\mathrm{i}k_{P(l+1)}} \left[2 - \mathrm{e}^{-\mathrm{i}k_{P(l+1)}} - \mathrm{e}^{\mathrm{i}k_{Pl}} \right] \left(\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pl,P(l+1)}}} \right) + \mathrm{e}^{\mathrm{i}k_{Pl}} \left[2 - \mathrm{e}^{-\mathrm{i}k_{Pl}} - \mathrm{e}^{\mathrm{i}k_{P(l+1)}} \right] \left(\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{P(l+1),Pl}}} \right) \right]
\end{aligned}
$$

Let us now have a look at the expression in the last line, and let us rewrite it using Eq. 52. If we prove that this expression is always equal to 0, then $t(l) = 0$, which proves the lemma.
If

$$2\cot\left(\frac{\varphi_{j,q}}{2}\right) = \cot\left(\frac{k_j}{2}\right) - \cot\left(\frac{k_q}{2}\right), \tag{51}$$

then, by a derivation analogous to the one in Appendix A.2, we can write

$$\mathrm{e}^{\mathrm{i}\varphi_{j,q}} = -\frac{2\mathrm{e}^{\mathrm{i}(k_j-k_q)} - \mathrm{e}^{-\mathrm{i}k_q} - \mathrm{e}^{\mathrm{i}k_j}}{2 - \mathrm{e}^{-\mathrm{i}k_q} - \mathrm{e}^{\mathrm{i}k_j}}. \tag{52}$$

The first step is observing that $\varphi_{Pl,P(l+1)} = -\varphi_{P(l+1),Pl}$, so there is a relative $-$-sign between the two terms in that last expression. The steps after that consist of taking everything under the square roots and simplifying the expression.

$$
\begin{aligned}
&\mathrm{e}^{\mathrm{i}k_{P(l+1)}}\left[2-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}\right]\left(\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{Pl,P(l+1)}}}\right)+\mathrm{e}^{\mathrm{i}k_{Pl}}\left[2-\mathrm{e}^{-\mathrm{i}k_{Pl}}-\mathrm{e}^{\mathrm{i}k_{P(l+1)}}\right]\left(\pm\sqrt{\mathrm{e}^{\mathrm{i}\varphi_{P(l+1),Pl}}}\right)\\
&=\pm\left[\mathrm{e}^{\mathrm{i}k_{P(l+1)}}\left[2-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}\right]\sqrt{-\frac{2\mathrm{e}^{\mathrm{i}\left(k_{Pl}-k_{P(l+1)}\right)}-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}}{2-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}}}\right.\\
&\qquad\left.-\,\mathrm{e}^{\mathrm{i}k_{Pl}}\left[2-\mathrm{e}^{-\mathrm{i}k_{Pl}}-\mathrm{e}^{\mathrm{i}k_{P(l+1)}}\right]\sqrt{-\frac{2\mathrm{e}^{\mathrm{i}\left(k_{P(l+1)}-k_{Pl}\right)}-\mathrm{e}^{-\mathrm{i}k_{Pl}}-\mathrm{e}^{\mathrm{i}k_{P(l+1)}}}{2-\mathrm{e}^{-\mathrm{i}k_{Pl}}-\mathrm{e}^{\mathrm{i}k_{P(l+1)}}}}\right]\\
&=\pm\left[\left[2-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}\right]\sqrt{-\frac{2\mathrm{e}^{\mathrm{i}\left(k_{Pl}+k_{P(l+1)}\right)}-\mathrm{e}^{\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}\left(k_{Pl}+2k_{P(l+1)}\right)}}{2-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}}}\right.\\
&\qquad\left.-\left[2-\mathrm{e}^{-\mathrm{i}k_{Pl}}-\mathrm{e}^{\mathrm{i}k_{P(l+1)}}\right]\sqrt{-\frac{2\mathrm{e}^{\mathrm{i}\left(k_{P(l+1)}+k_{Pl}\right)}-\mathrm{e}^{\mathrm{i}k_{Pl}}-\mathrm{e}^{\mathrm{i}\left(k_{P(l+1)}+2k_{Pl}\right)}}{2-\mathrm{e}^{-\mathrm{i}k_{Pl}}-\mathrm{e}^{\mathrm{i}k_{P(l+1)}}}}\right]\\
&=\pm\left[\sqrt{-\left(2\mathrm{e}^{\mathrm{i}\left(k_{Pl}+k_{P(l+1)}\right)}-\mathrm{e}^{\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}\left(k_{Pl}+2k_{P(l+1)}\right)}\right)\left(2-\mathrm{e}^{-\mathrm{i}k_{P(l+1)}}-\mathrm{e}^{\mathrm{i}k_{Pl}}\right)}\right.\\
&\qquad\left.-\sqrt{-\left(2\mathrm{e}^{\mathrm{i}\left(k_{P(l+1)}+k_{Pl}\right)}-\mathrm{e}^{\mathrm{i}k_{Pl}}-\mathrm{e}^{\mathrm{i}\left(k_{P(l+1)}+2k_{Pl}\right)}\right)\left(2-\mathrm{e}^{-\mathrm{i}k_{Pl}}-\mathrm{e}^{\mathrm{i}k_{P(l+1)}}\right)}\right]=0.
\end{aligned}
$$

Thus, $t(l)=0$ and this completes our proof. □

This Lemma has the following remark as a consequence.

Remark 3.9. According to Lemma 3.8, if $\varphi_{j,l}$ is given by Eq. 49, then, by Theorem 3.7, the equations for our coefficients (Eq. 41) are satisfied by the Bethe Ansatz (Eq. 43). In other words, we found the expression for the phase angle $\varphi_{j,l}$ in the Bethe Ansatz, namely

$$2\cot\left(\frac{\varphi_{j,l}}{2}\right)=\cot\left(\frac{k_j}{2}\right)-\cot\left(\frac{k_l}{2}\right). \tag{53}$$

◇

Just like in the $r=2$ case, we now want to discover the possible $\{k\}$'s by imposing the periodicity condition:

$$
\begin{aligned}
&a(n_1,\dots,n_r)=a(n_2,\dots,n_r,n_1+N)\\
\Longleftrightarrow\ &\sum_{P\in\mathcal{P}}\exp\left[\mathrm{i}\sum_{j=1}^{r}k_{Pj}n_j+\frac{1}{2}\mathrm{i}\sum_{j<q}\varphi_{Pj,Pq}\right]=\sum_{P\in\mathcal{P}}\exp\left[\mathrm{i}\sum_{j=1}^{r-1}\left[k_{Pj}n_{j+1}\right]+\mathrm{i}k_{Pr}(n_1+N)+\frac{1}{2}\mathrm{i}\sum_{j<q}\varphi_{Pj,Pq}\right].
\end{aligned} \tag{54}
$$

Again, we make the argument that this relation must be true for all $(n_1,\dots,n_r)\in\{1,\dots,N\}^r$, so the coefficients before the n_j's must match. We can look at taking a random $P\in\mathcal{P}$ for the left side, and then taking $P'(k) := P(k+1)$ on the right side. Then there must be an $m \in \mathbb{Z}$ such that for every $P \in \mathcal{P}$:

$$\begin{aligned}
\frac{1}{2}\sum_{j<q}\varphi_{Pj,Pq} &= Nk_{P1} + \frac{1}{2}\sum_{j<q}\varphi_{P(j+1),P(q+1)} - 2\pi m \\
\iff Nk_{P1} - 2\pi m &= \frac{1}{2}\left[\sum_{j<q}\varphi_{Pj,Pq} - \sum_{j<q}\varphi_{P(j+1),P(q+1)}\right] \\
&= \frac{1}{2}\left[\sum_{1\le j<q\le r}\varphi_{Pj,Pq} - \sum_{2\le j<q\le r}\varphi_{Pj,Pq} - \sum_{j=1}^{r-1}\varphi_{P(j+1),P1}\right] \\
&= \frac{1}{2}\left[\sum_{j=2}^{r}\varphi_{P1,Pj} + \sum_{j=1}^{r-1}\varphi_{P1,P(j+1)}\right] = \sum_{l=1}^{r}\varphi_{P1,l},
\end{aligned}$$

where we used $\varphi_{j,l} = -\varphi_{l,j}$. But this is valid for every $P \in \mathcal{P}$, so

$$\forall j \in \{1,\dots,r\} \ : \ Nk_j = 2\pi m + \sum_{l=1}^{r}\varphi_{j,l}. \tag{55}$$

Unfortunately, these equations are very involved, and we can only get approximate solutions. This is not the goal of this thesis, so we will terminate the discussion here.

In principle, we have an equation for the k_j's, which will give us the energy of the system by plugging them into Eq. 48. It will also give us the eigenvectors of $\mathcal{H}$. But these eigenvectors are also the eigenvectors of any operator M that commutes with $\mathcal{H}$. Operators that commute with the Hamiltonian are conserved quantities, as is mentioned earlier. Thus, we know the eigenvectors, and thus the eigenvalues, of any operator that is conserved in time.

What we also have is an expression for the phase angle $\varphi_{j,l}$, and this will turn out to be valuable in a whole other field of research: Square Ice.

Section 3.1 is based on [1], and from there the chapter is based on [2], but the majority of the proofs are my work. I found Lemma 3.6 by myself and found it interesting enough to state as a separate lemma. With the exception of Johan van de Leur's suggestion of considering the permutation $P \circ (x,y)$ with $x \neq y \in \{1,\dots,r\}$ in the proof of Lemma 3.8, all the proofs in this chapter are my own work.

4 The Square Ice model

As is discussed in [10], d-dimensional quantum systems have strong connections with $(d+1)$-dimensional classical systems. As we have discussed a 1-dimensional quantum system in the above, we now want to consider a 2-dimensional classical system to see if we can apply the Bethe Ansatz here as well. We will use the structure of water ice as an example. Measurements suggest that ice has a non-zero entropy at absolute zero. The goal of this chapter will be to find this entropy.

4.1 Introduction

In this chapter, we will introduce the Square Ice model, which is a model for ice (solid H_2O) at absolute zero, i.e. 0 K. As we know, ice has a hexagonal structure (which is visible in snowflakes, for example). To be precise, the space group is No. 186 in the International Union of Crystallography classification, and the structure is seen in Figure 1, in which all balls represent oxygen atoms. As you can see, each oxygen atom has bonds with its four nearest-neighbouring oxygen atoms. If we neglect the not-nearest-neighbour interactions, then this motivates the simplified picture where we have a square lattice with points, that represent the oxygen atoms, that all have four neighbours. Here we have the start of our 2-dimensional square ice model.

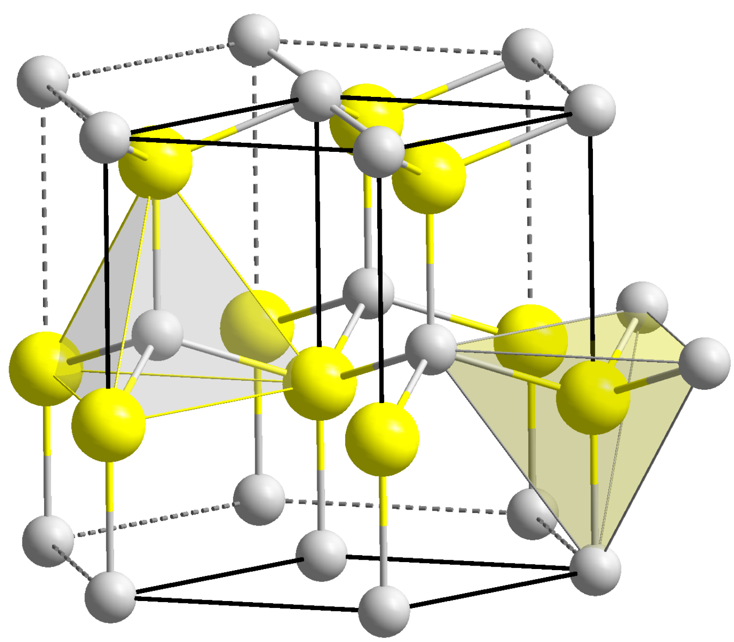

Figure 1: The structure of spacegroup No. 186. In the case of ice, the yellow and grey balls both represent oxygen atoms. Source: [17].

The bonds between the oxygen atoms are hydrogen bonds: each bond consists of one hydrogen atom. The distance between the nearest-neighbour oxygen atoms in ice is more than 2.7 Å ([15]), but the bond between hydrogen and oxygen atoms in water is roughly 0.96 Å ([9]), which is significantly less than half the distance between the oxygen atoms. This means that the hydrogen atom between two nearest-neighbour oxygen atoms has two options: being closer to one of them or to the other.

When we represent oxygen atoms by dots and the hydrogen bond between them by a line segment, we indicate the position of the hydrogen atom by an arrow: if the arrow is pointing from oxygen atom A to B, this means that the hydrogen atom is closer to B than to A.

Let us have a lattice of $N \times M$ oxygen atoms (which we will call simply atoms in the following) with periodic boundary conditions for both the horizontal and the vertical sides. We call this type of periodic boundary conditions toroidal boundary conditions, due to the glueing pattern one makes when constructing a torus from a square. In other words, we put our lattice on a torus.

Definition 4.1. Define Ω to be the set of all possible states a system can be in. The entropy S of this system is defined to be

$$S := k_b \log(|\Omega|), \tag{56}$$

where $k_b := 1.380649 \cdot 10^{23}$ J/K is the Boltzmann constant. ◁

In our case, Ω is the number of ways we can arrange the arrows in our lattice, because at absolute zero, the entropy due to thermodynamical effects is zero according to the Third Law of Thermodynamics. Thus, we only have the entropy from the number of configurations that our system can take on. We mention that in a unit cell of our lattice, there is one vertex and there are two line segments. Therefore, there are MN vertices and $2MN$ line segments in our system. Without imposing any extra rules, then, the entropy of this lattice system is given by

$$S = k_b \log(2^{2MN}) = MNk_b \log(4),$$

because each line segment can 'choose' between two directions for its arrow to point in. Let us write the actual entropy of our system as

$$S = MNk_b \log(W). \tag{57}$$

Early measurements on heat capacity in 1933 by Giauque and Ashley ([3]) indicate that

$$W = 1.51 \pm 0.04 \text{ (measurement)}, \tag{58}$$

and Nagle estimated in 1966 ([5]) that

$$W = 1.540 \pm 0.001 \text{ (estimation)}. \tag{59}$$

The first thing we notice, is that if we do not impose any rules, then $S = MNk_b \log(4)$, so $W = 4$. This is clearly significantly larger than the experimentally verified value for W, so there must be more constraints on how many configurations the arrows can be in. Therefore, let us introduce some rules regarding these arrows. Under normal conditions, water has a pH of around 7. This means that the concentration $C_{H_3O^+}$ of H_3O^+ atoms is

$$C_{H_3O^+} = 10^{-\text{pH}} \simeq 10^{-7}.$$

Furthermore, water is electrically neutral, so the concentration of OH^- will also be 10^{-7}. Therefore, we will neglect the presence of these ions in our model: every oxygen atom has two hydrogen atoms close to it. In our lattice, then, this means that every vertex has two incoming arrows and two outgoing ones. The possible configurations around a vertex are shown in Figure 2. This certainly reduces the number of possible configurations of the arrows, and the question is now how many there are left, and if this matches the estimation of Eq. 59. First, let us define explicitly what our model is.

Definition 4.2. The Square Ice model is an $N \times M$ lattice, with toroidal boundary conditions, of vertices that are connected to their nearest neighbours by line segments. Each line segment has an orientation, indicated by an arrow, that is pointed from the middle of the line segment towards one of the two vertices that it connects. Every vertex is connected to two arrows pointed towards it and two arrows pointing away from it, which is known as the ice rule. ◁

The ice rule leaves us with six possible vertex configurations, shown in Figure 2.

Now, let us look at the line segments in the sense that we have M (horizontal) rows of vertical line segments, and M rows of horizontal line segments. We let φ denote a configuration of a row of vertical line segments. We do this by saying

$$\mathscr{G} := \bigotimes_{j=1}^{N} \{\uparrow, \downarrow\} \tag{60}$$

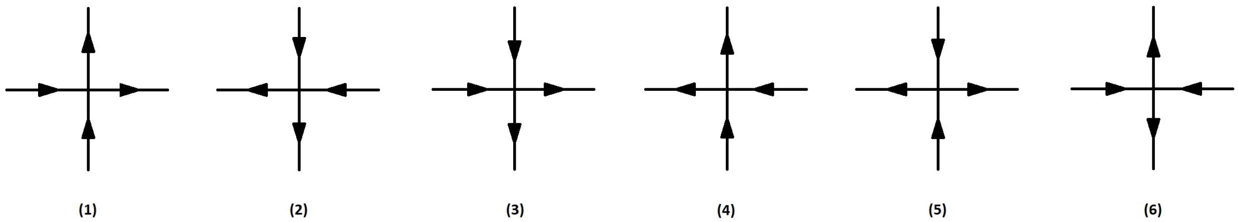

Figure 2: The six vertices that meet the ice rule.

and letting $\varphi \in \mathscr{G}$, where we will write

$$|\,\sigma_1 \dots \sigma_N\,\rangle := \bigotimes_{j=1}^{N} \sigma_j,$$

where $\sigma_j \in \{\uparrow,\downarrow\}$ for $j \in \{1,\dots,N\}$. As an example for the notation of $|\,\sigma_1 \dots \sigma_N\,\rangle$, a row of vertical line segments where all arrows point upwards will be denoted by $\varphi = |\uparrow \dots \uparrow\rangle$. Note the similarity with the spin chain again. Let us now define an inner product on $\mathscr{G}$, in a fashion similar to the inner product on the spin space $\mathscr{H}$.

Definition 4.3. For $\mathscr{G}_s := \{\uparrow,\downarrow\}$, define the inner product $\langle\,.\,|\,.\,\rangle$ as

$$\begin{aligned} &\langle\,.\,|\,.\,\rangle \;:\; \mathscr{G}_s \times \mathscr{G}_s \to \mathbb{R}, \\ &\langle\uparrow\,|\,\uparrow\rangle = \langle\downarrow\,|\,\downarrow\rangle = 1\;,\;\langle\uparrow\,|\,\downarrow\rangle = 0. \end{aligned}$$

The inner product between two vectors $v_1, v_2 \in \{a\,|\uparrow\rangle + b\,|\downarrow\rangle \;\mid a, b \in \mathbb{R}\}$ is computed by writing v_1 and v_2 as a linear combination of basis vectors. ◁

It is easy to see that $\langle\,.\,|\,.\,\rangle$ is an inner product, and if we define the inner product on the tensor product space $\mathscr{G}$ similar to the inner product on $\mathscr{H}$, then all possible $\varphi \in \mathscr{G}$ form an orthonormal basis. We will denote the i-th basis vector of $\mathscr{G}$ as e_i.
Let φ_k be the configuration of row k of vertical line segments, with $k \in \{1,\dots,M\}$. Remember that we want to count the number of possible states the ice lattice can be in. To this end, let us introduce some notation. We write

$$\vec{\varphi} := \begin{pmatrix} \varphi_1 \\ \vdots \\ \varphi_M \end{pmatrix} \in \mathscr{G}^M \tag{61}$$

for the configuration of all the vertical line segments in the lattice.

Definition 4.4. Suppose the configurations of vertical line segments φ_j and φ_{j+1} are given for a certain $j \in \{1,\dots,M\}$ (where we keep in mind the periodic boundary conditions $M+1 \equiv 1$). We consider the row of horizontal line segments that is between the two rows of vertical line segments of which the configurations are given.
Then we define $B(\varphi_j, \varphi_{j+1}) \in \mathbb{N} \cup \{0\}$ as the number of configurations of this row such that the ice rule is satisfied at each vertex in this row.
We define

$$A_{i,j} := B(e_i, e_j) \tag{62}$$

and we see A as a $2^N \times 2^N$ matrix, because $\mathscr{G}$ has 2^N basis vectors. We call A the transfer matrix. ◁

We see again the similarity with the spin chain matrix A, which indicated how similar two spin configurations were, as opposed to this matrix A which indicates how two rows of vertical line segments produce possible configurations for our lattice.

Suppose $\vec{\varphi}$, i.e. the configuration of all our vertical arrows, is given. Then the number of possible configurations (for our horizontal arrows, and thus for our whole system) will be

$$\prod_{j=1}^{M} B(\varphi_j, \varphi_{j+1}).$$

Thus, if we do not know the configurations of the vertical line segments, then we have to sum this expression over all possible $\vec{\varphi}$, i.e. all the possible configurations of the vertical line segments. Then the number of possible configurations will be given by

$$|\Omega| = \sum_{\vec{\varphi} \in \mathscr{G}^M} \prod_{j=1}^{M} B(\varphi_j, \varphi_{j+1}). \tag{63}$$

According to Eq. 56, to find the entropy of our lattice, we need to find B, or A. We start by mentioning that the diagonal elements of A are $A_{j,j}$. But when two rows of vertical line segments are identical, then the horizontal row between them can only be in one of two states: all arrows pointing to the left or all arrows to the right. This is easily seen by putting one left-arrow somewhere in this horizontal row: the ice rule makes us put a left-arrow on neighbouring horizontal line segments as well, and we continue doing this until the whole horizontal row is filled with left-arrows. The same argument can be made for right-arrows. Thus, $\forall \varphi \in \mathscr{G} \ : \ B(\varphi, \varphi) = 2$, and thus

$$\forall j \in \{1, \ldots, 2^N\} \ : \ A_{j,j} = 2.$$

Now suppose there is only one differing arrow between φ_j and φ_{j+1}. Say this is at vertex v in the horizontal row, and the up-arrow in the bottom row of vertical line segments is changed into a down-arrow in the top row of vertical line segments. Then, outside this special vertex v, the horizontal row inbetween must still be either all to the left or to the right pointing arrows. Let us say that they are pointing to the left. However, at the vertex itself, we have one arrow pointing upwards and one pointing downwards. This means that we need one arrow pointing to the left and one pointing to the right, according to the ice rule (see also Figure 2). In our case, this means that vertex v looks like (5) in Figure 2. This cannot be a possible configuration, because outside this vertex, all arrows are pointing to the left: there must be another vertex u at which the right arrows change to left arrows again. This vertex, then, must look like (6) in Figure 2, i.e. a down-arrow in the bottom row is changed into an up-arrow in the top row. In particular, there cannot be another vertex of type (5) inbetween our vertices. Let us state this result, which we have proven by the above discussion, in a lemma.

Lemma 4.5. *Consider a row of horizontal line segments and look at the vertex types in Figure 2. Between every vertex of type (5), there must be a vertex of type (6), and between every vertex of type (6), there must be a vertex of type (5).*

Note that in such a row, we cannot change the horizontal arrows (without altering the vertical arrows, which are given to be fixed), because at a vertex of type (5) or (6), this would violate the ice rule. Thus, for φ_j, φ_{j+1} and if there is at least one vertex of type (5) (and (6)) in the row of horizontal line segments between them, and this row meets Lemma 4.5, then $A(\varphi_j, \varphi_{j+1}) = 1$. If a row of horizontal line segments does not meet Lemma 4.5, then $A(\varphi_j, \varphi_{j+1}) = 0$. In summary, for $\varphi_j \neq \varphi_{j+1} \in \mathscr{G}$:

$$B(\varphi_j, \varphi_j) = 2;$$

$$B(\varphi_j, \varphi_{j+1}) = \begin{cases} 1 & \text{if the row of horizontal line segments between } \varphi_j \text{ and } \varphi_{j+1} \text{ meets Lemma 4.5;} \\ 0 & \text{otherwise.} \end{cases}$$

Or for A, for $j \neq l \in \{1, \ldots, 2^N\}$ (imagining that e_j and e_l would be the configurations of neighbouring rows):

$$A_{j,j} = 2 \tag{64}$$

$$A_{j,l} = \begin{cases} 1 & \text{if the row of horizontal line segments between } e_j \text{ and } e_l \text{ would meet Lemma 4.5;} \\ 0 & \text{otherwise.} \end{cases} \tag{65}$$

The next question we should ask ourselves, is how many φ_j, φ_{j+1} let the row of horizontal line segments meet Lemma 4.5, given a row consists of N (oxygen) atoms.
If there are zero vertices of type (5) or (6), then $\varphi_j = \varphi_{j+1}$, so we will not count this. If there is one vertex of type (5) and one of type (6), then there are $N(N-1)$ ways of placing them in our row of N atoms. If there are two vertices of type (5) and (6) each, then we have $\binom{N}{4}$ ways of distributing them. However, we have to assign type (5) and (6) to the vertices alternatingly. We can choose ((5),(6),(5),(6)), but also ((6),(5),(6),(5)), so we have two possibilities, so there are $2\binom{N}{4}$ possible arrangements satisfying the ice rule. Let us generalize this result.

Lemma 4.6. *There are*

$$2\binom{N}{2k}$$

ways to distribute k vertices of type (5) and (6) each over N lattice sites such that the ice rule is obeyed. In total, there are

$$2^N - 2$$

ways to distribute vertices of type (5) and (6) over N lattice sites, not counting not putting any at all.

Proof. To choose $2k$ lattice sites that we want to distribute our type (5) and (6) vertices over (k of each type), we have $\binom{N}{2k}$ possibilities. If the sites are chosen, to assign the vertex types, we can start with either (5) or (6), and to obey the ice rule we have to alternate them from there, so we have two possibilities for that operation. Therefore, we have a total of

$$2\binom{N}{2k}$$

possibilities to distribute k vertices of type (5) and (6) each over N lattice sites such that the ice rule is obeyed.
The total number of ways to distribute vertices of type (5) and (6) over N lattice sites is then

$$\sum_{k=1}^{\lfloor N/2 \rfloor} 2\binom{N}{2k}.$$

If N is even, then we let $N = 2n$ and

$$\begin{aligned}\sum_{k=1}^{\lfloor N/2 \rfloor} 2\binom{N}{2k} &= \sum_{k=1}^{n} 2\binom{N}{2k} = \sum_{k=1}^{N} \left(1+(-1)^k\right)\binom{N}{k} = \left[\sum_{k=0}^{N}\binom{N}{k} + \sum_{k=0}^{N}(-1)^k\binom{N}{k}\right] - 2\binom{N}{0} \\ &= \left[2^N + (1-1)^N\right] - 2 = 2^N - 2.\end{aligned}$$

If N is odd, then we let $N = 2n+1$ and

$$\begin{aligned}\sum_{k=1}^{\lfloor N/2 \rfloor} 2\binom{N}{2k} &= \sum_{k=1}^{n} 2\binom{N}{2k} = \left[\sum_{k=0}^{2n}\binom{N}{k} + \sum_{k=0}^{2n}(-1)^k\binom{N}{k}\right] - 2\binom{N}{0} \\ &= \left[2^N + (1-1)^N\right] - \left[\binom{N}{N} + (-1)^N\binom{N}{N}\right] - 2 = 2^N - 2.\end{aligned}$$

□

This lemma tells us that there are $2^N - 2$ combinations of e_j, e_l that will give $A_{j,l} = 1$. We already know that there are 2^N possible $\varphi \in \mathscr{G}$, so there are 2^N combinations of e_j, e_l that will give $A_{j,l} = 2$. In short, the 2^N diagonal entries of A are 2, another $2^N - 2$ entries are 1, and the rest is 0.
Furthermore, we notice another implication of the ice rule. If there are as many vertices of type (5) in a row of horizontal line segments as of type (6), then φ_j and φ_{j+1} must have the same number of up-arrows. This means that A working on a $\varphi \in \mathscr{G}$ will give a linear combination of $\varphi_j \in \mathscr{G}$ that all have the same number of up-arrows as φ. Thus, A is block-diagonal if we order our basis vectors e_j to how many up-arrows they contain. Also, A must be symmetrical, because $A_{j,l} = A_{l,j}$. Note again the similarities with the representation of the Hamiltonian. Summarized, we have the following properties for A.

Remark 4.7. A is symmetrical, block-diagonal, and all its entries are real and non-negative. In turn, this means that A has only real eigenvalues and that it is diagonalizable. ◇

Now we know a lot more about our transfer matrix, let us try to simplify Eq. 63 somewhat. To do this, we use the following expression for the trace of a power of a matrix.

Remark 4.8. For a matrix V and $L \in \mathbb{N}$, the following identity holds:

$$\left(V^L\right)_{\sigma\sigma'} = \sum_{\sigma_1,\ldots,\sigma_{L-1}} V_{\sigma\sigma_1} V_{\sigma_1\sigma_2} \ldots V_{\sigma_{L-1}\sigma'}.$$

◇

Now we can state the following.

Theorem 4.9. *The number of states our lattice can be in is*

$$|\Omega| = \mathrm{Tr}\left(A^M\right). \tag{66}$$

Proof. Using Remark 4.8, we can immediately write the trace of A^M as:

$$\begin{aligned}\mathrm{Tr}\left(A^M\right) &= \sum_{\sigma=1}^{2^N} \left(A^M\right)_{\sigma\sigma} = \sum_{\sigma,\sigma_1,\ldots,\sigma_{M-1}=1}^{2^N} A_{\sigma\sigma_1} A_{\sigma_1\sigma_2} \ldots A_{\sigma_{M-1}\sigma} = \sum_{\sigma_1,\ldots,\sigma_M=1}^{2^N} A_{\sigma_1\sigma_2} \ldots A_{\sigma_{M-1}\sigma_M} A_{\sigma_M\sigma_1} \\ &= \sum_{\sigma_1,\ldots,\sigma_M=1}^{2^N} \prod_{j=1}^{M} A_{\sigma_j,\sigma_{j+1}} = \sum_{\sigma_1,\ldots,\sigma_M=1}^{2^N} \prod_{j=1}^{M} B(e_{\sigma_j}, e_{\sigma_{j+1}}).\end{aligned}$$

But we are summing over all M-tuples of basis vectors e_i, so we can replace the summation over all the M sigmas by a summation over all elements $\vec{\varphi}$ in $\mathscr{G}^M$:

$$\mathrm{Tr}\left(A^M\right) = \sum_{\vec{\varphi}\in\mathscr{G}^M} \prod_{j=1}^{M} B(\varphi_j, \varphi_{j+1}) = |\Omega|,$$

where the last equal sign comes from Eq. 63. □

Thus, to find the entropy, we have to find the trace of A^M, which means we have to find the eigenvalues of A^M. However, if λ is an eigenvalue of A, then λ^M is an eigenvalue of A^M. This is a one-to-one correspondence, so it suffices to solve the eigenvalue equation

$$A \,|\, \psi \,\rangle = E \,|\, \psi \,\rangle \,. \tag{67}$$

Just like the diagonalization of the Hamiltonian of the spin chain, this is not an easy task, and we are going to need an ansatz again. First, let us introduce some notation that is similar to the notation used in the spin chain problem.
Let a row configuration φ with r down-arrows and $N - r$ up-arrows be given. The down-arrows are located

at arrow numbers $n_1, \ldots, n_r$ with $1 \le n_1 < \cdots < n_r \le N$. We notate this configuration as $|\, n_1, \ldots, n_r \,\rangle$. We write our eigenvector $|\, \psi \,\rangle$ as

$$|\, \psi \,\rangle = \sum_{1 \le n_1 < \cdots < n_r \le N} a(n_1, \ldots, n_r)\, |\, n_1, \ldots, n_r \,\rangle\,.$$

We want to have expressions for $a(n_1, \ldots, n_r)$ again, so we start out by writing down the eigenvalue equation.

$$A\, |\, \psi \,\rangle = \sum_{1 \le n_1 < \cdots < n_r \le N} a(n_1, \ldots, n_r) A\, |\, n_1, \ldots, n_r \,\rangle = E \sum_{1 \le n_1 < \cdots < n_r \le N} a(n_1, \ldots, n_r)\, |\, n_1, \ldots, n_r \,\rangle\,.$$

We have to figure out what A does with a basis vector $|\, n_1, \ldots, n_r \,\rangle$. Clearly, we want to get 2 times $|\, n_1, \ldots, n_r \,\rangle$, and we want every state $|\, m_1, \ldots, m_{r'} \,\rangle$, that lets the row of horizontal line segments between the rows corresponding to $|\, n_1, \ldots, n_r \,\rangle$ and $|\, m_1, \ldots, m_{r'} \,\rangle$ meet Lemma 4.5, exactly once. We see that meeting Lemma 4.5 is equivalent to requiring that $r = r'$ and that

$$n_1 \le m_1 \le n_2 \le m_2 \le \cdots \le n_r \le m_r \le N$$

or the same statement but with the n's switched with the m's. We can see this because if there are two down-arrows in one vertical row at positions x and y while there are only up-arrows at x and y and inbetween in the other vertical row, then we would need two consecutive vertices of type (5) or (6) (depending on if the down-arrows are in the upper or lower row). Thus, n_x can be anything from m_{x-1} to m_x, or in the other case, from m_x to m_{x+1}. We can write all of this as

$$A\, |\, n_1, \ldots, n_r \,\rangle = \sum_{m_1=1}^{n_1} \sum_{m_2=n_1}^{n_2} \cdots \sum_{m_r=n_{r-1}}^{n_r} |\, m_1, \ldots, m_r \,\rangle + \sum_{m_1=n_1}^{n_2} \sum_{m_2=n_2}^{n_3} \cdots \sum_{m_r=n_r}^{N} |\, m_1, \ldots, m_r \,\rangle\,, \tag{68}$$

where kets in which not all m_i are different must be interpreted as zero. Thus, the eigenvalue equation becomes

$$\sum_{1 \le n_1 < \cdots < n_r \le N} a(n_1, \ldots, n_r) \Bigg[\sum_{m_1=1}^{n_1} \cdots \sum_{m_r=n_{r-1}}^{n_r} |\, m_1, \ldots, m_r \,\rangle + \sum_{m_1=n_1}^{n_2} \cdots \sum_{m_r=n_r}^{N} \big[\, |\, m_1, \ldots, m_r \,\rangle \,\big] - E\, |\, n_1, \ldots, n_r \,\rangle \Bigg] = 0. \tag{69}$$

We notice that

$$\sum_{1 \le n_1 < \cdots < n_r \le N} a(n_1, \ldots, n_r) \sum_{m_1=1}^{n_1} \cdots \sum_{m_r=n_{r-1}}^{n_r} |\, m_1, \ldots, m_r \,\rangle = \sum_{1 \le n_1 < \cdots < n_r \le N} |\, n_1, \ldots, n_r \,\rangle \sum_{m_1=n_1}^{n_2} \cdots \sum_{m_r=n_r}^{N} a(m_1, \ldots, m_r),$$

so Eq. 69 becomes

$$\sum_{1 \le n_1 < \cdots < n_r \le N} |\, n_1, \ldots, n_r \,\rangle \left[\sum_{m_1=n_1}^{n_2} \cdots \sum_{m_r=n_r}^{N} a(m_1, \ldots, m_r) + \sum_{m_1=1}^{n_1} \cdots \sum_{m_r=n_{r-1}}^{n_r} a(m_1, \ldots, m_r) - E a(n_1, \ldots, n_r) \right] = 0.$$

But all the basis vectors are independent, so again we get an equation for every basis vector and we end up with

$$\boxed{\begin{aligned} &E a(n_1, \ldots, n_r) = \sum_{m_1=1}^{n_1} \sum_{m_2=n_1}^{n_2} \cdots \sum_{m_r=n_{r-1}}^{n_r} a(m_1, \ldots, m_r) + \sum_{m_1=n_1}^{n_2} \sum_{m_2=n_2}^{n_3} \cdots \sum_{m_r=n_r}^{N} a(m_1, \ldots, m_r), \\ &\forall j \in \{1, \ldots, r\} \;:\; a(n_1, \ldots, n_j, \ldots, n_r) = a(n_1, \ldots, n_j + N, \ldots, n_r), \end{aligned}} \tag{70}$$

where we added the periodic boundary conditions that we require from the lattice. Note that, just like in Eq. 68, coefficients in which not all m_i are different must be interpreted as zero. Note also the similarity with Eq. 41.

4.2 Solving the equation

It is time again to employ the Bethe Ansatz for the form of the coefficients $a(n_1, \dots, n_r)$. For this, we recall Definition 3.4. The **Bethe Ansatz** for general r and N now reads

Bethe Ansatz

$$a(n_1, \dots, n_r) = \sum_{P \in \mathcal{P}} \exp\left[\mathrm{i} \sum_{j=1}^{r} k_{Pj} n_j + \frac{1}{2} \mathrm{i} \sum_{j<q} \varphi_{Pj,Pq} \right] \tag{71}$$

where $\varphi_{j,l}$ is a priori just a real function of j and l of which we will derive the properties later. If we find all the solutions to our problem, then the ansatz is correct and we are done, and if we do not, then the ansatz is incorrect and we need to find the rest of the solutions.

Let us start by mentioning that the Bethe Ansatz (Eq. 71) states that the coefficients are a sum of plane waves

$$\exp\left[\mathrm{i} \sum_{j=1}^{r} k_{Pj} n_j + \frac{1}{2} \mathrm{i} \sum_{j<q} \varphi_{Pj,Pq} \right].$$

Therefore, let us take the easiest first step possible, and that is to insert the simplest possible form for $a(m_1, \dots, m_r)$ (i.e. the one for which $P = \mathrm{id}$ and $\varphi_{j,q} \equiv 0$, which is a plane wave),

$$\exp\left[\mathrm{i} \sum_{j=1}^{r} k_j n_j \right],$$

into Eq. 70 and see if this elementary example miraculously satisfies Eq. 70 for some E:

$$E \exp\left[\mathrm{i} \sum_{j=1}^{r} k_j n_j \right] = \sum_{m_1=n_1}^{n_2} \cdots \sum_{m_r=n_r}^{N} \exp\left[\mathrm{i} \sum_{j=1}^{r} k_j m_j \right] + \sum_{m_1=1}^{n_1} \cdots \sum_{m_r=n_{r-1}}^{n_r} \exp\left[\mathrm{i} \sum_{j=1}^{r} k_j m_j \right]. \tag{72}$$

We have to keep in mind to not count the terms where not all the m_i's are different. However, we see something more interesting here. For this plane wave to satisfy Eq. 70, i.e. for Eq. 72 to be true for some $E \in \mathbb{R}$, we need that the terms on the right are both (complex) multiples of the plane wave itself. This means that, first of all, all the terms on the right that do not depend on all the n_j's have to cancel each other out: we can just ignore counting those in the summations. Now we know this, we can comfortably go ahead and simplify the expression in Eq. 72 by noticing that (if we set $n_0 := 1$ and $n_{r+1} := N$ for now)

$$\begin{aligned}
\prod_{j=1}^{r} \frac{\mathrm{e}^{\mathrm{i}k_j n_{j-1}} - \mathrm{e}^{\mathrm{i}k_j (n_j+1)}}{1 - \mathrm{e}^{\mathrm{i}k_j}} &= \prod_{j=1}^{r} \mathrm{e}^{\mathrm{i}k_j n_{j-1}} \frac{1 - \left(\mathrm{e}^{\mathrm{i}k_j}\right)^{(n_j+1-n_{j-1})}}{1 - \mathrm{e}^{\mathrm{i}k_j}} = \prod_{j=1}^{r} \mathrm{e}^{\mathrm{i}k_j n_{j-1}} \left(\sum_{m=0}^{n_j - n_{j-1}} \mathrm{e}^{\mathrm{i}k_j m} \right) \\
&= \prod_{j=1}^{r} \left(\sum_{m=0}^{n_j - n_{j-1}} \mathrm{e}^{\mathrm{i}k_j (m + n_{j-1})} \right) = \prod_{j=1}^{r} \left(\sum_{m_j = n_{j-1}}^{n_j} \exp\left[\mathrm{i}k_j m_j\right] \right) \\
&= \sum_{m_1=n_1}^{n_2} \cdots \sum_{m_r=n_r}^{N} \exp\left[\mathrm{i} \sum_{j=1}^{r} k_j m_j \right]
\end{aligned}$$

and similarly

$$\prod_{j=1}^{r} \frac{\mathrm{e}^{\mathrm{i}k_j n_j} - \mathrm{e}^{\mathrm{i}k_j (n_{j+1}+1)}}{1 - \mathrm{e}^{\mathrm{i}k_j}} = \sum_{m_1=1}^{n_1} \cdots \sum_{m_r=n_{r-1}}^{n_r} \exp\left[\mathrm{i} \sum_{j=1}^{r} k_j m_j \right].$$

If we substitute these product expressions into Eq. 72, and we still impose that every term on the right has to depend on all the $k_j n_j$'s, then the only term that survives in the product

$$\prod_{j=1}^{r} \frac{\mathrm{e}^{\mathrm{i}k_j n_{j-1}} - \mathrm{e}^{\mathrm{i}k_j(n_j+1)}}{1-\mathrm{e}^{\mathrm{i}k_j}}$$

is the term we get when we choose to multiply all the $\mathrm{e}^{\mathrm{i}k_j(n_j+1)}$ with each other. Likewise, the only term that survives in the product

$$\prod_{j=1}^{r} \frac{\mathrm{e}^{\mathrm{i}k_j n_j} - \mathrm{e}^{\mathrm{i}k_j(n_{j+1}+1)}}{1-\mathrm{e}^{\mathrm{i}k_j}}$$

is the term we get when we choose to multiply all the $\mathrm{e}^{\mathrm{i}k_j n_j}$ with each other. Eq. 72 now becomes

$$E \exp\left[\mathrm{i}\sum_{j=1}^{r} k_j n_j\right] = \left(\prod_{j=1}^{r} \frac{1}{1-\mathrm{e}^{\mathrm{i}k_j}}\right)\left(1+(-1)^r \exp\left[\mathrm{i}\sum_{j=1}^{r} k_j\right]\right) \exp\left[\mathrm{i}\sum_{j=1}^{r} k_j n_j\right]. \tag{73}$$

This means that this would have an eigenvalue of

$$E = \left(\prod_{j=1}^{r} \frac{1}{1-\mathrm{e}^{\mathrm{i}k_j}}\right)\left(1+(-1)^r \exp\left[\mathrm{i}\sum_{j=1}^{r} k_j\right]\right) = \left(\prod_{j=1}^{r} \frac{1}{1-\mathrm{e}^{\mathrm{i}k_j}}\right)\left(1+(-1)^r\right), \tag{74}$$

where we used that the sum of all the k_j's is an integer multiple of 2π, according to the same translational argument made in the previous chapters. The following lemma is a citation from page 168 of [8], where I inserted the referred equations myself.

Lemma 4.10 (Citation)**.** *For every set of numbers $\{k_1, \ldots, k_r\}$ satisfying*

$$\forall j \in \{1, \ldots, r\} \ : \ \mathrm{e}^{\mathrm{i}k_j N} = (-1)^r \prod_{l=1}^{r} \left[\frac{\mathrm{e}^{k_j} - 1 - \mathrm{e}^{\mathrm{i}(k_j+k_l)}}{\mathrm{e}^{k_l} - 1 - \mathrm{e}^{\mathrm{i}(k_j+k_l)}}\right] \tag{75}$$

and such that no $k_j = 0$, we have a solution to the eigenvalue problem with an eigenvalue given by Eq. 74.

Proof. See {[8], pp 165-168} for the full proof. □

In a similar way as in the previous chapter, we can show that

$$\frac{\mathrm{e}^{k_j} - 1 - \mathrm{e}^{\mathrm{i}(k_j+k_l)}}{\mathrm{e}^{k_l} - 1 - \mathrm{e}^{\mathrm{i}(k_j+k_l)}} = \mathrm{e}^{-\mathrm{i}\varphi_{j,l}}. \tag{76}$$

We can easily see that $k_j \neq 0$ should hold, because otherwise the first factor of the right-hand side of the eigenvalue equation (Eq. 73) would diverge. Note that Lemma 4.10 gives us all the solutions (by counting how many solutions it gives us), so every solution $\{k_1, \ldots, k_r\}$ satisfies Eq. 75. A closer look at this equation lets us rewrite it as

$$\forall j \in \{1, \ldots, r\} \ : \ N k_j = -\pi r + 2\pi(j-1) - \sum_{l=1}^{r} \varphi_{k_j,k_l} \tag{77}$$

by taking the logarithm. Note that

$$k_j \in \mathbb{R}. \tag{78}$$

We can now state the following minor result.

Lemma 4.11. *The k_j's are symmetrically distributed, i.e.*

$$\forall j \in \{1, \ldots, r\} \ : \ k_j = -k_{r-j+1}. \tag{79}$$

Proof. We can calculate

$$N\left(k_j + k_{r-j+1}\right) = -\sum_{l=1}^{r}\left[\varphi_{k_j,k_l} + \varphi_{k_{r-j+1},k_l}\right] = -\sum_{l=1}^{r}\left[\varphi_{k_j,k_l} + \varphi_{k_{r-j+1},k_{r-l+1}}\right]$$
$$= -\sum_{l=1}^{r}\left[\varphi_{k_j,k_l} + \varphi_{k_l,k_j}\right] = -\sum_{l=1}^{r}\left[\varphi_{k_j,k_l} - \varphi_{k_j,k_l}\right] = 0$$

where we used that $\varphi_{k_j,k_l} = -\varphi_{k_l,k_j}$ from Eq. 76. □

We will use this later.
This is the point at which we want to narrow down our discussion to only infinitely big systems, i.e. we assume that $M, N \to \infty$. We do this because only in this limit is this problem solvable, and the physical application of real water ice will have $MN \simeq 10^{23}$, so $M, N \simeq 10^{11}$, so this is the system we are the most interested in.

4.3 Assuming a large system

From now on, we take the limit $N \to \infty$ and then $M \to \infty$. In this large system, we have $|\{k\}|, r, N \to \infty$, and therefore, we assume that the k's act as if they form a density function $\rho(k)$.

Definition 4.12. If there exists a density function of k, then we define it more accurately as

$$\rho(k) = \lim_{\substack{N\to\infty \\ N\mathrm{d}k=C}} \frac{1}{N\mathrm{d}k}\Big|\left\{k_j \in \{k\} \;\Big|\; k \le k_j < k + \mathrm{d}k\Big|\right\}\Big|, \tag{80}$$

where $C \in \mathbb{R}_{>0}$ ◁

We can now write Eq. 77 as

$$\begin{aligned}
k_j &= \frac{1}{N}\left[-\pi r + 2\pi(j-1)\right] - \frac{1}{N}\sum_{l=1}^{r}\varphi_{k_j,k_l} \\
&= \frac{\pi}{N}(2j - r - 2) - \sum_{q=k_1}^{k_r}\frac{1}{N}\varphi_{k_j,q} \\
&\overset{N\to\infty}{\to} \frac{\pi}{N}(2j - r - 2) - \int_a^b \frac{1}{N}\varphi_{k_j,q}\left|\left\{k_l \in \{k\} \;\big|\; q \le k_l < q + \mathrm{d}q\big|\right\}\right| \\
&= \frac{\pi}{N}(2j - r - 2) - \int_a^b \varphi_{k_j,q}\rho(q)\mathrm{d}q,
\end{aligned}$$

where we used Definition 4.12 in the last step, and $a, b \in \mathbb{R}$ are the boundaries of the integral that we will figure out later. First, let us take the derivative to k_j of the above equation, which we can do because we're assuming a large system and a continuous set of $\{k\}$:

$$\begin{aligned}
1 &= \frac{\mathrm{d}\frac{\pi}{N}(2j - r - 2)}{\mathrm{d}k_j} - \frac{\mathrm{d}}{\mathrm{d}k_j}\int_a^b \varphi_{k_j,q}\rho(q)\mathrm{d}q \\
&= \pi\frac{\partial(2j - r - 2)/N}{\partial j}\frac{\mathrm{d}j}{\mathrm{d}k_j} - \int_a^b \frac{\partial\varphi_{k_j,q}\rho(q)}{\partial k_j}\mathrm{d}q \\
&= \frac{2\pi}{N}\frac{\mathrm{d}j}{\mathrm{d}k_j} - \int_a^b \frac{\partial\varphi_{k_j,q}\rho(q)}{\partial k_j}\mathrm{d}q \\
&= \lim_{\mathrm{d}k\to 0}\frac{2\pi}{N}\frac{j(k_j + \mathrm{d}k) - j(k_j)}{\mathrm{d}k} - \int_a^b \frac{\partial\varphi_{k_j,q}\rho(q)}{\partial k_j}\mathrm{d}q \\
&= \lim_{\mathrm{d}k\to 0} 2\pi\frac{\left|\left\{k_l \in \{k_1, \ldots, k_r\} \;\big|\; k_l \le j < k_l + \mathrm{d}k\right\}\right|}{N\mathrm{d}k} - \int_a^b \frac{\partial\varphi_{k_j,q}\rho(q)}{\partial k_j}\mathrm{d}q,
\end{aligned}$$

and using Definition 4.12, we get

$$1 = 2\pi\rho(k_j) - \int_a^b \frac{\partial \varphi_{k_j,q}\rho(q)}{\partial k_j} \mathrm{d}q.$$

But the k_j's are symmetrically distributed (Lemma 4.11), so there exists a $Q \in \mathbb{R}$ such that

$$1 = 2\pi\rho(k_j) - \int_{-Q}^{Q} \frac{\partial \varphi_{k_j,q}}{\partial k_j} \rho(q) \mathrm{d}q. \tag{81}$$

We notice that we include all the k_j's (i.e. $k_1, \ldots, k_r$) in our calculations (see the summation in Eq. 77), so we determine Q from

$$\int_{-Q}^{Q} \rho(q)\, \mathrm{d}q = \frac{1}{N} \left|\left\{k_l \in \{k\} \;\middle|\; -Q \leq k_l < Q\right\}\right| = \frac{|\{k\}|}{N} = \frac{r}{N}. \tag{82}$$

Let us step back for a second now and remind ourselves what the goal of this calculation is, which is to find the entropy of the square ice system. According to Theorem 4.9 and Definition 4.1,

$$S = k_b \log\left(\mathrm{Tr}\left(A^M\right)\right) = k_b \log\left(\sum_{E\in\sigma_A} E^M\right), \tag{83}$$

where σ_A denotes the spectrum of A. As we are assuming a large system here, $M \to \infty$, so to find the entropy, we need to find the eigenvalues of A with the biggest absolute value. From here, we want to make a claim, which we will prove later.

Hypothesis 3. *The eigenvalues of A that are greatest in absolute value lie in the subspace $r = N/2$.*

Of course we will be careful not to use any facts based on this hypothesis to prove the hypothesis. We assume that the hypothesis is true from this point on, and immediately, we find that the largest eigenvalue is unique.

Lemma 4.13. *There exists a unique eigenvalue $E_{\max}$ of A of which the absolute value is strictly bigger than all other eigenvalues of A.*

Proof. The $r = N/2$ subspace, which we will call $A_{N/2}$ here, has no non-trivial invariant subspace, i.e. if A works on a vector with r arrows pointing down, then the outcome will be a superposition of vectors with r arrows pointing down. We already knew this. This means that the block $r = N/2$, i.e. $A_{N/2}$, is an irreducible matrix. We also know that A is a reducible matrix. To summarize what we know: A is nonnegative and reducible, $A_{N/2}$ is nonnegative and irreducible and $\mathrm{Tr}\left(A_{N/2}\right) > 0$ because the diagonal elements are all 2. By Corollary 2.2.28 of [11], the matrix $A_{N/2}$ is primitive[6] because it is irreducible and its trace is positive. Now denote the spectral radius of a matrix X by $\rho_s(X)$. Then, by Theorem 2.1.7 of [11], $\rho_s\left(A_{N/2}\right)$ is greater in absolute value than any other eigenvalue, because $A_{N/2}$ is nonnegative and primitive. We call the eigenvalue of $A_{N/2}$ that is biggest in absolute value $E_{\max}$, and because we assume Hypothesis 3, this proves the lemma. □

We recall that we wrote the entropy of our system as

$$S = MNk_b \log(W),$$

so, looking at Eq. 83, the following must hold:

$$\log(W) = \lim_{N\to\infty} \frac{1}{N} \log\left(E_{\max}\right). \tag{84}$$

[6] A matrix X is primitive if and only if there exists an $m \in \mathbb{N}$ such that X^m is positive, i.e. X^m has only positive entries.

But we have an expression for the eigenvalues $E(r)$ as a function of r in Eq. 74, so we can actually calculate this:

$$\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right) = \lim_{N\to\infty}\frac{1}{N}\log\left(\left(\prod_{j=1}^{r}\frac{1}{1-\mathrm{e}^{\mathrm{i}k_j}}\right)\left(1+(-1)^r\right)\right)$$
$$= \lim_{N\to\infty}\frac{1}{N}\log\left(\prod_{j=1}^{r}\frac{1}{1-\mathrm{e}^{\mathrm{i}k_j}}\right)+\frac{1}{N}\log\left[1+(-1)^r\right].$$

But, we can choose r to be even. In this large system this is not a problem: we are taking the limit $N\to\infty$, so taking $r' := 2r$ and $N' := 2N$ will not change the properties of our system, and r' will always be even. Also, r is of the scale of N, so we can omit the second term. Furthermore, according to Lemma 4.11, we can order the k_j's such that we have

$$\prod_{j=1}^{r}\frac{1}{1-\mathrm{e}^{\mathrm{i}k_j}} = \prod_{j=1}^{r/2}\frac{1}{\left(1-\mathrm{e}^{\mathrm{i}k_j}\right)\left(1-\mathrm{e}^{-\mathrm{i}k_j}\right)} = \prod_{j=1}^{r/2}\left|\frac{1}{\left(1-\mathrm{e}^{\mathrm{i}k_j}\right)}\right|^2 = \prod_{j=1}^{r}\left|\frac{1}{\left(1-\mathrm{e}^{\mathrm{i}k_j}\right)}\right|.$$

We are left with

$$\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right) = -\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{r}\log\left|1-\mathrm{e}^{\mathrm{i}k_j}\right|$$
$$= -\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{r}\log\left|\frac{1}{i}\left(\mathrm{e}^{-\mathrm{i}k_j/2}-\mathrm{e}^{\mathrm{i}k_j/2}\right)\right|$$
$$= -\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{r}\log\left|2\sin\left(k_j/2\right)\right|$$
$$= -\frac{1}{2}\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{r}\log(4\sin^2(k_j/2))$$
$$= -\frac{1}{2}\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{r}\log(2-2\cos(k_j)).$$

If we now make the same conversion to an integral form as we did earlier, we get

$$\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right) = -\frac{1}{2}\int_{-Q}^{Q}\log\left[2-2\cos\left(q\right)\right]\rho(q)\,\mathrm{d}q. \tag{85}$$

Lieb ([8]) now suggests a coordinate transformation that we will use here as well. He sets

$$\mu := \frac{2}{3}\pi \tag{86}$$

and defines α by

$$\mathrm{e}^{\alpha} := \frac{\mathrm{e}^{\mathrm{i}\mu}+\mathrm{e}^{\mathrm{i}k_j}}{1+\mathrm{e}^{\mathrm{i}\mu+\mathrm{i}k_j}} \tag{87}$$

such that

$$\mathrm{e}^{\mathrm{i}k_j} = \frac{\mathrm{e}^{\mathrm{i}\mu}-\mathrm{e}^{\alpha}}{\mathrm{e}^{\mathrm{i}\mu+\alpha}-1}. \tag{88}$$

We see that

$$\mathrm{e}^{\alpha} = \frac{(\mathrm{e}^{\mathrm{i}\mu}+\mathrm{e}^{\mathrm{i}k_j})(1+\mathrm{e}^{-\mathrm{i}\mu-\mathrm{i}k_j})}{(1+\mathrm{e}^{\mathrm{i}\mu+\mathrm{i}k_j})(1+\mathrm{e}^{-\mathrm{i}\mu-\mathrm{i}k_j})} = \frac{\mathrm{e}^{\mathrm{i}\mu}+\mathrm{e}^{-\mathrm{i}k_j}+\mathrm{e}^{\mathrm{i}k_j}+\mathrm{e}^{-\mathrm{i}\mu}}{|1+\mathrm{e}^{\mathrm{i}\mu+\mathrm{i}k_j}|^2} = \frac{2(\cos(\mu)+\cos(k_j))}{|1+\mathrm{e}^{\mathrm{i}\mu+\mathrm{i}k_j}|^2}.$$

Like {[6] Eq. 9 and Eq. 10}, we will **assume** that

$$\textbf{Assumption: } \forall j \in \{1, \ldots, r\} \ : \ -(\pi - \mu) < k_j < \pi - \mu \quad \text{where } \mu = \frac{2}{3}\pi \text{ as in the above.} \tag{89}$$

Again, if we find all the solutions, then this assumption is justified.
We see that $\mathrm{e}^{\alpha} \in \mathbb{R}$ and $\mathrm{e}^{\alpha} > 0$, so $\alpha \in \mathbb{R}$ and α runs from $-\infty$ to ∞.
Lieb ([8]) also suggests introducing a few functions.

Definition 4.14. Define the following functions.

$$R \ : \ \mathbb{R} \to \mathbb{R}, \ R(\alpha)\mathrm{d}\alpha := 2\pi\rho(k_j)\mathrm{d}k_j, \tag{90}$$

$$\xi \ : \ \mathbb{R} \to \mathbb{R}, \ \xi(\alpha) := \frac{\sin(\mu)}{\cosh(\alpha) - \cos(\mu)}, \tag{91}$$

$$K \ : \ \mathbb{R} \to \mathbb{R}, \ K(\alpha) := \frac{\sin(2\mu)}{2\pi(\cosh(\alpha) - \cos(2\mu))}. \tag{92}$$

◁

With this transformation and these new functions, the integral equation Eq. 81 becomes

$$R(\alpha) = 2\pi\rho(k_j)\frac{\mathrm{d}k_j}{\mathrm{d}\alpha} = \frac{\mathrm{d}k_j}{\mathrm{d}\alpha} + \frac{\mathrm{d}k_j}{\mathrm{d}\alpha}\int_{-Q}^{Q} \frac{\partial\varphi_{k_j,q}}{\partial k_j}\rho(q)\mathrm{d}q = \frac{\mathrm{d}k_j}{\mathrm{d}\alpha} + \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\partial\varphi_{k_j,q}}{\partial\alpha}R(\beta)\,\mathrm{d}\beta.$$

In Appendix B.1 it is shown that from Eq. 88 it follows that

$$\frac{\mathrm{d}k_j}{\mathrm{d}\alpha} = \frac{\sin(\mu)}{\cosh(\alpha) - \cos(\mu)}.$$

However, to proceed from here, we will have to figure out an expression for $\varphi_{k_j,q}$. With rewriting of Eq. 76 similar to how we did it in the previous chapters, we get the following expression:

$$\cot\left(\frac{\varphi_{k,q}}{2}\right) = \frac{\cos\left[(k+q)/2\right] - \frac{1}{2}\cos\left[(k-q)/2\right]}{\frac{1}{2}\sin\left[(k-q)/2\right]}. \tag{93}$$

In Appendix B.2 it is shown that then

$$\frac{\partial\varphi}{\partial\beta} = \frac{\sin(2\mu)}{\cosh(\alpha-\beta) - \cos(2\mu)} = -\frac{\partial\varphi}{\partial\alpha}.$$

Thus, we get for $R(\alpha)$, keeping in mind that $\mu = \frac{2}{3}\pi$:

$$\begin{aligned} R(\alpha) &= \frac{\sin(\mu)}{\cosh(\alpha) - \cos(\mu)} - \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\sin(2\mu)}{\cosh(\alpha-\beta) - \cos(2\mu)}R(\beta)\,\mathrm{d}\beta \\ &= \xi(\alpha) - \int_{-\infty}^{\infty} K(\alpha-\beta)R(\beta)\,\mathrm{d}\beta. \end{aligned} \tag{94}$$

Again, we remind ourselves of the fact that we want to know the entropy, so we want to know $E_{\max}$, so we want to solve Eq. 85, which we can now rewrite in terms of α as

$$\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right) = -\frac{1}{4\pi}\int_{-\infty}^{\infty}\log\left(1 - \frac{3}{1+2\cosh(\alpha)}\right)R(\alpha)\,\mathrm{d}\alpha, \tag{95}$$

as shown in Appendix B.3. We can now prove that Hypothesis 3 was correct.

Lemma 4.15. *The largest eigenvalue corresponds to an eigenvector with $r = N/2$.*

Proof. Let us begin by mentioning that if $r = N/2$, then the integration limits in Eq. 95 are from $-\infty$ to ∞. Thus, if $r < N/2$, then the integration domain can only get smaller.
We also know that

$$R(\alpha) = 2\pi\rho(k_j)\frac{\mathrm{d}k_j}{\mathrm{d}\alpha} = 2\pi\rho(k_j)\frac{\sin(\mu)}{\cosh(\alpha) - \cos(\mu)} > 0,$$

because $\sin(\mu) = \frac{1}{2}\sqrt{3} > 0$ and $\cosh(\alpha) - \cos(\mu) \geq \frac{3}{2} > 0$. Then, by the argumentation in ([7] 2.C, page 329) and by Eq. (9b) in [7],

$$\frac{\mathrm{d}R(\alpha)}{\mathrm{d}b} > 0,$$

where $(-b, b)$ is the integration domain over α. Thus, if $r \neq N/2$, then the integration domain must be smaller than (or equal to) $(-\infty, \infty)$, and $R(\alpha)$ will be smaller than (or equal to) its value at $r = N/2$. This means that $\log(E(r))$ will be smaller than or equal to the $\log(E(r))$ at $r = N/2$, and because the logarithm is an increasing function, this means that the maximum eigenvalue $E(r)$ will be of an eigenvector with $r = N/2$, which was to be proven. □

Looking at Eq. 95, we see that we want to know $R(\alpha)$, so we want to solve Eq. 94. This can be done using Fourier transformations, and the full proof of the following Lemma is shown in Appendix B.4.

Lemma 4.16. *The solution to Eq. 94 is given by*

$$R(\alpha) = \frac{\pi}{2\mu\cosh\left(\frac{\pi\alpha}{2\mu}\right)}. \tag{96}$$

Proof. Please see Appendix B.4. □

Now we can continue our calculation in Eq. 95, using $\mu = \frac{2}{3}\pi$:

$$\begin{aligned}\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right) &= -\frac{1}{4\pi}\int_{-\infty}^{\infty}\log\left(1 - \frac{3}{1 + 2\cosh(\alpha)}\right)\frac{\pi}{2\mu\cosh\left(\frac{\pi\alpha}{2\mu}\right)}\,\mathrm{d}\alpha \\ &= -\frac{3}{16\pi}\int_{-\infty}^{\infty}\log\left(1 - \frac{3}{1 + 2\cosh(\alpha)}\right)\frac{1}{\cosh\left(\frac{3\alpha}{4}\right)}\,\mathrm{d}\alpha.\end{aligned}$$

We see that we are dealing with $\cosh(3\alpha/4) = f(\mathrm{e}^{\alpha/4})$, so we make the substitution $x = \mathrm{e}^{\alpha/4}$, which gives us $4\mathrm{d}x/x = \mathrm{d}\alpha$, so we are left with

$$\begin{aligned}\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right) &= -\frac{3}{4\pi}\int_{0}^{\infty}\frac{1}{x}\log\left(1 - \frac{3}{1 + x^4 + x^{-4}}\right)\frac{2}{x^3 + x^{-3}}\mathrm{d}x \\ &= -\frac{3}{2\pi}\int_{0}^{\infty}\log\left(\frac{x^8 - 2x^4 + 1}{x^4 + x^8 + 1}\right)\frac{x^2}{x^6 + 1}\mathrm{d}x \\ &= -\frac{3}{4\pi}\int_{-\infty}^{\infty}\log\left(\frac{(x^2 - 1)^2(x^2 + 1)^2}{x^8 + x^4 + 1}\right)\frac{x^2}{x^6 + 1}\mathrm{d}x \\ &= -\frac{3}{2\pi}\int_{-\infty}^{\infty}\log\left[(x + 1)(x - 1)(x + i)(x - i)\right]\frac{x^2}{x^6 + 1}\mathrm{d}x \\ &\quad + \frac{3}{4\pi}\int_{-\infty}^{\infty}\log\left(x^8 + x^4 + 1\right)\frac{x^2}{x^6 + 1}\mathrm{d}x.\end{aligned}$$

We want to employ complex analysis here, so we want to know the residues of the integrand. This is straightforward but a lot of effort, so we refer to Appendix B.5 for the full calculation of the integral. The result derived there is

$$\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right) = \frac{3}{2}\log\left(\frac{4}{3}\right). \tag{97}$$

Now, according to Eq. 84:

$$W = \left(\frac{4}{3}\right)^{3/2}. \tag{98}$$

If we evaluate this numerically, we get, to five significant figures,

$$W \simeq 1.5396. \tag{99}$$

This is in agreement with the measurements of Giauque and Ashley in Eq. 58, but it is also in excellent agreement with the estimation by Nagle provided in Eq. 59, which reads $W = 1.540 \pm 0.001$.

We set out to find out what the entropy of our system was, and we found the answer. The entropy of our system is given by Eq. 57:

$$\boxed{S = \frac{3}{2} M N k_b \log\left(\frac{4}{3}\right).}$$

The overall method in this chapter is based on [8]: the theorems and lemmas are inspired by remarks in this paper, while the proofs are my work.

5 Conclusion

The goal of this thesis was to investigate two physical models and their corresponding main questions, and use the Bethe Ansatz to answer these questions mathematically. We found that in both models, the Bethe Ansatz turned out to not only give us a few solutions, but actually all of them. In the Heisenberg model of spins, in the special case of only two spins down, we constructed the Bethe Ansatz quite intuitively, and we were able to set up equations that were solvable numerically. The generalization to more spins down was a logical step from there, one which we could not have guessed if we did not already do the special case first. We showed that all wave functions are of the form of the Bethe Ansatz. Unfortunately, we were not able to calculate any exact solutions for a general number of spins down. However, in principle we got the eigenfunctions of the Hamiltonian $\mathcal{H}$, and thus its eigenvalues, and with that we also got the eigenvalues of any operator that is a conserved quantity.

In the Square Ice model, we found an equation for the eigenvalues of the M-th power of our transfer matrix, and it looked a lot like the eigenvalue equation of our Hamiltonian in the Heisenberg model. Naturally, we used the Bethe Ansatz again, and we found that indeed all configurations of ice can be written in this form. We were even able to calculate exact solutions if we let the size of our lattice go to infinity. This was a reasonably good approximation, as most physical systems we are concerned about consist of around 10^{23} atoms, which corresponds to 10^{23} lattice sites in our model, which makes the length and width of our lattice about 10^{11} vertices.

In short, using the Bethe Ansatz, we were able to calculate the energy of a Heisenberg spin chain, and the entropy of Square Ice. We found an exact solution for the latter, given an infinitely big system. Clearly, the Bethe Ansatz is very useful indeed in different fields of physics and mathematics, and seemingly different systems with different problems can sometimes be solved in a very similar way.

Appendices

A Proofs regarding the Heisenberg spin chain model

A.1 Proving $|A| = |B|$

We prove that

$$\left|\frac{A}{B}\right| := \left|-\frac{2e^{\mathrm{i}k_1} - 1 - e^{\mathrm{i}(k_1+k_2)}}{2e^{\mathrm{i}k_2} - 1 - e^{\mathrm{i}(k_1+k_2)}}\right| = 1.$$

Proof. This is just a matter of smartly rewriting things:

$$\begin{aligned}\frac{2e^{\mathrm{i}k_1} - 1 - e^{\mathrm{i}(k_1+k_2)}}{2e^{\mathrm{i}k_2} - 1 - e^{\mathrm{i}(k_1+k_2)}} &= \frac{2e^{\mathrm{i}\frac{k_1-k_2}{2}} - e^{-\mathrm{i}\frac{k_1+k_2}{2}} - e^{\mathrm{i}\frac{k_1+k_2}{2}}}{2e^{-\mathrm{i}\frac{k_1-k_2}{2}} - e^{-\mathrm{i}\frac{k_1+k_2}{2}} - e^{\mathrm{i}\frac{k_1+k_2}{2}}} = \frac{e^{\mathrm{i}\frac{k_1-k_2}{2}} - \cos\left(\frac{k_1+k_2}{2}\right)}{e^{-\mathrm{i}\frac{k_1-k_2}{2}} - \cos\left(\frac{k_1+k_2}{2}\right)} \\ &= \frac{\cos\left(\frac{k_1-k_2}{2}\right) - \cos\left(\frac{k_1+k_2}{2}\right) + \mathrm{i}\sin\left(\frac{k_1-k_2}{2}\right)}{\cos\left(-\frac{k_1-k_2}{2}\right) - \cos\left(\frac{k_1+k_2}{2}\right) + \mathrm{i}\sin\left(-\frac{k_1-k_2}{2}\right)}.\end{aligned}$$

This means for the norm that

$$\left|\frac{2e^{\mathrm{i}k_1} - 1 - e^{\mathrm{i}(k_1+k_2)}}{2e^{\mathrm{i}k_2} - 1 - e^{\mathrm{i}(k_1+k_2)}}\right|^2 = \frac{\left[\cos\left(\frac{k_1-k_2}{2}\right) - \cos\left(\frac{k_1+k_2}{2}\right)\right]^2 + \sin^2\left(\frac{k_1-k_2}{2}\right)}{\left[\cos\left(-\frac{k_1-k_2}{2}\right) - \cos\left(\frac{k_1+k_2}{2}\right)\right]^2 + \sin^2\left(-\frac{k_1-k_2}{2}\right)} = 1,$$

which proves that $\left|\frac{A}{B}\right| = 1$. □

A.2 Proving the relation for φ

If we write $A = e^{\mathrm{i}\varphi/2}$ and $B = e^{-\mathrm{i}\varphi/2}$, then we want to know how φ depends on k_1 and k_2. We determine this dependence in the following, using $A = 2e^{\mathrm{i}k_1} - 1 - e^{\mathrm{i}(k_1+k_2)}$ and $B = -\left(2e^{\mathrm{i}k_2} - 1 - e^{\mathrm{i}(k_1+k_2)}\right)$. We can choose A and B like this, because now $|A| = |B|$, and the overall phase angle of A and B does not matter, because it does not change the physics of our problem. We calculate

$$\begin{aligned}2\cot\left(\frac{\varphi}{2}\right) &= 2\mathrm{i}\,\frac{e^{\mathrm{i}\varphi/2} + e^{-\mathrm{i}\varphi/2}}{e^{\mathrm{i}\varphi/2} - e^{-\mathrm{i}\varphi/2}} = 2\mathrm{i}\,\frac{A+B}{A-B} = 2\mathrm{i}\,\frac{e^{\mathrm{i}k_1} - e^{\mathrm{i}k_2}}{e^{\mathrm{i}k_1} + e^{\mathrm{i}k_2} - 1 - e^{\mathrm{i}(k_1+k_2)}} \\ &= \mathrm{i}\left[\frac{e^{\mathrm{i}k_1/2} + e^{-\mathrm{i}k_1/2}}{e^{\mathrm{i}k_1/2} - e^{-\mathrm{i}k_2/2}} - \frac{e^{\mathrm{i}k_2/2} + e^{-\mathrm{i}k_2/2}}{e^{\mathrm{i}k_2/2} - e^{-\mathrm{i}k_2/2}}\right] = \cot\left(\frac{k_1}{2}\right) - \cot\left(\frac{k_2}{2}\right).\end{aligned}$$

A.3 Energy of $r = 2$ case with neighbouring spins down

We restate Eq. 17, writing the coefficients in the form of the Bethe Ansatz, and derive the energy of the $r = 2$ case with the two spins down neighbouring each other.

$$\begin{aligned}&\frac{2}{J}(E - E_0)\left(Ae^{\mathrm{i}((k_1+k_2)n+k_2)} + Be^{\mathrm{i}((k_1+k_2)n+k_1)}\right) \\ &= 2\left(Ae^{\mathrm{i}((k_1+k_2)n+k_2)} + Be^{\mathrm{i}((k_1+k_2)n+k_1)}\right) - A\left(e^{-\mathrm{i}k_1} + e^{\mathrm{i}k_2}\right)e^{\mathrm{i}((k_1+k_2)n+k_2)} - B\left(e^{-\mathrm{i}k_2} + e^{\mathrm{i}k_1}\right)e^{\mathrm{i}((k_1+k_2)n+k_1)} \\ \Longleftrightarrow\ &\frac{2}{J}(E - E_0)\left(\frac{A}{B}e^{\mathrm{i}k_2} + e^{\mathrm{i}k_1}\right) = 2\left(\frac{A}{B}e^{\mathrm{i}k_2} + e^{\mathrm{i}k_1}\right) - \frac{A}{B}\left(e^{-\mathrm{i}k_1} + e^{\mathrm{i}k_2}\right)e^{\mathrm{i}k_2} - \left(e^{-\mathrm{i}k_2} + e^{\mathrm{i}k_1}\right)e^{\mathrm{i}k_1}.\end{aligned}$$

We recall now that $\frac{A}{B} = -\frac{2e^{\mathrm{i}k_1} - 1 - e^{\mathrm{i}(k_1+k_2)}}{2e^{\mathrm{i}k_2} - 1 - e^{\mathrm{i}(k_1+k_2)}}$, so we will substitute this into our equation so we can express E in terms of E_0, J, k_1 and k_2.

$$\begin{aligned}&\frac{2}{J}(E - E_0)\left(-\frac{2e^{\mathrm{i}k_1} - 1 - e^{\mathrm{i}(k_1+k_2)}}{2e^{\mathrm{i}k_2} - 1 - e^{\mathrm{i}(k_1+k_2)}}e^{\mathrm{i}k_2} + e^{\mathrm{i}k_1}\right) \\ &= 2\left(-\frac{2e^{\mathrm{i}k_1} - 1 - e^{\mathrm{i}(k_1+k_2)}}{2e^{\mathrm{i}k_2} - 1 - e^{\mathrm{i}(k_1+k_2)}}e^{\mathrm{i}k_2} + e^{\mathrm{i}k_1}\right) + \frac{2e^{\mathrm{i}k_1} - 1 - e^{\mathrm{i}(k_1+k_2)}}{2e^{\mathrm{i}k_2} - 1 - e^{\mathrm{i}(k_1+k_2)}}\left(e^{-\mathrm{i}k_1} + e^{\mathrm{i}k_2}\right)e^{\mathrm{i}k_2} - \left(e^{-\mathrm{i}k_2} + e^{\mathrm{i}k_1}\right)e^{\mathrm{i}k_1}\end{aligned}$$

Multiplying both sides with B now yields

$$\begin{aligned}
&\frac{2}{J}(E-E_0)\left(e^{\mathrm{i}k_2}+e^{\mathrm{i}(k_1+2k_2)}-e^{\mathrm{i}k_1}-e^{\mathrm{i}(2k_1+k_2)}\right)\\
&=4\left(e^{\mathrm{i}k_2}+e^{\mathrm{i}(k_1+2k_2)}-e^{\mathrm{i}k_1}-e^{\mathrm{i}(2k_1+k_2)}\right)+e^{\mathrm{i}(k_1-k_2)}-e^{\mathrm{i}(k_2-k_1)}+2e^{2\mathrm{i}k_1}-2e^{2\mathrm{i}k_2}-e^{\mathrm{i}(k_1+3k_2)}+e^{\mathrm{i}(k_2+3k_1)}\\
\iff &\frac{2}{J}(E-E_0)=4-\frac{\left(e^{-\mathrm{i}(k_1+k_2)}+2+e^{\mathrm{i}(k_1+k_2)}\right)\left(e^{2\mathrm{i}k_1}-e^{2\mathrm{i}k_2}\right)}{\left(1+e^{\mathrm{i}(k_1+k_2)}\right)\left(e^{\mathrm{i}k_1}-e^{\mathrm{i}k_2}\right)}
\end{aligned}$$

Now we mention that $a^2-b^2=(a+b)(a-b)$, so we can divide some things out:

$$\begin{aligned}
\frac{2}{J}(E-E_0)&=4-\frac{\left(e^{-\mathrm{i}(k_1+k_2)}+2+e^{\mathrm{i}(k_1+k_2)}\right)\left(e^{\mathrm{i}k_1}+e^{\mathrm{i}k_2}\right)}{1+e^{\mathrm{i}(k_1+k_2)}}\\
&=4-\frac{\left(e^{\mathrm{i}(k_1+k_2)/2}+e^{-\mathrm{i}(k_1+k_2)/2}\right)^2\left(e^{\mathrm{i}k_1}+e^{\mathrm{i}k_2}\right)}{\left(e^{\mathrm{i}(k_1+k_2)/2}+e^{-\mathrm{i}(k_1+k_2)/2}\right)e^{\mathrm{i}(k_1+k_2)/2}}\\
&=4-\left(e^{\mathrm{i}(k_1+k_2)/2}+e^{-\mathrm{i}(k_1+k_2)/2}\right)\left(e^{\mathrm{i}k_1}+e^{\mathrm{i}k_2}\right)e^{-\mathrm{i}(k_1+k_2)/2}\\
&=4-\left(2\cos(k_1)+2\cos(k_2)\right).
\end{aligned}$$

We get for the energy of the system with neighbouring spins down for $r=2$:

$$E-E_0=J\sum_{j=1}^{2}\left[1-\cos(k_j)\right]. \tag{100}$$

A.4 Proving the partial derivatives of φ

We can write the relation for φ as follows:

$$\varphi=2\,\mathrm{arccot}\left(\frac{1}{2}\left[\cot\left(\frac{k_1}{2}\right)-\cot\left(\frac{k_2}{2}\right)\right]\right). \tag{101}$$

A few derivatives that are handy to know are:

$$\frac{\mathrm{d}\,\mathrm{arccot}(x)}{\mathrm{d}x}=-\frac{1}{1+x^2}\ ,\ \frac{\mathrm{d}\cot(x)}{\mathrm{d}x}=-\frac{1}{\sin^2(x)}.$$

We compute, for $k_1,k_2\in\mathbb{R}-2\pi\mathbb{Z}$:

$$\begin{aligned}
\frac{\partial\varphi}{\partial k_1}&=2\frac{-1}{1+\left(\frac{1}{2}\left[\cot\left(\frac{k_1}{2}\right)-\cot\left(\frac{k_2}{2}\right)\right]\right)^2}\cdot\frac{-1}{2}\frac{1}{\sin^2\left(\frac{k_1}{2}\right)}\cdot\frac{1}{2}\\
&=\frac{1}{2}\frac{1}{1+\left(\frac{1}{2}\left[\cot\left(\frac{k_1}{2}\right)-\cot\left(\frac{k_2}{2}\right)\right]\right)^2}\frac{1}{\sin^2\left(\frac{k_1}{2}\right)}>0,\\
\frac{\partial\varphi}{\partial k_2}&=-\frac{1}{2}\frac{1}{1+\left(\frac{1}{2}\left[\cot\left(\frac{k_1}{2}\right)-\cot\left(\frac{k_2}{2}\right)\right]\right)^2}\frac{1}{\sin^2\left(\frac{k_2}{2}\right)}<0.
\end{aligned}$$

B Proofs regarding the Square Ice model

B.1 Proving $\frac{\mathrm{d}k_j}{\mathrm{d}\alpha} = \frac{\sin(\mu)}{\cosh(\alpha)-\cos(\mu)}$

We write $k_j = k$ and we calculate, using Eq. 88

$$\begin{aligned}
\frac{\mathrm{d}k}{\mathrm{d}\alpha} &= \frac{\mathrm{d}k}{\mathrm{d}e^{\mathrm{i}k}}\frac{\mathrm{d}e^{\mathrm{i}k}}{\mathrm{d}e^{\alpha}}\frac{\mathrm{d}e^{\alpha}}{\mathrm{d}\alpha} = -\mathrm{i}\frac{e^{\alpha}}{e^{\mathrm{i}k}}\frac{\mathrm{d}\left(\frac{e^{\mathrm{i}\mu}-x}{e^{\mathrm{i}\mu}x-1}\right)}{\mathrm{d}x}\Bigg|_{x=e^{\alpha}} \\
&= \mathrm{i}\frac{e^{\alpha}}{e^{\mathrm{i}k}}\frac{\left(e^{\mathrm{i}\mu}e^{\alpha}-1\right)+\left(e^{\mathrm{i}\mu}-e^{\alpha}\right)e^{\mathrm{i}\mu}}{\left(e^{\mathrm{i}\mu}e^{\alpha}-1\right)^2} \\
&= \mathrm{i}e^{\alpha}\frac{\left(e^{\mathrm{i}\mu}e^{\alpha}-1\right)\left(-1+e^{2\mathrm{i}\mu}\right)}{\left(e^{\mathrm{i}\mu}-e^{\alpha}\right)\left(e^{2\mathrm{i}\mu}-2e^{\mathrm{i}\mu}e^{\alpha}+1\right)}.
\end{aligned}$$

Dividing both the numerator and the denominator by $e^{\mathrm{i}\mu}e^{\alpha}$ gives us

$$\begin{aligned}
\frac{\mathrm{d}k}{\mathrm{d}\alpha} &= \mathrm{i}\frac{-1+e^{2\mathrm{i}\mu}+e^{-\mathrm{i}\mu}e^{-\alpha}-e^{\mathrm{i}\mu}e^{-\alpha}}{e^{2\mathrm{i}\mu}-2e^{\mathrm{i}\mu}e^{-\alpha}+e^{-2\alpha}-e^{\mathrm{i}\mu}e^{\alpha}+2-e^{-\mathrm{i}\mu}e^{-\alpha}} \\
&= -\frac{\left[-1+e^{2\mathrm{i}\mu}+e^{-\mathrm{i}\mu}e^{-\alpha}-e^{\mathrm{i}\mu}e^{-\alpha}\right]\left[e^{\alpha}+e^{-\alpha}-e^{\mathrm{i}\mu}-e^{-\mathrm{i}\mu}\right]}{\left[e^{2\mathrm{i}\mu}-2e^{\mathrm{i}\mu}e^{-\alpha}+e^{-2\alpha}-e^{\mathrm{i}\mu}e^{\alpha}+2-e^{-\mathrm{i}\mu}e^{-\alpha}\right]\left[e^{\mathrm{i}\mu}-e^{-\mathrm{i}\mu}\right]}\frac{\sin(\mu)}{\cosh(\alpha)-\cos(\mu)} \\
&= \frac{\sin(\mu)}{\cosh(\alpha)-\cos(\mu)}.
\end{aligned}$$

B.2 Proving $\frac{\partial\varphi_{k_j,q}}{\partial\beta} = \frac{\sin(2\mu)}{\cosh(\alpha-\beta)-\cos(2\mu)}$

We will write $k_j = k$, and we will first rewrite $\varphi_{k,q}$ to a nice form before we take the derivative.

Lemma B.1. *We can rewrite $\varphi_{k,q}$ as*

$$\varphi_{k,q} = 2\arctan\left[\cot(\mu)\tanh\left(\frac{\beta-\alpha}{2}\right)\right].$$

Proof. We start with Eq. 93 and, using $\mu = \frac{2\pi}{3}$, we see that

$$\begin{aligned}
\varphi_{k,q} &= 2\arctan\left[\frac{-\cos(\mu)\sin[(k-q)/2]}{\cos[(k+q)/2]+\cos(\mu)[(k-q)/2]}\right] \\
&= 2\arctan\left[\frac{\sin[(q-k)/2]}{\cos[(q-k)/2]+\frac{1}{\cos(\mu)}\cos[(k+q)/2]}\right] \\
&= 2\arctan\left[\frac{1}{i}\frac{e^{\mathrm{i}q}-e^{\mathrm{i}k}}{e^{\mathrm{i}q}+e^{\mathrm{i}k}+\frac{1+e^{\mathrm{i}k}e^{\mathrm{i}q}}{\cos(\mu)}}\right] \\
&= 2\arctan\left[\frac{\cos(\mu)}{\sin(\mu)}\frac{e^{\mathrm{i}q}\left(e^{-\mathrm{i}\mu}-e^{\mathrm{i}\mu}\right)+e^{\mathrm{i}k}\left(e^{\mathrm{i}\mu}-e^{-\mathrm{i}\mu}\right)}{e^{\mathrm{i}q}\left(e^{-\mathrm{i}\mu}+e^{\mathrm{i}\mu}\right)+e^{\mathrm{i}k}\left(e^{\mathrm{i}\mu}+e^{-\mathrm{i}\mu}\right)+2+2e^{\mathrm{i}k}e^{\mathrm{i}q}}\right] \\
&= 2\arctan\left[\frac{\cos(\mu)}{\sin(\mu)}\frac{\frac{1+e^{\mathrm{i}\mu}e^{\mathrm{i}k}}{e^{\mathrm{i}\mu}+e^{\mathrm{i}k}}\frac{e^{\mathrm{i}\mu}+e^{\mathrm{i}q}}{1+e^{\mathrm{i}\mu}e^{\mathrm{i}q}}-1}{\frac{1+e^{\mathrm{i}\mu}e^{\mathrm{i}k}}{e^{\mathrm{i}\mu}+e^{\mathrm{i}k}}\frac{e^{\mathrm{i}\mu}+e^{\mathrm{i}q}}{1+e^{\mathrm{i}\mu}e^{\mathrm{i}q}}+1}\right]
\end{aligned}$$

Now we can use Eq. 87 to calculate

$$\begin{aligned}
\varphi_{k,q} &= 2\arctan\left[\frac{\cos(\mu)}{\sin(\mu)}\frac{e^{-\alpha}e^{\beta}-1}{e^{-\alpha}e^{\beta}+1}\right] \\
&= 2\arctan\left[\cot(\mu)\tanh\left(\frac{\beta-\alpha}{2}\right)\right],
\end{aligned}$$

which proofs the lemma. □

Lemma B.2. *The derivative* $\frac{\partial \varphi_{k_j,q}}{\partial \beta}$ *is given by*

$$\frac{\partial \varphi_{k_j,q}}{\partial \beta} = \frac{\sin(2\mu)}{\cosh(\alpha-\beta)-\cos(2\mu)}.$$

Proof. Using the result from the previous lemma, we can calculate

$$\begin{aligned}\frac{\partial \varphi_{k_j,q}}{\partial \beta} &= 2\frac{\partial}{\partial \beta}\left(\arctan\left[\cot(\mu)\tanh\left(\frac{\beta-\alpha}{2}\right)\right]\right)\\ &= \frac{2\sin(\mu)\cos(\mu)}{2\cos^2(\mu)\sinh^2\left(\frac{\beta-\alpha}{2}\right)+2\sin^2(\mu)\cosh^2\left(\frac{\beta-\alpha}{2}\right)}\end{aligned}$$

But

$$\begin{aligned}\sinh^2(x) &= \frac{\cosh(2x)-1}{2},\\ \cosh^2(x) &= \frac{\cosh(2x)+1}{2},\\ 2\sin(x)\cos(x) &= \sin(2x),\\ \sin^2(x)-\cos^2(x) &= -\cos(2x),\end{aligned}$$

so

$$\begin{aligned}\frac{\partial \varphi_{k_j,q}}{\partial \beta} &= \frac{\sin(2\mu)}{\cos^2(\mu)\left(\cosh(\beta-\alpha)-1\right)+\sin^2(\mu)\left(\cosh\left(\beta-\alpha\right)+1\right)}\\ &= \frac{\sin(2\mu)}{\cosh(\alpha-\beta)-\cos(2\mu)},\end{aligned}$$

which was to be proven. □

B.3 Rewriting $\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right)$

We can rewrite Eq. 85 with the transformation of Eq. 88 as follows. We will use the definition of R (Eq. 90) and $\mu = 2\pi/3$ in the derivation.

$$\begin{aligned}&\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right) = -\frac{1}{2}\int_{-Q}^{Q}\log\left(2-2\cos\left(q\right)\right)\rho(q)\,\mathrm{d}q = -\frac{1}{2}\int_{-Q}^{Q}\log\left(2-\left(e^{\mathrm{i}q}+e^{-\mathrm{i}q}\right)\right)\rho(q)\,\mathrm{d}q\\ &= -\frac{1}{4\pi}\int_{-\infty}^{\infty}\log\left(2-\left(\frac{e^{\mathrm{i}\mu}-e^{\alpha}}{e^{\mathrm{i}\mu+\alpha}-1}+\frac{e^{\mathrm{i}\mu+\alpha}-1}{e^{\mathrm{i}\mu}-e^{\alpha}}\right)\right)R(\alpha)\,\mathrm{d}\alpha\\ &= -\frac{1}{4\pi}\int_{-\infty}^{\infty}\log\left(1-\frac{\left(e^{\mathrm{i}\mu}+e^{-\mathrm{i}\mu}+1\right)\left(e^{\alpha}+e^{-\alpha}\right)-4-\left(e^{\mathrm{i}\mu}+e^{-\mathrm{i}\mu}\right)}{e^{\mathrm{i}\mu}+e^{-\mathrm{i}\mu}-\left(e^{\alpha}+e^{-\alpha}\right)}\right)R(\alpha)\,\mathrm{d}\alpha\end{aligned}$$

Now we see that the value of μ fixes $e^{\mathrm{i}\mu}+e^{-\mathrm{i}\mu}=-1$ to get

$$\lim_{N\to\infty}\frac{1}{N}\log\left(E(r)\right) = -\frac{1}{4\pi}\int_{-\infty}^{\infty}\log\left(1-\frac{3}{1+2\cosh(\alpha)}\right)R(\alpha)\,\mathrm{d}\alpha,$$

which is how it is rewritten in Eq. 95.

B.4 Proof of Lemma 4.16

B.4.1 Expressions for integrals

In the proof of the Lemma, we will need to calculate two integrals explicitly, to know

$$\int_{-\infty}^{\infty}\frac{e^{\mathrm{i}\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\,\mathrm{d}\beta, \tag{102}$$

$$\int_{-\infty}^{\infty} \frac{e^{i\gamma\beta}}{\cosh(\gamma)}\, d\gamma. \tag{103}$$

We will calculate these integrals in this section. Hereafter, in Section B.4.2, we will prove Lemma 4.16 using these integrals. To calculate these integrals, we need the Residue Theorem, which we state here after introducing some terminology.

Definition B.3. Let $f : \mathbb{C} \to \mathbb{C}$ have a Laurent expansion at z_0:

$$f(z) = \sum_{-\infty}^{\infty} a_n (z - z_0)^n.$$

The residue of f at z_0 is the coefficient a_{-1} and we notate it by $\mathrm{Res}_{z_0} f = a_{-1}$. ◁

Theorem B.4 (Residue Theorem)**.** *Let U be an open subset of $\mathbb{C}$, γ a closed path in U that is homologous to a point in U, and let f be an analytic function on U except at $n \in \mathbb{N}$ points b_j ($j \in \{1, \dots, n\}$) in $U - \mathrm{Image}(\gamma)$. Then ([14], p. 112)*

$$\int_\gamma f = 2\pi i \sum_{j=1}^{n} \mathrm{Res}_{b_j} f. \tag{104}$$

Obviously, for $\beta \in \mathbb{C}$ and at $|\beta| \to \infty$, the integrand in Eq. 102 goes to zero exponentially in the upper half-plane, so we can integrate along the upper half-plane. We need to calculate the residues, and we can do this by using Cauchy's Integral formula ([14], p. 84):

$$\mathrm{Res}_b(f) = \frac{1}{2\pi i} \int_\gamma f(z)\, dz, \tag{105}$$

where γ denotes *any* closed path that goes around the pole b, and only b, exactly once. In our case, the poles are, for $n \in \mathbb{N}$, at $\beta = i\mu + 2\pi i n$, so if we write $C(z, r)$ as the circle with centre $z \in \mathbb{C}$ and radius $r \in \mathbb{R}$, then we have:

$$\begin{aligned}
\mathrm{Res}_{\beta=i\mu+2\pi in}\left(\frac{e^{i\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\right) &= \frac{1}{2\pi i}\int_{C(i\mu+2\pi in,\varepsilon)} \frac{e^{i\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\, d\beta \\
&= \frac{1}{2\pi i}\int_0^{2\pi} \frac{\varepsilon i e^{i\theta} e^{-(\mu+2\pi n)\gamma + i\varepsilon e^{i\theta}\gamma}}{\cosh(i\mu+\varepsilon e^{i\theta})-\cos(\mu)}\, d\theta \\
&= \frac{\varepsilon i e^{-(\mu+2\pi n)\gamma}}{2\pi i}\int_0^{2\pi} \frac{e^{i\theta} e^{i\varepsilon e^{i\theta}\gamma}}{\sinh(i\mu)\sinh(\varepsilon e^{i\theta}) + \cosh(i\mu)\cosh(\varepsilon e^{i\theta}) - \cos(\mu)}\, d\theta
\end{aligned}$$

Now we let $\varepsilon \to 0$, and we have

$$\mathrm{Res}_{\beta=i\mu+2\pi in}\left(\frac{e^{i\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\right) = \frac{e^{-\mu\gamma}e^{-2\pi n\gamma}}{i\sin(\mu)}$$

We also have poles at $\beta = -i\mu + 2\pi i n$ for $n \in \mathbb{N} - \{0\}$, and their residues can be calculated in a similar manner, from which we get

$$\mathrm{Res}_{\beta=-i\mu+2\pi i+2\pi in}\left(\frac{e^{i\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\right) = -\frac{e^{(\mu-2\pi)\gamma}e^{-2\pi n\gamma}}{i\sin(\mu)}.$$

Now we note that the integrand is analytic outside its poles, so we can calculate the integral using the Residue Theorem (Theorem B.4) as follows:

$$\begin{aligned}
&\int_{-\infty}^{\infty} \frac{e^{i\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\, d\beta = \int_{\text{upper half-plane}} \frac{e^{i\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\, d\beta \\
&= \sum_{n=0}^{\infty} 2\pi i \left[\mathrm{Res}_{\beta=i(\mu+2\pi n)}\left(\frac{e^{i\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\right) + \mathrm{Res}_{\beta=-i\mu+2\pi in+2\pi in}\left(\frac{e^{i\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\right)\right] \\
&= 2\pi \frac{e^{-\mu\gamma} - e^{(\mu-2\pi)\gamma}}{\sin(\mu)} \sum_{n=0}^{\infty} \left(e^{-2\pi\gamma}\right)^n = 2\pi \frac{e^{-\mu\gamma} - e^{(\mu-2\pi)\gamma}}{\sin(\mu)} \frac{1}{1-e^{-2\pi\gamma}} = \frac{2\pi}{\sin(\mu)} \frac{\sinh\left[(\pi-\mu)\gamma\right]}{\sinh(\pi\gamma)}.
\end{aligned}$$

Now let us have a look at the second integral.

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}\gamma\beta}}{\cosh(\gamma)}\,\mathrm{d}\gamma = \int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}\gamma\beta}}{\cos(\mathrm{i}\gamma)}\,\mathrm{d}\gamma.$$

We see, from the fact that $\beta > 0$, that this time, we also integrate along the upper half-plane, because the integrand goes to zero there as $|\gamma| \to \infty$. Clearly, the poles are at $\mathrm{i}\gamma = -\pi/2 - \pi n$ The residue of the integrand at a pole is again given by Eq. 105:

$$\begin{aligned}
\mathrm{Res}_{\mathrm{i}\gamma=-\pi/2-\pi n}\left(\frac{e^{\mathrm{i}\gamma\beta}}{\cos(\mathrm{i}\gamma)}\right) &= \lim_{\varepsilon\to 0}\frac{1}{2\pi\mathrm{i}}\int_{C(\mathrm{i}\mu,\varepsilon)} \frac{\mathrm{e}^{\mathrm{i}\gamma\beta}}{\cos(\mathrm{i}\gamma)}\,\mathrm{d}\gamma \\
&= \lim_{\varepsilon\to 0}\frac{1}{2\pi\mathrm{i}}\int_{\theta=0}^{2\pi} \frac{\varepsilon\mathrm{i}\mathrm{e}^{\mathrm{i}\theta}\mathrm{e}^{-(\pi/2+\pi n-\mathrm{i}\varepsilon\mathrm{e}^{\mathrm{i}\theta})\beta}}{\cos\left[\pi/2+\pi n-\mathrm{i}\varepsilon\mathrm{e}^{\mathrm{i}\theta}\right]}\,\mathrm{d}\theta \\
&= \lim_{\varepsilon\to 0}\frac{\varepsilon\mathrm{e}^{-\pi\beta/2}}{2\pi}\int_{\theta=0}^{2\pi} \frac{\mathrm{e}^{\mathrm{i}\theta}\mathrm{e}^{-\pi n\beta}}{\sin(\pi/2+\pi n)\sin(\mathrm{i}\varepsilon\mathrm{e}^{\mathrm{i}\theta})}\,\mathrm{d}\theta \\
&= \frac{(-1)^n\mathrm{e}^{-\pi\beta/2}\mathrm{e}^{-\pi n\beta}}{\mathrm{i}}.
\end{aligned}$$

Again, the conditions of Theorem B.4 are met, and we can calculate the integral from Eq. 103:

$$\begin{aligned}
\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}\gamma\beta}}{\cosh(\gamma)}\,\mathrm{d}\gamma &= \int_{\text{upper half-plane}} \frac{\mathrm{e}^{\mathrm{i}\gamma\beta}}{\cosh(\gamma)}\,\mathrm{d}\gamma = 2\pi\mathrm{i}\sum_{n=0}^{\infty}\mathrm{Res}_{\mathrm{i}\gamma=-\pi/2-\pi n}\left(\frac{\mathrm{e}^{\mathrm{i}\gamma\beta}}{\cos(\mathrm{i}\gamma)}\right) \\
&= 2\pi\mathrm{e}^{-\pi\beta/2}\sum_{n=0}^{\infty}(-1)^n\mathrm{e}^{-\pi n\beta} = 2\pi\mathrm{e}^{-\pi\beta/2}\left[\sum_{n=0}^{\infty}\mathrm{e}^{-2\pi n\beta} - \sum_{n=0}^{\infty}\mathrm{e}^{-2\pi n\beta-\pi\beta}\right] \\
&= 2\pi\left[\frac{\mathrm{e}^{\pi\beta/2}-\mathrm{e}^{-\pi\beta/2}}{\mathrm{e}^{\pi\beta}-\mathrm{e}^{-\pi\beta}}\right] = \frac{\pi}{\cosh(\pi\beta/2)}.
\end{aligned}$$

To summarize, we calculated the following integrals, which we will use in the next section:

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}\beta\gamma}}{\cosh(\beta)-\cos(\mu)}\,\mathrm{d}\beta = \frac{2\pi}{\sin(\mu)}\frac{\sinh\left[(\pi-\mu)\gamma\right]}{\sinh(\pi\gamma)}, \tag{106}$$

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}\gamma\beta}}{\cosh(\gamma)}\,\mathrm{d}\gamma = \frac{\pi}{\cosh(\pi\beta/2)}. \tag{107}$$

B.4.2 Proof of the Lemma

We prove that the solution to Eq. 94 is given by

$$R(\alpha) = \frac{\pi}{2\mu\cosh\left(\frac{\pi\alpha}{2\mu}\right)}. \tag{108}$$

Proof. We note that for $\mu = 2\pi/3$ (which is the case we are interested in),

$$K = -\frac{1}{2\pi}\xi,$$

so from Eq. 94, it follows that

$$R(\alpha) = \xi(\alpha) - (R*K)(\alpha) = \xi(\alpha) + \frac{1}{2\pi}(R*\xi)(\alpha),$$

where $*$ is the convolution product. Let us now define a Fourier transformation.

Definition B.5. We define the Fourier transform $\hat{f}$ of a smooth function f as

$$\hat{f}(\gamma) := \int_{-\infty}^{\infty} f(x) e^{-2\pi \mathrm{i} x \gamma} \, \mathrm{d}x.$$

Note that the inverse Fourier transform f of $\hat{f}$ is now given by

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\gamma) e^{2\pi \mathrm{i} x \gamma} \, \mathrm{d}\gamma.$$

◁

The Fourier transformation of a convolution product is ([4])

$$\widehat{a * b} = \hat{a} \cdot \hat{b},$$

where the $\cdot$ indicates the regular multiplication of one-dimensional functions. We use this fact to our advantage by Fourier transforming our equation, to get

$$\hat{R}(\gamma) = \hat{\xi}(\gamma) + \frac{1}{2\pi} \hat{R}(\gamma) \hat{\xi}(\gamma)$$
$$\iff \hat{R}(\gamma) = \frac{\hat{\xi}(\gamma)}{1 - \frac{1}{2\pi} \hat{\xi}(\gamma)}.$$

Thus, to figure out R, we have to figure out $\hat{\xi}$. We can calculate, using Eq. 106:

$$\hat{\xi}(\gamma) = \sin(\mu) \int_{-\infty}^{\infty} \frac{e^{-2\pi \mathrm{i} \beta \gamma}}{\cosh(\beta) - \cos(\mu)} \, \mathrm{d}\beta$$
$$\implies \hat{\xi}\left(\frac{-\gamma}{2\pi}\right) = \sin(\mu) \int_{-\infty}^{\infty} \frac{e^{\mathrm{i}\beta\gamma}}{\cosh(\beta) - \cos(\mu)} \, \mathrm{d}\beta = 2\pi \frac{\sinh\left[(\pi - \mu)\gamma\right]}{\sinh(\pi\gamma)} = \frac{\pi}{\cosh(\mu\gamma) + \frac{1}{2}},$$

where we have used $\mu = 2\pi/3$ to get the last equality. We can now calculate $\hat{R}$:

$$\hat{R}\left(\frac{-\gamma}{2\pi}\right) = \frac{\hat{\xi}\left(\frac{-\gamma}{2\pi}\right)}{1 - \frac{1}{2\pi}\hat{\xi}\left(\frac{-\gamma}{2\pi}\right)} = \frac{\pi}{\cosh(\mu\gamma)}$$
$$\implies \hat{R}(\gamma) = \frac{\pi}{\cosh(2\pi\mu\gamma)}.$$

The last step is to inverse Fourier transform this equation and evaluating the resulting integral using Eq. 107.

$$R(\alpha) = \int_{-\infty}^{\infty} \hat{R}(\gamma) e^{2\pi \mathrm{i} \alpha \gamma} \, \mathrm{d}\gamma = \int_{-\infty}^{\infty} \frac{e^{2\pi \mathrm{i}\alpha\gamma} \pi}{\cosh(2\pi\mu\gamma)} \, \mathrm{d}\gamma$$
$$= \frac{1}{2\mu} \int_{-\infty}^{\infty} \frac{e^{\mathrm{i}\gamma(\alpha/\mu)}}{\cosh(\gamma)} \, \mathrm{d}\gamma = \frac{\pi}{2\mu \cosh\left(\frac{\pi\alpha}{2\mu}\right)},$$

which proves the lemma. □

B.5 Calculation of the integral $\lim_{N\to\infty} \frac{1}{N} \log\left(E(r)\right)$

The integral we will calculate is restated, with z substituted for x because we want to make clear we are working in the complex plane:

$$\frac{3}{4\pi}\left[-2\int_{-\infty}^{\infty} \log\left[(z+\mathrm{i})(z-\mathrm{i})\right] \frac{z^2}{z^6+1} \mathrm{d}z - \int_{-\infty}^{\infty} \log\left[(z+1)^2(z-1)^2\right] \frac{z^2}{z^6+1} \mathrm{d}z + \int_{-\infty}^{\infty} \log\left(z^8+z^4+1\right) \frac{z^2}{z^6+1} \mathrm{d}z\right].$$

We will start with the right-most term.

B.5.1 Looking at $\int_{-\infty}^{\infty} \log\left(z^8+z^4+1\right) \frac{z^2}{z^6+1} \mathrm{d}z$

We notice that

$$\log\left(1+z^4+z^8\right) = \log\left(z-e^{\mathrm{i}\pi/6}\right) + \log\left(z-e^{\mathrm{i}\pi/3}\right) + \log\left(z-e^{2\mathrm{i}\pi/3}\right) + \log\left(z-e^{5\mathrm{i}\pi/6}\right) + \log\left(z-e^{-5\mathrm{i}\pi/6}\right) + \log\left(z-e^{-2\mathrm{i}\pi/3}\right) + \log\left(z-e^{-\mathrm{i}\pi/3}\right) + \log\left(z-e^{-\mathrm{i}\pi/6}\right), \quad (109)$$

where all the terms are of the form $\log(z-z_0)$ with $z_0 \in \mathbb{C}-\mathbb{R}$. Thus, first we will take a look at this general form. The integral we want to calculate is

$$\int_{-\infty}^{\infty} f(z)\,\mathrm{d}z := \int_{-\infty}^{\infty} \log(z-z_0)\frac{z^2}{z^6+1}\,\mathrm{d}z.$$

We want to do this with closed integral curves over the half-plane in the complex plane, but we want to avoid the singularity of the logarithm. This means that depending on if the imaginary part of z_0, which we denote with $\Im(z_0)$, is positive or negative, we choose the lower or the upper half-plane, respectively.

If $\Im(z_0) > 0$, then we integrate over the lower half-plane. We are looking for the residues of $1/(z^6+1)$, so we write it out:

$$z^6+1 = \left(z-e^{\mathrm{i}\pi/6}\right)(z-i)\left(z-e^{5\mathrm{i}\pi/6}\right)\left(z-e^{-5\mathrm{i}\pi/6}\right)(z+i)\left(z-e^{-\mathrm{i}\pi/6}\right). \quad (110)$$

Now we want to employ the Residue Theorem (Theorem B.4) again. Let $C_>$ denote the path that goes along the upper half-plane and $C_<$ the one along the lower half-plane but in opposite direction as to conform to the direction of integration over the real axis, with radius R. We want to let $R \to \infty$, and indeed, if $|z| = R$, then $\lim_{R\to\infty} 2\pi R f(z) = 0$. This means that

$$\int_C f = \int_{-\infty}^{\infty} f(z)\,\mathrm{d}z.$$

We use the Residue Theorem but we want to avoid including the logarithmic singularity in our contour, so depending on if the imaginary part of z_0, written $\Im(z_0)$, is positive or negative, we integrate over $C_<$ or over $C_>$, respectively, and we calculate

$$\begin{aligned}
\int_{C_<} f &= -2\pi\mathrm{i}\left[\mathrm{Res}_{e^{-\mathrm{i}\pi/6}} f + \mathrm{Res}_{-\mathrm{i}} f + \mathrm{Res}_{e^{-5\mathrm{i}\pi/6}} f\right] \\
&= -2\pi\mathrm{i}\left[\frac{e^{-\mathrm{i}\pi/3}\log\left(e^{-\mathrm{i}\pi/6}-z_0\right)}{(-\mathrm{i})\left(e^{-\mathrm{i}\pi/6}-\mathrm{i}\right)\left(\sqrt{3}\right)\left(2e^{-\mathrm{i}\pi/6}\right)\left(e^{\mathrm{i}\pi/6}\right)}\right. \\
&\qquad + \frac{-1\log(-i-z_0)}{\left(-\mathrm{i}-e^{\mathrm{i}\pi/6}\right)(-2\mathrm{i})\left(-e^{5\mathrm{i}\pi/6}-\mathrm{i}\right)\left(e^{-\mathrm{i}\pi/6}\right)\left(e^{-5\mathrm{i}\pi/6}\right)} \\
&\qquad \left. + \frac{e^{\mathrm{i}\pi/3}\log\left(e^{-5\mathrm{i}\pi/6}-z_0\right)}{\left(2e^{-5\mathrm{i}\pi/6}\right)\left(e^{-5\mathrm{i}\pi/6}-\mathrm{i}\right)(-\mathrm{i})\left(e^{5\mathrm{i}\pi/6}\right)\left(-\sqrt{3}\right)}\right] \\
&= \frac{\pi}{3}\left[\log\left(z_0^2+\mathrm{i}z_0-1\right) - \log\left(-\mathrm{i}-z_0\right)\right].
\end{aligned}$$

Similarly, if $\Im(z_0) < 0$, then we integrate along the upper half-plane, and we get

$$\int_{C_>} f = \frac{\pi}{3}\left[\log\left(z_0^2-\mathrm{i}z_0-1\right) - \log\left(\mathrm{i}-z_0\right)\right]. \quad (111)$$

We now look at Eq. 109 again and we calculate

$$\begin{aligned}\int_{-\infty}^{\infty} \log\left(z^8+z^4+1\right)\frac{z^2}{z^6+1}\mathrm{d}z = \frac{\pi}{3}\Bigg[&\log\left(\mathrm{i}\sqrt{3}-1\right)+\log\left(\frac{\mathrm{i}}{2}\left(\sqrt{3}+1\right)-\frac{1}{2}\left(\sqrt{3}+3\right)\right)\\
&+\log\left(-\frac{\mathrm{i}}{2}\left(\sqrt{3}+1\right)-\frac{1}{2}\left(\sqrt{3}+3\right)\right)+\log\left(-\mathrm{i}\sqrt{3}-1\right)\\
&-\log\left(-\mathrm{i}-e^{\mathrm{i}\pi/6}\right)-\log\left(-\mathrm{i}-e^{e^{\mathrm{i}\pi/3}}\right)-\log\left(-\mathrm{i}-e^{2\mathrm{i}\pi/3}\right)\\
&-\log\left(-\mathrm{i}-e^{5\mathrm{i}\pi/6}\right)+\log\left(\mathrm{i}\sqrt{3}-1\right)\\
&+\log\left(\frac{\mathrm{i}}{2}\left(\sqrt{3}+1\right)-\frac{1}{2}\left(\sqrt{3}+3\right)\right)\\
&+\log\left(-\frac{\mathrm{i}}{2}\left(\sqrt{3}+1\right)-\frac{1}{2}\left(\sqrt{3}+3\right)\right)+\log\left(-\mathrm{i}\sqrt{3}-1\right)\\
&-\log\left(\mathrm{i}-e^{-5\mathrm{i}\pi/6}\right)-\log\left(\mathrm{i}-e^{-2\mathrm{i}\pi/3}\right)\\
&-\log\left(\mathrm{i}-e^{-\mathrm{i}\pi/3}\right)-\log\left(\mathrm{i}-e^{-\mathrm{i}\pi/6}\right)\Bigg]\\
=\frac{2\pi}{3}\log\left(\frac{8}{3}\right).&\end{aligned}$$

Next, we will do the left-most term, with the purely imaginary singularities.

B.5.2 Looking at $\int_{-\infty}^{\infty}\log\left[(z+\mathbf{i})(z-\mathbf{i})\right]\frac{z^2}{z^6+1}\,\mathrm{d}z$

We can use the same equations for $\int_{C_<}$ and $\int_{C_>}$ as before, so we calculate

$$\int_{-\infty}^{\infty}\log\left[(z+\mathrm{i})(z-\mathrm{i})\right]\frac{z^2}{z^6+1}\,\mathrm{d}z=\frac{\pi}{3}\left[\log(-3)-\log(-2\mathrm{i})+\log(-3)-\log(2\mathrm{i})\right]=\frac{2\pi}{3}\log\left(\frac{3}{2}\right).$$

Now let us look at the remaining term.

B.5.3 Looking at $\int_{-\infty}^{\infty}\log\left[(z+1)^2(z-1)^2\right]\frac{z^2}{z^6+1}\mathrm{d}z$

We can rewrite this, writing the real part of $z\in\mathbb{C}$ as $\Re(z)$, as

$$\begin{aligned}\int_{-\infty}^{\infty}\log\left[(z+1)^2(z-1)^2\right]\frac{z^2}{z^6+1}\mathrm{d}z&=2\int_{-\infty}^{\infty}\log|(z+1)(z-1)|\frac{z^2}{z^6+1}\mathrm{d}z\\
&=2\Re\left(\int_{-\infty}^{\infty}\log(z+1)\frac{z^2}{z^6+1}\mathrm{d}z+\int_{-\infty}^{\infty}\log(z-1)\frac{z^2}{z^6+1}\mathrm{d}z\right)\end{aligned}$$

Here, we cannot use our previous contour along the upper half-plane, because the singularities are on the real axis. We can use the contour $\mathscr{C}$ shown in Figure 3.

The part of the integral along $A_\pm$ can be computed as follows, for $f(z)=\log(z\pm1)\frac{z^2}{z^6+1}$:

$$\left|\lim_{\varepsilon\to0}\int_{A_\pm}f(z)\,\mathrm{d}z\right|=\left|\lim_{\varepsilon\to0}\int_0^{\pi}f(\varepsilon e^{\mathrm{i}\varphi}\pm1)\mathrm{i}e^{\mathrm{i}\varphi}\varepsilon\,\mathrm{d}\varphi\right|\leq\left|\lim_{\varepsilon\to0}\varepsilon\log(\varepsilon)\right|=0$$

The part of the integral along $|z|=R$ also goes to zero as $R\to\infty$, as we have seen before. Thus,

$$\int_{-\infty}^{\infty}f(z)\,\mathrm{d}z=\int_{\mathscr{C}}f(z).$$

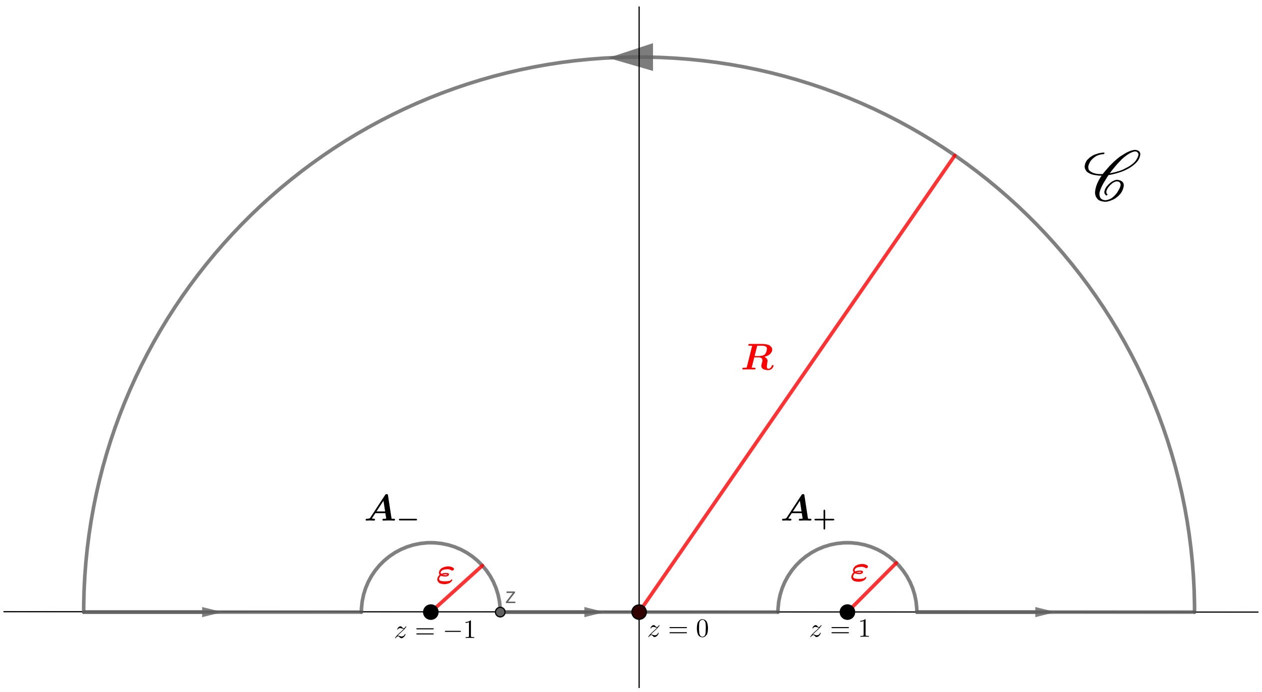

Figure 3: The contour $\mathscr{C}$ along which we calculate the integral of Section B.5.3. The red markings indicate the radii of the half circles.

But we have the same singularities from z^6+1 in $\mathscr{C}$ as in our previous upper half-plane contour $C_>$! This means that we can use Eq. 111 again, and we calculate

$$2\Re\left(\sum_{+,-}\int_{-\infty}^{\infty}\log(z\pm 1)\frac{z^2}{z^6+1}\mathrm{d}z\right)=2\Re\left(\sum_{+,-}\int_{\mathscr{C}}\log(z\pm 1)\frac{z^2}{z^6+1}\mathrm{d}z\right)=2\Re\left(\sum_{+,-}\int_{C_>}\log(z\pm 1)\frac{z^2}{z^6+1}\mathrm{d}z\right)$$
$$=2\Re\left(\sum_{+,-}\frac{\pi}{3}\left[\log(1\mp\mathrm{i}-1)-\log(\mathrm{i}\mp 1)\right]\right)=-\frac{2\pi}{3}\log(2).$$

B.5.4 Calculation of the whole integral

We can now calculate the whole integral by using the results from the previous sections.

$$\frac{3}{4\pi}\left[-2\int_{-\infty}^{\infty}\log\left[(z+\mathrm{i})(z-\mathrm{i})\right]\frac{z^2}{z^6+1}\mathrm{d}z-\int_{-\infty}^{\infty}\log\left[(z+1)^2(z-1)^2\right]\frac{z^2}{z^6+1}\mathrm{d}z+\int_{-\infty}^{\infty}\log\left(z^8+z^4+1\right)\frac{z^2}{z^6+1}\mathrm{d}z\right]$$
$$=\frac{3}{4\pi}\left[-\frac{4\pi}{3}\log\left(\frac{3}{2}\right)+\frac{2\pi}{3}\log(2)+\frac{2\pi}{3}\log\left(\frac{8}{3}\right)\right]=\frac{3}{2}\log\left(\frac{4}{3}\right).$$

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