Reflection Positivity in Heisenberg and Ice-Type Models

by

Jort de Groot

To obtain the degree of Bachelor of Science in Applied Mathematics and Applied Physics
at the Delft University of Technology

Student number:	4704916
Supervisors:	Dr. B. Janssens (EEMCS)
	Dr. A.R. Akhmerov (TNW)
Other committee members:	Dr. J.L.A. Dubbeldam (EEMCS)
	Dr. ir. J.M. Thijssen (TNW)

Delft, July 2020

Abstract

This thesis gives a thorough description of the mathematical tool called reflection positivity, which can be used to prove the occurrence of phase transitions in physical models. A major result, although already known, is a theorem that gives tractable conditions on the Hamiltonian such that the Boltzmann functional is reflection positive. In this thesis, the theorem is used to give conditions on free parameters in four different models, such that the model is reflection positive with respect to certain chosen reflections. The evaluated models are (a) the antiferromagnetic quantum Heisenberg model; (b) the spin ice model; (c) the 6-vertex model and (d) the 16-vertex model. For the Heisenberg model we found that for reflections in a reflection plane there are certain parameter values such that the Boltzmann functional is reflection positive, this is an already known and published result. For the spin ice model we found that for the spin invariant reflection there is no symmetry that yields a reflection positive Boltzmann functional, this is a new result. For both the 6-vertex and 16-vertex model we showed that, for certain energy values, the Boltzmann functional is reflection positive with respect to reflections in the diagonal, which are also new results. In the case of the 16-vertex model, this boils down to checking whether or not a matrix is positive semidefinite. Using this result we showed that energy values that allow for the existence of magnetic monopoles do not yield a reflection positive Boltzmann functional. A topic for further research is investigating the occurrence of phase transitions in the models that are shown to be reflection positive, for which chessboard estimates seem to be a promising approach. Furthermore, in this thesis it was not rigorously proved that the spin ice model with a spin inverting reflection gives a reflection positive Boltzmann functional for rotational symmetry or symmetry in a reflection plane. This is believed to be true, but does require further investigation.

Contents

1

Introduction

Ice melts at around 273 Kelvin, while other materials melt at different temperatures. The magnetization of ferromagnets is lost at high temperatures. These are examples of fascinating phenomena in equilibrium statistical mechanics, called phase transitions. In physics there are a lot of approximate methods to explain or otherwise justify phase transitions, but a thorough mathematical description exists only for a few simple cases, and then only for simplified versions.

One of those mathematical approaches to phase transitions in lattice spin models is based on the technique of reflection positivity. This is a technique in statistical physics that was developed in the late 1970s by Dyson, Lieb, Simon, Fröhlich, Israel and Spencer [DLS78, FILS78, FSS76]. Using reflection positivity, one can usually utilize two types of arguments to prove phase transitions. The first one is to derive the infrared bound, where spin interactions are interpreted as a random walk. The second is using the so called chessboard estimates, where the Cauchy-Schwartz theorem is utilized to be able to draw conclusions about a model as a whole by evaluating only a small part of the model.

Reflection positivity is not only used to prove phase transitions. In fact, the technique was first developed in the early 1970s in constructive quantum field theory by Osterwalder, Schrader, Glimm, Jaffe and Spencer [OS73b, OS73a, OS75, GJS74, GJS75]. At first, the similarity between the two fields was not obvious. However, recently a general framework for reflection positivity was introduced by Jaffe and Janssens, in the extensive work 'reflection positive doubles' [JJ17]. Janssens is one of the supervisors of this thesis.

In order to prove reflection positivity for a physical model, one generally needs to make three choices. The first two are often determined by the model itself, those are the considered lattice and the description of the Boltzmann functional. The final choice is what reflection one is going to evaluate. A prerequisite is often that the lattice is reflection invariant, which means it possesses some sort of symmetry.

In the work of Jaffe and Janssens it is shown that under a few conditions checking reflection positivity boils down to checking some tractable conditions on the Hamiltonian. Specifically, one needs to check whether the Hamiltonian can be split up in three parts such that the first only contains interactions on one side of the reflection plane, the second is the reflection of the first and the third is contained in the so-called reflection positive cone.

In this thesis we aim at proving or disproving reflection positivity in different models using one of the two methods described above. The first model we evaluate is the antiferromagnetic quantum Heisenberg model, where we treat both the nearest neighbour and the long-range variant for a reflection in a reflection plane. This result is already known and used, as described in [FSS76, DLS76], moreover it is treated as an example in [JJ17]. For the second, third and fourth model we aim at proving new results. The second model is the spin ice model described in [CMS08], where we look into all possible reflections that leave the considered pyrochlore lattice invariant. The third and fourth model are ice type models being the 6-vertex and 16-vertex model, respectively, based on the description in [Bax73]. Here we look into diagonal reflections.

In Chapter 2 we provide the reader with the necessary definitions and theorems from different fields of mathematics and physics, that are used intensively throughout this thesis. In Chapter 3 we give a description of reflection positivity, all definitions and theorems of this chapter are directly from [JJ17], or slight simplifications. In Chapter 4 we show how reflection positivity can be used to prove phase transitions. This chapter is based on a set of lecture notes given in [Bis09].

Finally, in Chapters 5, 6, 7 and 8 the Heisenberg model, spin ice model, 6-vertex model and 16-vertex model are treated in respective order. Reflection positivity is evaluated for different types of reflections, that are suited for the specific models.

This thesis has been written as part of the double bachelor's degree Applied Mathematics and Applied Physics at the Delft University of Technology.

2

Mathematical and Physical tools

This chapter is devoted to cover material from different fields of mathematics and physics that is used throughout this thesis. Necessary definitions and theorems are formulated in the sections below. In this chapter, most of the stated theorems are proved for completeness. Reading these proofs is not necessary for understanding the thesis, however, the reader is invited to do so.

In Section 2.1, the concept of a $*$-algebra is introduced, which is used intensively throughout this thesis. In Section 2.2, some equivalence relations regarding positive semidefinite matrices are proved. Then, in Section 2.3, some useful definitions and theorems concerning quotient spaces and positive semidefinite forms are formulated. In Section 2.4, material in the field of analysis and probability theory is treated. Finally, in Section 2.5, some terms regarding lattice statistical physics are introduced.

2.1. Algebras, rings and fields

In this thesis we use the notions of a field and an algebra over a field extensively, therefore these definitions will be properly defined. For more concepts from abstract algebra we refer to a general textbook such as [HGK04, Gij17].

Let us start by defining a 'ring'.

Definition 2.1 ([HGK04])**.** A *ring* is a nonempty set A together with two binary algebraic operations, $'+'$ and $'\cdot'$, that we call addition and multiplication, respectively, such that for all $a, b, c \in A$ the following axioms are satisfied:

1) $a + (b + c) = (a + b) + c$ (associativity of addition);
2) $a + b = b + a$ (commutativity of addition);
3) there exists an element $0 \in A$, such that $a + 0 = 0 + a = a$ (existence of a zero element);
4) there exists an element $x \in A$, such that $a + x = 0$ (existence of "inverses" for addition);
5) $(a + b) \cdot c = a \cdot c + b \cdot c$ (right distributivity);
6) $a \cdot (b + c) = a \cdot b + a \cdot c$ (left distributivity).

We will write ab instead of $a \cdot b$ to indicate multiplication. A ring with some additional structure is called a field, which is properly defined as follows.

Definition 2.2 ([HGK04])**.** A division ring D is a nonzero ring (i.e. a ring containing more elements then only the zero element) for which all nonzero elements form a group under multiplication. A commutative division ring is called a *field*.

With these definitions we can define an algebra.

Definition 2.3 ([HGK04])**.** An *algebra* over a field k is a set A which is both a ring and a vector space in such a manner that the additive group structures are the same, and the axiom

$$(\lambda a)b = a(\lambda b) = \lambda(ab), \tag{2.1}$$

is satisfied for all $\lambda \in k$ and $a, b \in A$.

In this thesis we mainly work with a $*$*-algebra* $\mathfrak{A}$ over the complex numbers, which is an associative algebra with involution $*$ over a commutative ring R ($\mathbb{C}$) with involution $\bar{\ }$, satisfying $(ab)^* = b^* a^*$ and $(\lambda a + \mu b)^* = \bar{\lambda} a^* + \bar{\mu} b^*$ for all $a, b \in \mathfrak{A}$ and $\lambda, \mu \in R$ (or $\mathbb{C}$). Finally, we will need a subalgebra.

Definition 2.4 ([HGK04])**.** A *subalgebra* over a field k is a subset S of an algebra A, that carries over and is closed under the operations on A.

2.2. Positive semidefinite matrices

In this thesis, positive semidefinite matrices will be used extensively. In this section, we treat some properties of positive semidefinite matrices used in further proofs. We will freely use some basic concepts of linear algebra, that can be looked up in literature such as [Ver17]. For a standard inner product there are two possibilities: it can be defined such that it is linear in the left or in the right component. We will use the convention often used by physicists, which is an inner product that is linear in the right component.

We first define what it means for a matrix to be positive semidefinite.

Definition 2.5. A Hermitian matrix $A \in M_n(\mathbb{C})$ is called *positive semidefinite* if for every $\mathbf{z} \in \mathbb{C}^n$

$$\mathbf{z}^* A\mathbf{z} \geq 0. \tag{2.2}$$

Note that this definition is also applicable for matrices with real components. An important equivalence relation for positive semidefinite matrices is given in the next theorem.

Theorem 2.1. Let $A \in M_n(\mathbb{C})$ be a Hermitian matrix, then the following are equivalent.

a. The matrix A is positive semidefinite.
b. All eigenvalues of A are nonnegative.
c. The matrix can be written as $R^* R$ for some (not necessarily square) matrix R.

Proof. "$a \Rightarrow b$" Let the eigenvalues of A be given by $\lambda_1, ..., \lambda_n$. Since the matrix A is Hermitian, we can choose a basis $\mathcal{B} = \{\mathbf{q}_1, ..., \mathbf{q}_n\}$ of $\mathbb{C}^n$ consisting of eigenvectors of A. Since A is positive semidefinite, it follows that for $i = 1,,, n$, $\mathbf{q}_i^* A\mathbf{q}_i = \lambda_i |\mathbf{q}_i|^2 \geq 0$, from which we conclude that the eigenvalues are nonnegative.

"$b \Rightarrow c$" Suppose all eigenvalues are nonnegative (and thus real). Since A is Hermitian, we can write $A = Q^* DQ$, where $Q \in M_n(\mathbb{C})$ and D is a diagonal matrix with eigenvalues on the diagonal. Since all eigenvalues are nonnegative, we can find a Hermitian matrix C such that $D = C^2$. But then $A = D^* C^* CD = R^* R$, where $R = CD$. Note that possible zero rows in R, resulting from identically zero eigenvalues, can be removed, causing a non-square matrix R.

"$c \Rightarrow a$" Suppose that we can write $A = R^* R$ for some matrix R, and let $\mathbf{z} \in \mathbb{C}^n$. Then $\mathbf{z}^* R^* R\mathbf{z} = (R\mathbf{z})^* R\mathbf{z} = |R\mathbf{z}|^2 \geq 0$. Since $\mathbf{z}$ arbitrary, this proves the claim. □

Another useful property of positive semidefinite matrices, is that they can be written as sums of projection matrices.

Definition 2.6. Let $\mathbf{u}, \mathbf{v} \in \mathbb{C}^n$. The *projection* of $\mathbf{u}$ on $\mathbf{v}$ is given by

$$P_{\mathbf{v}}(\mathbf{u}) = \frac{\langle \mathbf{v}, \mathbf{u} \rangle}{\langle \mathbf{v}, \mathbf{v} \rangle} \mathbf{v}, \tag{2.3}$$

where $\langle\cdot,\cdot\rangle$ denotes the Euclidean inner product. This is a linear transformation, and can thus be written as $P_{\mathbf{v}}(\mathbf{u}) = P_{\mathbf{v}}\mathbf{u}$, where $P_{\mathbf{v}}$ is the *projection matrix* on $\mathbf{v}$ given by

$$P_{\mathbf{v}} := \hat{\mathbf{v}}\hat{\mathbf{v}}^*, \tag{2.4}$$

where $\hat{\mathbf{v}}$ is the vector pointing in the direction of $\mathbf{v}$ with unit length, $\hat{\mathbf{v}} = \frac{\mathbf{v}}{|\mathbf{v}|}$.

Theorem 2.2. Projection matrices are positive semidefinite.

Proof. The proof follows immediately from Theorem 2.1. □

A straightforward yet useful property of projection matrices is the fact that they have one eigenvalue equal to 1, and the rest of the eigenvalues are equal to 0. This can be shown by choosing an orthogonal basis of $\mathbb{R}^n$ containing the vector on which is projected.

Theorem 2.3. Let $A \in M_n(\mathbb{C})$ be a Hermitian matrix. Then A is positive semidefinite if and only if we can write $P = \sum_{i=1}^k a_i P_{\mathbf{q}_i}$, where a_i are positive constants and $P_{\mathbf{q}_i}$ are projection matrices.

Proof. "⇒" A is Hermitian, so we can decompose $A = QDQ^*$, where $Q = [\mathbf{q}_1, \ldots, \mathbf{q}_n]$ and D is a diagonal matrix with the non-negative eigenvalues $\lambda_1, \ldots, \lambda_n$ of A on the diagonal. But then $A = \lambda_1 \mathbf{q}_1\mathbf{q}_1^* + \ldots + \lambda_n \mathbf{q}_n \mathbf{q}_n^*$ which is a positive sum of projection matrices.

"⇐" Suppose we can write $A = \sum_{i=1}^k a_i P_{\mathbf{q}_i}$ as described, and let $\mathbf{z} \in \mathbb{C}^n$ be arbitrary. Then

$$\mathbf{z}^* A\mathbf{z} = \mathbf{z}^*(\sum_{i=1}^k a_i P_{\mathbf{q}_i})\mathbf{z} = \sum_{i=1}^k a_i(\mathbf{z}^* P_{\mathbf{q}_i}\mathbf{z}),$$

and since projection matrices are positive semidefinite, this is a sum of positive coefficients and thus positive. □

2.3. Quotient spaces and positive semidefinite forms

Throughout this thesis we will not only use positive semidefinite matrices; sometimes we will talk about a positive semidefinite form. In this section we show that the quotient space of a vector space with the kernel of a positive semidefinite form induces a normed vector space, where the norm comes from an inner product. From this vector space one can construct a Hilbert space. We, furthermore, prove the Cauchy-Schwartz inequality for positive semidefinite forms.

The definition of a *vector space* and a *subspace* can be found on page 16 and 27, respectively, of [Ver17]. Note that a vector space has great resemblance with an algebra. In particular, an algebra is a vector space operated with multiplication of the elements. Using subspaces we can construct more vector spaces.

Definition 2.7. If V is a vector space over a field K and W is a subspace of V, then we define V/W as the *quotient space*, containing all cosets $[\mathbf{v}]$, where $[\mathbf{v}] = \mathbf{v} + W = \{\mathbf{v} + \mathbf{w} : \mathbf{w} \in W\}$.

In particular, quotient spaces are vector spaces, which is shown in the following theorem.

Theorem 2.4. Let V be a vector space over a field K and let W be a subspace of V, then the quotient space V/W is also a vector space with operations

1. $[\mathbf{v}] + [\mathbf{w}] = [\mathbf{v} + \mathbf{w}]$ for all $[\mathbf{v}], [\mathbf{w}]$ in V/W
2. $c[\mathbf{v}] = [c\mathbf{v}]$ for all c in K and $[\mathbf{v}]$ in V/W

Proof. The proof consists of two parts. First we show that the operations are well-defined, then we show that the operations satisfy the eight axioms.

We show that addition and scalar multiplication are independent of the chosen representative. For this, let $\mathbf{v}$ and $\mathbf{u}$ be representatives for $[\mathbf{v}]$ and $[\mathbf{u}]$ respectively, then $[\mathbf{v}]+[\mathbf{u}] = [\mathbf{v}+\mathbf{u}]$. Now suppose we had chosen other representatives **v'** and **u'**, then it is enough to show that $[\mathbf{v'}+\mathbf{u'}] \subseteq [\mathbf{v}+\mathbf{u}]$. Since $\mathbf{v'} \in [\mathbf{v}]$, we can write $\mathbf{v'} = \mathbf{v}+\mathbf{w}_1$ with $\mathbf{w}_1 \in W$. Similarly $\mathbf{u'} = \mathbf{u}+\mathbf{w}_2$. We find $[\mathbf{v'}+\mathbf{u'}] = \{\mathbf{v'}+\mathbf{u'}+\mathbf{w} : \mathbf{w} \in W\} = \{\mathbf{v}+\mathbf{u}+\mathbf{w}_1+\mathbf{w}_2+\mathbf{w} : \mathbf{w} \in W\} \subseteq \{\mathbf{v}+\mathbf{u}+\mathbf{w} : \mathbf{w} \in W\} = [\mathbf{v}+\mathbf{u}]$, where associativity of vector spaces and the definition of subspaces is used.

Now let **v** be a representative for $[\mathbf{v}]$ and let $c \in K$, then $c[\mathbf{v}] = [c\mathbf{v}]$. Suppose that **v'** is another representative for $[\mathbf{v}]$, then it is enough to show that $[c\mathbf{v'}] \subseteq [c\mathbf{v}]$. Since $\mathbf{v'} \in [\mathbf{v}]$, we can write $\mathbf{v'} = \mathbf{v}+\hat{\mathbf{w}}$ with $\hat{\mathbf{w}} \in W$. Then $[c\mathbf{v'}] = \{c\mathbf{v'}+\mathbf{w} : \mathbf{w} \in W\} = \{c(\mathbf{v}+\hat{\mathbf{w}})+\mathbf{w} : \mathbf{w} \in W\} = \{c\mathbf{v}+c\hat{\mathbf{w}}+\mathbf{w} : \mathbf{w} \in W\} \subseteq \{c\mathbf{v}+\mathbf{w} : \mathbf{w} \in W\}$, where we have used the distributive property of vector spaces and the definition of subspaces. It is thus shown that addition and scalar multiplication are well-defined.

What remains is to show that the eight axioms are satisfied, which follows quickly from the fact that V is a vector space. We conclude that V/W is indeed a vector space. □

Definition 2.8. A *sesquilinear form* S on a vector space V over $\mathbb{C}$ is a function $S : V \times V \to \mathbb{C}$ that is linear in one argument, and antilinear in the other:

- $B(\mathbf{u}+\mathbf{u'},\mathbf{v}) = B(\mathbf{u},\mathbf{v}) + B(\mathbf{u'},\mathbf{v})$
- $B(\mathbf{u},\mathbf{v}+\mathbf{v'}) = B(\mathbf{u},\mathbf{v}) + B(\mathbf{u},\mathbf{v'})$
- $B(\bar{c}\mathbf{u},\mathbf{v}) = B(\mathbf{u},c\mathbf{v}) = cB(\mathbf{u},\mathbf{v})$

We will now move to positive semidefinite forms. Let us first state some definitions.

Definition 2.9. A *positive semidefinite form* over a vector space V over $\mathbb{C}$ is a Hermitian sesquilinear form $\langle\cdot,\cdot\rangle : V \times V \to \mathbb{C}$ such that $\langle\mathbf{v},\mathbf{v}\rangle \geq 0$ for all **v** in V. Notice that because the form is Hermitian, we have $\langle\mathbf{v},\mathbf{v}\rangle \in \mathbb{R}$ for all **v** in V.

Definition 2.10. The *kernel* of a sesquilinear form S on a vector space V is the set $\text{Ker}(S) = \{\mathbf{u} \in V : S(\mathbf{u},\mathbf{v}) = 0 \text{ for all } \mathbf{v} \in V\}$.

A useful property of a kernel is the fact that it is a subspace.

Theorem 2.5. The kernel of a positive semidefinite form $\langle\cdot,\cdot\rangle$ on a vector space V over $\mathbb{C}$ is a subspace of V.

Proof. We show the three properties of a subspace.

Let **u** and **v** in $\text{Ker}(\langle\cdot,\cdot\rangle)$, and choose **w** in V arbitrary. Then $\langle\mathbf{u}+\mathbf{v},\mathbf{w}\rangle = \langle\mathbf{u},\mathbf{w}\rangle + \langle\mathbf{v},\mathbf{w}\rangle = 0+0 = 0$, so $\mathbf{u}+\mathbf{v} \in \text{Ker}(\langle\cdot,\cdot\rangle)$.

Let **v** in $\text{Ker}(\langle\cdot,\cdot\rangle)$, c in $\mathbb{C}$, and choose **w** in V arbitrary. Then $\langle c\mathbf{v},\mathbf{w}\rangle = \bar{c}\langle\mathbf{v},\mathbf{w}\rangle = \bar{c}0 = 0$ so $c\mathbf{v} \in \text{Ker}(\langle\cdot,\cdot\rangle)$. Notice that by choosing $c = 0$ it follows that $\mathbf{0} \in \text{Ker}(\langle\cdot,\cdot\rangle)$. □

Positive semidefinite forms satisfy the Cauchy-Schwartz inequality.

Theorem 2.6. Let $\langle\cdot,\cdot\rangle$ be a positive semidefinite form on a vector space V over $\mathbb{C}$. Then for every vector $\mathbf{v},\mathbf{w}$ in V the Cauchy-Schwarz inequality,

$$|\langle\mathbf{v},\mathbf{w}\rangle|^2 \leq \langle\mathbf{v},\mathbf{v}\rangle\langle\mathbf{w},\mathbf{w}\rangle, \tag{2.5}$$

is satisfied.

Proof. Let t in $\mathbb{R}$ and choose $\mathbf{v},\mathbf{w} \in V$ arbitrary. We find

$$\begin{aligned}
0 \leq& \langle\mathbf{v} - t\overline{\langle\mathbf{v},\mathbf{w}\rangle}\mathbf{w}, \mathbf{v} - t\overline{\langle\mathbf{v},\mathbf{w}\rangle}\mathbf{w}\rangle \\
=& \langle\mathbf{v},\mathbf{v}\rangle - \langle\mathbf{v}, t\overline{\langle\mathbf{v},\mathbf{w}\rangle}\mathbf{w}\rangle - \langle t\overline{\langle\mathbf{v},\mathbf{w}\rangle}\mathbf{w},\mathbf{v}\rangle + \langle t\overline{\langle\mathbf{v},\mathbf{w}\rangle}\mathbf{w}, t\overline{\langle\mathbf{v},\mathbf{w}\rangle}\mathbf{w}\rangle \\
=& \langle\mathbf{v},\mathbf{v}\rangle - t\overline{\langle\mathbf{v},\mathbf{w}\rangle}\langle\mathbf{v},\mathbf{w}\rangle - t\langle\mathbf{v},\mathbf{w}\rangle\langle\mathbf{w},\mathbf{v}\rangle + t^2\overline{\langle\mathbf{v},\mathbf{w}\rangle}\langle\mathbf{v},\mathbf{w}\rangle\langle\mathbf{w},\mathbf{w}\rangle \\
=& \langle\mathbf{v},\mathbf{v}\rangle - 2t|\langle\mathbf{v},\mathbf{w}\rangle|^2 + t^2|\langle\mathbf{v},\mathbf{w}\rangle|^2\langle\mathbf{w},\mathbf{w}\rangle.
\end{aligned}$$

Since this is a real parabola taking only non-negative values, it follows that the discriminant is non-positive, thus

$$4|\langle \mathbf{v}, \mathbf{w}\rangle|^4 - 4|\langle \mathbf{v}, \mathbf{w}\rangle|^2 \langle \mathbf{v}, \mathbf{v}\rangle\langle \mathbf{w}, \mathbf{w}\rangle \leq 0.$$

As $\mathbf{v}$ and $\mathbf{w}$ arbitrary, the Cauchy-Schwarz inequality follows. □

Theorem 2.7. The kernel of a positive semidefinite form is $\{\mathbf{0}\}$ if and only if the positive semidefinite form is an inner product.

Proof. Note that if the kernel of a positive semidefinite form on a vectorspace V equal is to $\{\mathbf{0}\}$, then for every $\mathbf{v} \neq \mathbf{0}$ in V there exists a $\mathbf{w} \neq \mathbf{0}$ sucht that $\langle \mathbf{v}, \mathbf{w}\rangle > 0$. Using the Cauchy-Schwarz inequality (2.5), this means $\langle \mathbf{v}, \mathbf{v}\rangle > 0$. Since $\mathbf{v}$ is arbitrary, it follows that the positive semidefinite form is an inner product. Now suppose that the positive semidefinite form is an inner product, then $\langle \mathbf{v}, \mathbf{v}\rangle > 0$ is satisfied for all $\mathbf{v} \neq \mathbf{0}$ in V, and thus the kernel equals $\{\mathbf{0}\}$. □

A positive semidefinite form on a vector space induces inner product spaces. Using these space one can construct Hilbert spaces, which is a complete, normed vector space, where the norm is induced by an inner product.

Theorem 2.8. Let $\langle\cdot,\cdot\rangle$ be a positive semidefinite form on a vector space V over $\mathbb{C}$. Then $\langle\cdot,\cdot\rangle$ induces a positive semidefinite form on the vector space $V/\mathrm{Ker}(\langle\cdot,\cdot\rangle)$. In particular it is positive definite.

Proof. Let $\mathbf{v}$ be a representative for $[\mathbf{v}]$ and $\mathbf{w}$ a representative for $[\mathbf{w}]$. Than $\langle[\mathbf{v}],[\mathbf{w}]\rangle = \langle \mathbf{v}, \mathbf{w}\rangle$. We show that this is well-defined on $V/\mathrm{Ker}(\langle\cdot,\cdot\rangle)$, and thus independent of the chosen representative. For this, let $\mathbf{v'}$ and $\mathbf{w'}$ be different representatives for $[\mathbf{v}]$ and $[\mathbf{w}]$ respectively. Since $\mathbf{v'} \in [\mathbf{v}]$ we find $\mathbf{v'} = \mathbf{v} + \mathbf{n}_1$ with $\mathbf{n}_1 \in \mathrm{Ker}(\langle\cdot,\cdot\rangle)$. Similarly $\mathbf{w'} = \mathbf{w} + \mathbf{n}_2$. Then $\langle \mathbf{v'}, \mathbf{w'}\rangle = \langle \mathbf{v}+\mathbf{n}_1, \mathbf{w}+\mathbf{n}_2\rangle = \langle \mathbf{v}, \mathbf{w}\rangle + \langle \mathbf{v}, \mathbf{n}_2\rangle + \langle \mathbf{n}_1, \mathbf{w}\rangle + \langle \mathbf{n}_1, \mathbf{n}_2\rangle = \langle \mathbf{v}, \mathbf{w}\rangle$ where all other terms are zero because $\mathbf{n}_1, \mathbf{n}_2 \in \mathrm{Ker}(\langle\cdot,\cdot\rangle)$.

Positive definiteness of the bilinear form follows because for $[\mathbf{v}]$ with representative $\mathbf{v} \notin \mathrm{Ker}(\langle\cdot,\cdot\rangle)$ we have $\langle[\mathbf{v}],[\mathbf{v}]\rangle = \langle \mathbf{v}, \mathbf{v}\rangle > 0$. □

2.4. Analysis and probability theory

In this thesis we use measures and functionals extensively. Recall that a σ-algebra on a set S is a family containing the empty set, the whole set S, complements of sets and countable unions of sets. With this we can define a measure.

Definition 2.11 ([Dud02])**.** A function $\mu : \mathcal{A} \to [0,\infty]$ on a σ-algebra is called a *measure* if it satisfies

1) $\mu(A) \geq 0$ for all $A \in \mathcal{A}$,
2) $\mu(\emptyset) = 0$
3) For any countable collection $(A_k)_{k\geq 1}$ of disjoint sets in $\mathcal{A}$,

$$\mu\left(\bigcup_{k=1}^{\infty} A_k\right) = \sum_{k=1}^{\infty} \mu(A_k). \tag{2.6}$$

We often work with a probability space, which is defined as follows.

Definition 2.12 ([Dud02])**.** A triple $(\Omega, \mathcal{A}, \mu)$ is called a *probability space* if $\mathcal{A}$ is a σ-algebra on the set Ω, and μ is a measure on $\mathcal{A}$ satisfying $\mu(\Omega) = 1$.

We can define measurable functions on a sample space, such a function is called a random variable. The set of all random variables acting on the probability space is an algebra $\mathfrak{A}$. The expectation $\mathbb{E} : \mathfrak{A} \to \mathbb{C}$ of a random variable is defined as

$$\mathbb{E}(A) = \int_{\Omega} A\, d\mu. \tag{2.7}$$

The expectation is an example of a functional.

Definition 2.13. A *linear functional* τ on a vector space V over a field K is a linear map $\tau : V \to K$.

Besides the expectation, an example of a functional is the trace of a matrix.

In most applications in this thesis, we investigate classical models, where we can either use the Gibbs measure or the Boltzmann functional. The Riesz representation theorem allows us to freely switch between measures and functionals. The statement of the Riesz representation theorem is as follows.

Theorem 2.9 ([Rud86])**.** Let X be a locally compact Hausdorff space, and let Λ be a positive linear functional on the space of compact supported continuous functions $C_c(X)$. Then there exists a σ-algebra $\mathfrak{M}$ in X which contains all Borel sets in X, and there exists a unique positive measure μ on $\mathfrak{M}$ which represents Λ in the sense that

$$\Lambda(f) = \int_X f\,d\mu, \qquad \text{for every } f \in C_c(X), \tag{2.8}$$

and which has the following additional properties

1. $\mu(K) < \infty$ for every compact set $K \subset X$.
2. For every $E \in \mathfrak{M}$, we have
$$\mu(E) = \inf\{\mu(V) : E \subset V, V \text{ open}.$$
3. The relation
$$\mu(E) = \sup\{\mu(K) : K \subset E, K \text{ compact}$$
holds for every open set E, and for every $E \in \mathfrak{M}$ with $\mu(E) < \infty$.
4. If $E \in \mathfrak{M}$, $A \subset E$, and $\mu(E) = 0$, then $A \in \mathfrak{M}$.

2.5. Lattice spin models

Throughout this thesis we use a lot of terms connected to lattice statistical physics. The ones that we use most extensively will be clarified here, for more information on the subject one can use e.g. [Sim13, Thi19]

There are several possible definitions of a lattice. In this thesis we use different definitions, depending on the considered model. The definition that imposes the least structure is the one that defines a lattice as a countable set of points in d-dimensional space. With this definition we often require the constraint that the lattice must have some sort of internal structure, such as being invariant under a reflection in a reflection plane. In other words, when the lattice is cut in half, the two parts need to be equal.

A definition that imposes more structure to the lattice is the following:

Definition 2.14 ([Sim13])**.** A *lattice* Λ is an infinite set of points defined by an integer sum of a set of linearly independent primitive lattice vectors.

In simple terms, every lattice point $\lambda \in \Lambda$ has the same surrounding. Such a lattice comes with a reciprocal lattice, that is defined as follows.

Definition 2.15 ([Sim13])**.** Given a (direct) lattice Λ, a point λ' is in the *reciprocal lattice* if and only if

$$e^{i\lambda\cdot\lambda'} = 1, \tag{2.9}$$

for all points $\lambda \in \Lambda$. Here the dot product $\lambda \cdot \lambda'$ means the standard inner product.

In a classical model, we often consider a *spin* S_λ on every lattice point λ. This is a random variable taking values in a closed subset Ω of $\mathbb{R}^\nu$ for some $\nu \geq 1$. In the case of a finite lattice, we sometimes need spins outside of this lattice to properly define the law of of S_Λ. The configuration of spins outside of the lattice will be referred to as S_{Λ^c}.

For a square $N \times \cdots \times N$ lattice, a special boundary condition is the periodic boundary condition. This wraps the lattice around a torus, which can nicely be visualized in two dimensions.

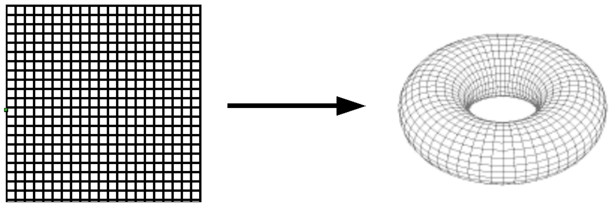

Figure 2.1: Visualization of a two-dimensional cubic lattice with periodic boundary condition.

The energy of a certain configuration of spins on a lattice, is described by the Hamiltonian. This Hamiltonian can often be written as a sum over the lattice points. In the most general form we have

$$H = \sum_{\lambda \in \Lambda} h_\lambda(S), \tag{2.10}$$

where S is the spin configuration in the lattice, and h_λ is the energy to which λ contributes.

For a finite number of possible spin configurations, we can define a probability on every configuration, in terms of the Hamiltonian. This probability is given by

$$\mathbb{P}(S) = \frac{e^{-\beta H(S)}}{Z}, \tag{2.11}$$

where Z is the partition function, a normalisation constant equal to the sum over all configurations at inverse temperature β, $Z = \sum_S e^{-\beta H(S)}$. This probability can also be written as a measure.

In case of an infinite amount of possible spin configurations we can not give a finite probability to every configuration. We then define the probability measure, called the Gibbs measure,

$$\mu_{\Lambda,\beta}^{(S_{\Lambda^c})}(dS_\Lambda) := \frac{e^{-\beta H_\Lambda(S)}}{Z_{\Lambda,\beta}(S_{\Lambda^c})} \prod_{x \in \Lambda} \mu_0(dS_x). \tag{2.12}$$

Here $S := (S_\Lambda, S_{\Lambda^c})$ is the spin configuration, with S_Λ the configuration of spins inside the lattice, and S_{Λ^c} the configuration of spins outside the lattice, the boundary spins.

By the Riesz representation theorem we can exchange the role of the Gibbs measure with a functional. The *expectation* of a random variable A is defined as

$$\mathbb{E}(A) := \int_\Omega A \mu_{\Lambda,\beta}^{(S_{\Lambda^c})}(dS_\Lambda) = \int_\Omega A \frac{e^{-\beta H_\Lambda(S)}}{Z_{\Lambda,\beta}(S_{\Lambda^c})} \prod_{x \in \Lambda} \mu_0(dS_x). \tag{2.13}$$

We call this expectation the Boltzmann functional τ_H. The background functional τ is the second integral without the fraction. When disregarding the partition function, which is a positive constant, we can thus define $\tau_H(A) = \tau(Ae^{-H})$.

This concludes this chapter. We will now move on to defining reflection positivity using the tools developed in this chapter.

3
Reflection positivity

In this chapter, an introduction to reflection positivity is given. The material is based on the framework described in 'reflection positive doubles' [JJ17] by Arthur Jaffe and Bas Janssens, the latter being one of the supervisors of this thesis.

We begin the chapter by developing a general framework for reflection positivity in Section 3.1, covering a wide variety of classical and quantum mechanical systems. We introduce the basic concepts needed to treat reflection positivity in a more specific setting than treated in [JJ17], because where Jaffe and Janssens developed a general framework for bosonic, fermionic and parafermionic systems, in this thesis we only work with bosonic systems. The consequence of this, is that we only talk about bosonic $*$-algebras, whereas Jaffe and Janssens developed their framework for the more general graded algebras. This makes the proofs somewhat more straightforward. In Section 3.2, we state and prove a theorem regarding reflection positivity. This theorem provides us with tractable conditions on the Hamiltonian, and can be used to prove reflection positivity.

I would like to emphasize that this chapter is merely a collection of already known definitions and results. The stated theorems and proofs are already known and published. For additional information on reflection positivity, see [JJ17] or [Bis09].

3.1. Defining reflection positivity

Let $\mathfrak{A}$ be a $*$-algebra. The algebra $\mathfrak{A}$ is required to be a locally convex topological algebra. This means that $\mathfrak{A}$ is a locally convex (Hausdorff) topological vector space, for which multiplication is separately continuous.

To define reflection positivity, we need a reflection $\Theta : \mathfrak{A} \to \mathfrak{A}$. This is defined in the following way.

Definition 3.1. A *reflection* $\Theta : \mathfrak{A} \to \mathfrak{A}$ is a continuous, anti-linear homomorphism which squares to the identity.

We could have chosen to make Θ a continuous, linear antihomomorphism. Then one should replace $\Theta(A)$ with $\Theta(A^*)$ in the remainder of this thesis.

Using this reflection, we let $\mathfrak{A}_+$ be a distinguished subalgebra of $\mathfrak{A}$, and write $\mathfrak{A}_- := \Theta(\mathfrak{A}_+)$ for its reflection. Now define $\mathfrak{A}_-\mathfrak{A}_+ := \{A_-A_+ : A_\pm \in \mathfrak{A}_\pm\}$. Then we require that the linear span of $\mathfrak{A}_-\mathfrak{A}_+$ is dense in $\mathfrak{A}$ and the elements of $\mathfrak{A}_\pm$ satisfy the commutation relation

$$A_-A_+ = A_+A_- \text{ for } A_\pm \in \mathfrak{A}_\pm. \tag{3.1}$$

If these requirements hold, we call $\mathfrak{A}$ the *double* of $\mathfrak{A}_+\mathfrak{A}_-$.

Reflection positivity is defined for reflection invariant functionals.

Definition 3.2. A functional $\varrho : \mathfrak{A} \to \mathbb{C}$ is *reflection invariant* if $\varrho(\Theta(A)) = \overline{\varrho(A)}$ for all $A \in \mathfrak{A}$.

Furthermore we need the notion of sesquilinear forms.

Definition 3.3. Let ϱ be a neutral functional on $\mathfrak{A}$. Then $\langle A, B\rangle_{\Theta,\varrho}$ is the sesquilinear form on $\mathfrak{A}_+$, with

$$\langle A, B\rangle_{\Theta,\varrho} = \varrho(\Theta(A)B), \tag{3.2}$$

for $A, B \in \mathfrak{A}_+$.

Now we are in the position to define reflection positivity.

Definition 3.4. Let $\varrho : \mathfrak{A} \to \mathbb{C}$ be a neutral linear functional. Then ϱ is *reflection positive* on $\mathfrak{A}_+$ with respect to Θ if the form (3.2) is positive semidefinite,

$$\langle A, A\rangle_{\Theta,\varrho} = \varrho(\Theta(A)A) \geq 0, \tag{3.3}$$

for all $A \in \mathfrak{A}_+$

Using these definitions we can formulate and prove some propositions.

Proposition 3.1. Let ϱ be a continuous functional on $\mathfrak{A}$. Then the sesquilinear form (3.2) is Hermitian on $\mathfrak{A}_+$ if and only if ϱ is reflection invariant.

Proof. Let $A, B \in \mathfrak{A}_+$. Using the commutation relation (3.1) we have $A\Theta(B) = \Theta(B)A$. Then $\langle B, A\rangle_{\Theta,\varrho} = \varrho(\Theta(B)A) = \varrho(A\Theta(B))$ and $\overline{\langle A, B\rangle} = \overline{\varrho(\Theta(A)B)}$. If we set $X = \Theta(A)B$ and $\Theta(X) = A\Theta(B)$, we see $\langle B, A\rangle = \overline{\langle A, B\rangle}$ for all $A, B \in \mathfrak{A}_+$ if and only if $\varrho(X) = \overline{\varrho(\Theta(X))}$ for all $X \in \mathfrak{A}_-\mathfrak{A}_+$. Now using continuity of the functional ϱ and the fact that $\mathfrak{A}_-\mathfrak{A}_+$ is dense in $\mathfrak{A}$, the result follows. □

Proposition 3.2. Every continuous, reflection positive functional $\varrho : \mathfrak{A} \to \mathbb{C}$ is reflection invariant.

Proof. Let $A, B \in \mathfrak{A}_+$, then since the functional is sesquilinear and positive semidefinite, we have

$$\langle A+B, A+B\rangle_{\Theta,\varrho} = \langle A, A\rangle_{\Theta,\varrho} + \langle A, B\rangle_{\Theta,\varrho} + \langle B, A\rangle_{\Theta,\varrho} + \langle B, B\rangle_{\Theta,\varrho} \geq 0,$$

so we find $\langle A, B\rangle + \langle B, A\rangle \in \mathbb{R}$. Since A, B arbitrary, we conclude that the sesquilinear form is Hermitian, and thus by Proposition 3.1 we conclude that it is reflection invariant. □

Proposition 3.3. Let $\varrho : \mathfrak{A} \to \mathbb{C}$ be a functional. Then ϱ is reflection positive on $\mathfrak{A}_+$ if and only if it is reflection positive on $\mathfrak{A}_-$.

Proof. Let $A, B \in \mathfrak{A}_-$, then we can define the sesquilinear form on $\mathfrak{A}_-$ by $\langle A, B\rangle_{\Theta,\varrho} := \varrho(\Theta(A)B)$. Now using the commutation relation we find $\langle A, B\rangle_{\Theta,\varrho} = \varrho(\Theta(A)B) = \varrho(B\Theta(A)) = \langle \Theta(B), \Theta(A)\rangle_{\Theta,\varrho}$ where $\Theta(A), \Theta(B) \in \mathfrak{A}_+$. Then reflection positivity of the sesquilinear form on $\mathfrak{A}_+$ is equivalent to reflection positivity of the sesquilinear form on $\mathfrak{A}_-$. □

Using a reflection positive functional, a quantum Hilbert space can be constructed. For this an inner product is needed. This inner product is formed by using the positive semidefinite sesquilinear form on the quotient space of the subalgebra $\mathfrak{A}_+$ and the kernel of the sesquilinear form. As proved in Section 2.3, this is valid.

Definition 3.5. Let ϱ be a reflection positive functional on $\mathfrak{A}$. Let $\mathcal{N} \subseteq \mathfrak{A}_+$ be the kernel of the positive semidefinite form $\langle A, B\rangle_{\Theta,\varrho}$. Then the *quantum Hilbert space* $\mathcal{H}_{\Theta,\varrho}$ is the closure of ${}^{\mathfrak{A}_+}\!/_{\mathcal{N}}$, with inner product induced by the positive definite form $\langle A, B\rangle_{\Theta,\varrho}$.

A useful tool to prove reflection positivity, is making use of the reflection-positive cone. In the bosonic setting, we define this cone as follows.

Definition 3.6. The *reflection-positive cone* $\mathcal{K}_+ \subseteq \mathfrak{A}$ is the set

$$\mathcal{K}_+ = \{\Theta(A)A | A \in \mathfrak{A}_+\}. \tag{3.4}$$

We denote the convex hull of $\mathcal{K}_+$ by $\text{co}(\mathcal{K}_+)$ and its closure by $\overline{\text{co}}(\mathcal{K}_+)$. We show that the set of continuous, reflection positive functionals on $\mathfrak{A}$ is precisely the *continuous dual cone* of $\overline{\text{co}}(\mathcal{K}_+)$ in $\mathfrak{A}$.

Proposition 3.4. Let $\varrho : \mathfrak{A} \to \mathbb{C}$ be a continuous, linear functional. Then the functional ϱ is reflection positive if and only if the functional ϱ is nonnegative on $\overline{\text{co}}(\mathcal{K}_+)$.

Since the proof for graded algebras is equal to the proof for our more specific bosonic algebra, this proposition won't be proved here, but can be read in [JJ17], Proposition $II.18$. The idea of the proof is that both statements are equivalent with the functional ϱ being nonnegative on $\mathcal{K}_+$, which follows from Definition 3.6 and continuity of ϱ.

We will go a bit more into depth on the reflection positive cone, since it is a useful tool for reflection positivity. First of all we prove that $\mathcal{K}_+$ is multiplicatively closed.

Theorem 3.5. The cone $\mathcal{K}_+$ is multiplicatively closed, and it is pointwise invariant under reflection.

Proof. To show that the cone is multiplicatively closed, we show $\mathcal{K}_+\mathcal{K}_+ \subseteq \mathcal{K}_+$. Let $A_1, A_2, B_1, B_2 \in \mathfrak{A}_+$, then

$$(\Theta(A_1)B_1)(\Theta(A_2)B_2) = \Theta(A_1)\Theta(A_2)B_1B_2 = \Theta(A_1A_2)B_1B_2. \tag{3.5}$$

To show that the one is pointwise invariant under reflection, we show that $\Theta|_{\mathcal{K}_+} = Id$. Let $A, B \in \mathfrak{A}_+$. Then the reflection of $\Theta(A)B$ equals is

$$\Theta(\Theta(A)B) = A\Theta(B) = \Theta(B)A. \tag{3.6}$$

In particular, $\Theta(A)A$ is reflection invariant. □

Theorem 3.5 needs to be extended to the closure $\overline{\text{co}}(\mathcal{K}_+)$ of the convex hull $\text{co}(\mathcal{K}_+)$ of $\mathcal{K}_+$, since we are mainly interested in continuous reflection positive functionals. A useful characterization of $\text{co}(\mathcal{K}_+)$ is given in the following proposition.

Proposition 3.6. Let $K \in \mathfrak{A}$. Then $K \in \text{co}(\mathcal{K}_+)$ if and only if both:

1) The element K can be written as a finite sum

$$K = \sum_{I,J \in \mathcal{I}} J_{IJ}\Theta(C_I)C_J, \tag{3.7}$$

with $C_I \in \mathfrak{A}_+$ labelled by a finite set $\mathcal{I}$.

2) Let $(J_{IJ})_{\mathcal{I}}$ be the matrix with entries J_{IJ}, labelled by $I, J \in \mathcal{I}$. Then $(J_{IJ})_{\mathcal{I}}$ is positive semi-definite.

Proof. "⇒" Every $K \in \text{co}(\mathcal{K}_+)$ can be written as a finite convex combination $K = \sum_{r\in\mathcal{I}} p_r\Theta(X_r)X_r$ of elements of $\mathcal{K}_+$. In particular, it is of the form (3.7) with $(J_{IJ}) = p_I\delta_{IJ}$.

"⇐" Suppose that K is of the form (3.7), then the matrix $(J_{IJ})_{\mathcal{I}}$ has nonnegative eigenvalues p_r. Now choose orthonormal eigenvectors $(x_I^r)_{I\in\mathcal{I}}$ and define $X_r = \sum_I x_I^r C_I$, then $X_r \in \mathfrak{A}_+$ and $K = \sum_r p_r\Theta(X_r)X_r \in \text{co}(\mathcal{K}_+)$. □

Now we can characterize the closure $\overline{\text{co}}(\mathcal{K}_+)$ of $\text{co}(\mathcal{K}_+)$ as follows:

Corollary 3.7. An element $K \in \mathfrak{A}$ is in $\overline{\text{co}}(\mathcal{K}_+)$ if and only if $K = \lim_{n\to\infty} K_n$, with $K_n \in \text{co}(\mathcal{K}_+)$ as in (3.7).

Corollary 3.8. The closed, convex cone $\overline{\text{co}}(\mathcal{K}_+)$ is multiplicatively closed, and it is pointwise invariant under reflection.

For the proof of the latter we refer to Corollary IV.6 in [JJ17] , since the proof for graded algebras is equal to the one for bosonic algebras.

In the applications in this thesis, the functionals τ_H are perturbations of a fixed functional τ by the Hamiltonian H. Here the Hamiltonian $H \in \mathfrak{A}$ is a reflection invariant operator, $\Theta(H) = H$, and $\tau : \mathfrak{A} \to \mathbb{C}$ is a continuous, reflection positive functional on $\mathfrak{A}$. If the exponential series for e^{-H} converges, then the *Boltzmann functional* $\tau_H : \mathfrak{A} \to \mathbb{C}$ is defined by

$$\tau_H(A) = \tau(Ae^{-H}). \tag{3.8}$$

The Boltzmann functional is continuous and reflection invariant, since both $A \mapsto Ae^{-H}$ and $A \mapsto \tau(A)$ are continuous, and both H and τ are reflection invariant. Furthermore, if τ_H is reflection positive for $H \in \mathfrak{A}$, then it is reflection positive for every shift $H' + \Delta I$ with $\Delta \in \mathbb{R}$, since $\tau_{H'} = e^{-\Delta}\tau_H$.

To show that τ_H is reflection positive, the first step is to show that the background functional τ is reflection positive. This can be done using the following factorization criterion.

Definition 3.7. Let $\tau : \mathfrak{A} \to \mathbb{C}$ be a continuous, reflection invariant functional. Then τ is *factorizing* if there exists a continuous functional τ_+ on $\mathfrak{A}_+$ such that

$$\tau(\Theta(A)B) = \overline{\tau_+(A)}\tau_+(B), \tag{3.9}$$

for all $A, B \in \mathfrak{A}_+$.

Since τ is reflection invariant, this is equivalent to

$$\tau(AB) = \tau_-(A)\tau_+(B), \tag{3.10}$$

for $A \in \mathfrak{A}_-, B \in \mathfrak{A}_+$. Here $\tau_-(B) := \overline{\tau_+(\Theta(B))}$ for $B \in \mathfrak{A}_-$. The factorizing functional τ is uniquely determined by $\tau_+ : \mathfrak{A}_+ \to \mathbb{C}$ since the span of $\mathfrak{A}_-\mathfrak{A}_+$ is dense in $\mathfrak{A}$. If the background functional is factorizing, it is reflection positive. This is shown in the following proposition.

Proposition 3.9. Every factorizing functional $\tau : \mathfrak{A} \to \mathbb{C}$ is reflection positive.

Proof. Let $A \in \mathfrak{A}_+$, then $\tau(\Theta(A)A) = \overline{\tau_+(A)}\tau_+(A) \geq 0$. □

A useful property to determine conditions on H such that τ_H is reflection positive, is the notion of strictly positive functionals.

Definition 3.8. The functional $\tau_+ : \mathfrak{A}_+ \to \mathbb{C}$ is *strictly positive* if

$$\tau_+(A^* A) > 0, \tag{3.11}$$

for all nonzero $A \in \mathfrak{A}_+$.

If τ is factorizing such that τ_+ is strictly positive, then the scalar product $\langle A, B\rangle = \tau_+(A^* B)$ on $\mathfrak{A}_+$ is nondegenerate.

One of the ways to determine whether the functional τ_H is reflection positive, is by using the matrix of coupling constants. For this, we require that $\mathfrak{A}_+$ has a countable Schauder basis.

Definition 3.9. A *Schauder basis* is a countable, ordered set $\{v_I\}_{I\in\mathcal{I}}$ of elements in $\mathfrak{A}_+$ such that every $A \in \mathfrak{A}_+$ has a unique expansion $A = \sum_{I\in\mathcal{I}} a_I v_I$.

Using the Gram-Schmidt procedure, a Schauder basis $\{C_I\}_{I\in\mathcal{I}}$ of $\mathfrak{A}_+$ with the following properties can be found:

B1. There is a unit $C_{I_0} = \mathbf{1}$, for some distinguished index $I_0 \in \mathcal{I}$.
B2. For all $I, J \in \mathcal{I}$, one has $\tau_+(C_I^* C_J) = \delta_{IJ}$, where δ is the Dirac delta function.
B3. The linear span of $\{C_I\}_{I\in\mathcal{I}}$ is dense in $\mathfrak{A}_+$.

Any set $\{C_I\}_{I\in\mathcal{I}}$ satisfying $B1-3$ is a Schauder basis, since every $A \in \mathfrak{A}_+$ has a unique expansion $A = \sum_{I\in\mathcal{I}} a_I C_I$, with $a_I = \tau(C_I^* A)$.

Using the orthogonal basis of $\mathfrak{A}_+$, we construct a basis of A by defining the operators

$$B_{IJ} = \Theta(C_I)C_J, \quad \text{and} \quad \hat{B}_{IJ} = \Theta(C_I^*)C_J^*. \tag{3.12}$$

These operators are dual in the sense that

$$\tau(\hat{B}_{IJ} B_{I'J'}) = \delta_{II'}\delta_{JJ'}, \tag{3.13}$$

which is easily shown by using the commutation relation and the fact that the functional is factorizing and that $\Theta(A)\Theta(B) = \Theta(AB)$.

As the linear span of $\mathfrak{A}_-\mathfrak{A}_+$ is dense in $\mathfrak{A}$, every $A \in \mathfrak{A}$ has a convergent expansion

$$A = \sum_{(I,J)\in\mathcal{I}\times\mathcal{I}} a_{IJ} B_{IJ}. \tag{3.14}$$

This sum requires an order on $\mathcal{I} \times \mathcal{I}$ which can be obtained in a natural way from the order on $\mathcal{I}$.

The expansion (3.14) of $A \in \mathfrak{A}$ is unique, and the coefficients $a_{IJ} = \tau(\hat{B}_{IJ} A)$ depend continuously on A, which is a consequence of (3.13).

Since $\Theta(B_{IJ}) = B_{JI}$, an operator $A \in \mathfrak{A}$ is reflection invariant, $\Theta(A) = A$, if and only if the matrix is $(a_{IJ})_{\mathcal{I}}$ is Hermitian.

Every Hamiltonian $H \in \mathfrak{A}$ has a unique expansion

$$-H = \sum_{(I,J)\in\mathcal{I}\times\mathcal{I}} J_{IJ}\Theta(C_I)C_J. \tag{3.15}$$

The matrix $(J_{IJ})_{\mathcal{I}}$ describes the couplings between $C_J \in \mathfrak{A}_+$ and $\Theta(C_I) \in \mathfrak{A}_-$.

Definition 3.10. The matrix $(J_{IJ})_{\mathcal{I}}$ is called the *matrix of coupling constants.*

In the matrix of coupling constants, the term $J_{I_0J_0}$ describes the coefficient of the identity. Furthermore the terms J_{I_0J} describes couplings inside $\mathfrak{A}_+$ and the terms J_{II_0} describe couplings inside $\mathfrak{A}_-$. The terms J_{IJ} with $I, J \neq I_0$ describe couplings between $\mathfrak{A}_-$ and $\mathfrak{A}_+$

Definition 3.11. The submatrix $(J^0_{IJ})_{\mathcal{I}\setminus\{I_0\}}$ of $(J_{IJ})_{\mathcal{I}}$, consisting of elements with $I, J \neq I_0$, is called the *matrix of coupling constants across the reflection plane.*

Proposition 3.10. If the matrix of coupling constants $(J_{IJ})_{\mathcal{I}}$ is Hermitian, then H is reflection invariant. If it is positive semidefinite, then $-H \in \overline{\text{co}}(\mathcal{K}_+)$

Proof. Reflection invariance follows from the fact that $A \in \mathfrak{A}$ is reflection invariant if and only if the matrix of its expansion is Hermitian. Furthermore, $-H \in \overline{\text{co}}(\mathcal{K}_+)$ since every finite partial sum of (3.15) is of the form (3.7) if the matrix $(J_{IJ})_{\mathcal{I}}$ is positive semidefinite. □

Using the developed framework, we can find necessary and sufficient conditions to prove reflection positivity.

3.2. Characterization of reflection positivity

We wish to determine whether or not τ_H is reflection positive in terms of tractable conditions on the Hamiltonian H. For this we assume

Q1. $\mathfrak{A}$ is a locally-convex, topological algebra.
Q2. $\mathfrak{A}$ is the double of $\mathfrak{A}_+$.
Q3. $\tau : \mathfrak{A} \to \mathbb{C}$ is continuous and reflection positive.
Q4. The algebra $\mathfrak{A}_+$ is a $*$-algebra, and $\mathfrak{A}_+$ admits an unconditional Schauder basis.
Q5. The functional $\tau : \mathfrak{A} \to \mathbb{C}$ factorizes into τ_+ and τ_-.
Q6. The functional $\tau_+ : \mathfrak{A}_+ \to \mathbb{C}$ is strictly positive.

If we furthermore require that the exponential $\exp : \mathfrak{A} \to \mathfrak{A}$ is continuous, and $\beta \mapsto \exp(-\beta H)$ is differentiable at zero, we can state the following theorem with necessary and sufficient conditions for reflection positivity of the Boltzmann functional. This theorem is used to prove reflection positivity in the applications of Chapter 5, 6, 7 and 8.

Theorem 3.11. Let τ be a continuous, factorizing functional on $\mathfrak{A}$, and suppose that τ_+ is strictly positive. Let $H \in \mathfrak{A}$ be a reflection invariant operator. Then the following are equivalent:

a. The Boltzmann functional $\tau_{\beta H}$ is reflection positive for all $0 \le \beta$.
b. There exists an $\epsilon > 0$ such that $\tau_{\beta H}$ is reflection positive for $0 \le \beta < \epsilon$.
c. The matrix $(J^0_{IJ})_{\mathcal{I}}$ of coupling constants across the reflection plane is positive semidefinite.
d. There is a decomposition $H = H_- + H_0 + H_+$, with $H_+ \in \mathfrak{A}_+$, with $-H_0 \in \overline{\mathrm{co}}(\mathcal{K}_+)$, and with $H_- = \Theta(H_+)$.

We will prove this theorem with help of a sufficient condition for reflection positivity, and a necessary condition.

If we only assume Q1-3 and the natural condition that $\exp : \mathfrak{A} \to \mathfrak{A}$ is continuous, already a sufficient condition for reflection positivity of the Boltzmann functional $\tau_H(A) = \tau(Ae^{-H})$ for an element $H \in \mathfrak{A}$ can be found. This sufficient condition will be constructed below.

Proposition 3.12. Let $A \mapsto \tau(A)$ be a continuous, reflection positive functional on $\mathfrak{A}$, and let $K_1, K_2 \in \overline{\mathrm{co}}(\mathcal{K}_+)$, Then the functionals

$$A \mapsto \tau(K_1 A), \quad A \mapsto \tau(AK_2), \quad \text{and} \quad A \mapsto \tau(K_1 A K_2),$$

are also continuous and reflection positive.

Proof. Using Proposition 3.4, it suffices to show that if $A \in \overline{\mathrm{co}}(\mathcal{K}_+)$, then also KA, AK, and KAK in $\overline{\mathrm{co}}(\mathcal{K}_+)$, which follows from Corollary 3.8. Since multiplication is separately continuous, the continuity follows from continuity of τ. □

Proposition 3.13. Suppose that $-H \in \overline{\mathrm{co}}(\mathcal{K}_+)$, and that the exponential series

$$\exp(-H) - I = \sum_{k=1}^{\infty} \frac{1}{k!}(-H)^k \tag{3.16}$$

converges in $\mathfrak{A}$. If τ is a continuous, reflection positive functional, then the Boltzmann functional $\tau_H(A) = \tau(Ae^{-H})$ is also continuous and reflection positive. Its reflection positive inner product dominates that of τ,

$$\langle A, A\rangle_{\Theta,\tau_H} \ge \langle A, A\rangle_{\Theta,\tau} \quad \text{for all } A \in \mathfrak{A}_+. \tag{3.17}$$

Proof. Since $\overline{\text{co}}(\mathcal{K}_+)$ is a closed convex cone, that is multiplicatively closed, we find that every partial sum of (3.16) is contained in the cone and thus $e^{-H} - I \in \overline{\text{co}}(\mathcal{K}_+)$. Now using Proposition 3.12, the functional $A \mapsto \tau(A(e^{-H} - I))$ is continuous and reflection positive. It follows that

$$\tau_H(\Theta(A)A) = \tau((\Theta(A)A)e^{-H}) \geq \tau(\Theta(A)A) \geq 0,$$

for all $A \in \mathfrak{A}_+$. In particular, τ_H is reflection positive. □

Theorem 3.14. Suppose that the exponential series $\exp(A) = \sum_{k=0}^{\infty} \frac{1}{k!} A^k$ converges for all $A \in \mathfrak{A}$, and that $\exp : \mathfrak{A} \to \mathfrak{A}$ is continuous. Let $\tau : \mathfrak{A} \to \mathbb{C}$ be a continuous, reflection positive functional. Let $H \in \mathfrak{A}$ admit a decomposition

$$H = H_- + H_0 + H_+, \tag{3.18}$$

with $H_+ \in \mathfrak{A}_+$, $-H_0 \in \overline{\text{co}}(\mathcal{K}_+)$, and with $H_- = \Theta(H_+)$. Then the Boltzmann functional $\tau_H(A) = \tau(Ae^{-H})$ is continuous and reflection positive.

Proof. For $\epsilon > 0$, define $H_\epsilon \in \mathfrak{A}$ by

$$H_\epsilon = H_0 - \Theta(\epsilon^{-1}I - \epsilon H_+)(\epsilon^{-1}I - \epsilon H_+).$$

Let $A \in \mathfrak{A}_+$. As $-H_\epsilon \in \overline{\text{co}}(\mathcal{K}_+)$, by Proposition 3.13 we have

$$\tau((\Theta(A)A)e^{-H_\epsilon}) \geq 0. \tag{3.19}$$

Since additive constants in the Hamiltonian do not change reflection positivity, we have $H'_\epsilon = H - \epsilon^2\Theta(H_+)H_+$, which satisfies

$$\tau((\Theta(A)A)e^{-H'_\epsilon}) \geq 0.$$

Since $\lim_{\epsilon\downarrow 0} H'_\epsilon = H$ and $\exp : \mathfrak{A} \to \mathfrak{A}$ is continuous, we conclude

$$\lim_{\epsilon\downarrow 0} \tau((\Theta(A)A)e^{-H'_\epsilon}) = \tau((\Theta(A)A)e^{-H}) \geq 0.$$

□

Remark 3.15. If H satisfies the condition of Theorem 3.14, then the Boltzmann functional $\tau_{\beta H}$ is reflection positive for all $\beta \geq 0$.

One might notice that this is the statement $d \Rightarrow a$ in Theorem 3.11. In addition to Q1-3 we now also assume Q4-6.

Lemma 3.16. Suppose that the exponential series for $\exp(-\beta H)$ converges, and is differentiable at $\beta = 0$. If $\tau_{\beta H}$ is reflection positive for all $\beta \in [0,\epsilon)$, then

$$\tau((\Theta(A)A)H) \leq 0, \tag{3.20}$$

for all $A \in \mathfrak{A}_+$ with $\tau(\Theta(A)A) = 0$.

Since the proof of this lemma is equal to the proof of Lemma V.8 in [JJ17], one can read it there.

Theorem 3.17. Suppose there exists an $\epsilon > 0$ such that the map $\beta \mapsto \exp(-\beta H)$ is well-defined on $\beta \in [0,\epsilon)$, and differentiable at $\beta = 0$. If $\tau_{\beta H}$ is reflection positive for all $\beta \in [0,\epsilon)$, then the matrix $(J^0_{IJ})_{\mathcal{I}\setminus\{I_0\}}$ of coupling constants across the reflection plane is positive semidefinite.

Proof. Let $A \in \mathfrak{A}_+$ with $\tau_+(A) = 0$. Since τ factorizes, we have $\tau(\Theta(A)A) = |\tau_+(A)|^2 = 0$. Now insert the expansion (3.15) into the expression (3.20), and use commutativity to find

$$0 \leq \sum_{I,J \in \mathcal{I}} J_{IJ} \tau((\Theta(A)A)(\Theta(C_I)C_J)) = \sum_{I,J \in \mathcal{I}} J_{IJ} \tau(\Theta(AC_I)AC_J) = \sum_{I,J \in \mathcal{I}} J_{IJ} \bar{\alpha}_I \alpha_J, \tag{3.21}$$

with $\alpha_I = \tau_+(AC_I)$. Note that $\alpha_{I_0} = \tau_+(A) = 0$. It suffices to check $0 \leq \sum_{I,J} J_{IJ} \bar{\chi}_I \chi_J$ for vectors $(\chi_I)_{\mathcal{I}}$ with finitely many nonzero entries. Our attention can be restricted to vectors for which $\chi_{I_0} = 0$, since we are interested in positivity of the submatrix $(J^0_{IJ})_{\mathcal{I} \setminus \{I_0\}}$ of coupling constants across the reflection plane.

Let $(\chi_I)_{\mathcal{I}}$ be a vector as described above, and set $A = \sum_{I \in \mathcal{I}} \chi_I C_I^*$. Note that $\tau_+(AC_I) = \chi_I$, since $\tau_+(C_I^* C_J) = \delta_{IJ}$. Combining this with (3.21), gives $0 \leq \sum_{I,J} J^0_{IJ} \bar{\chi}_I \chi_J$ as required. □

One might notice that this is the implication $b \Rightarrow c$ in Theorem 3.11. Now we are finally in the position to prove Theorem 3.11, so let us proceed.

Proof of Theorem 3.11. The implication $a \Rightarrow b$ is clear. The implication $b \Rightarrow c$ is Theorem 3.17. For $c \Rightarrow d$, note that since $H \in \mathfrak{A}$ is reflection invariant and $(J^0_{IJ})_{\mathcal{I} \setminus \{I_0\}}$ is positive semidefinite, we can decompose H as $H = H_+ + H_0 + H_-$ with $-H_0 \in \overline{\mathrm{co}}(\mathcal{K}_+)$, $H_+ \in \mathfrak{A}_+$ and $\Theta(H_+) = H_-$, where the operators H_0 and H_+ are given in terms of the matrix of coupling constants by

$$-H_0 = \sum_{I,J \in \mathcal{I} \setminus \{I_0\}} J^0_{IJ} \Theta(C_I) C_J, \tag{3.22}$$

$$-H_+ = \frac{1}{2} J_{I_0 J_0} \mathbf{1} + \sum_{J \in \mathcal{I} \setminus \{I_0\}} J_{I_0 J} C_J. \tag{3.23}$$

Finally implication $d \Rightarrow a$ is Theorem 3.15. □

In the applications described in this thesis, most important are the equivalencies $a \Longleftrightarrow c$ and $a \Longleftrightarrow d$, since c and d are properties of the Hamiltonian H that can concretely be examined.

With the proof of Theorem 3.11 the necessary material on reflection positivity is covered. It remains to show how these rather abstract properties of functionals can be used to prove phase transitions. That will be the topic of the next chapter.

4

Phase transitions

One of the main applications of reflection positivity, is establishing the occurrence of phase transitions. In this chapter a brief overview of how reflection positivity can be used to prove phase transitions is given. This generally boils down to two types of arguments one can make, the first is based on infrared bounds, while the second is based on chessboard estimates.

The chapter consists of three sections. In Section 4.1 we explain how a phase transition is mathematically defined. In Section 4.2 the method of proving phase transitions using the infrared bound is treated. Finally in section 4.3 it is explained what chessboard estimates are, and how they can be used to prove phase transitions.

This chapter is meant as a mere overview of how to use reflection positivity in practice. In this thesis, the theory will not be applied to the models that are studied, therefore the exact proofs of the stated theorems will not be discussed. For a more complete overview, where all definitions and theorems are stated in more detail, we refer the reader to the lecture notes provided by Marek Biskup [Bis09] or the book by Sacha Friedli and Yvan Velenik [FV17].

4.1. Defining phase transitions

To describe phase transitions, we will slightly alter the framework developed in Chapter 3.1, since we work with probability measures instead of functionals. Given a finite set $\Lambda \subset \mathbb{Z}^d$ together with a spin configuration $S_\Lambda := (S_x)_{x\in\Lambda}$, where S_x takes values in a probability space Ω for all $x \in \Lambda$, and given a Hamiltonian H_Λ and boundary condition S_{Λ^c}, the *Gibbs measure* in Λ is the probability measure on Ω^Λ given by

$$\mu_{\Lambda,\beta}^{(S_{\Lambda^c})}(dS_\Lambda) := \frac{e^{-\beta H_\Lambda(S)}}{Z_{\Lambda,\beta}(S_{\Lambda^c})} \prod_{x\in\Lambda} \mu_0(dS_x). \tag{4.1}$$

In Section 2.5 we have already shown that this measure is the 'dual' of the Boltzmann functional. To identify phase transitions, this measure needs to be extended to infinite volume, for which a distinguishing property of Gibbs measures is used.

Lemma 4.1. Let $\Lambda \subset \Delta \subset \mathbb{Z}^d$ be finite sets and let $S_{\Delta^c} \in \Omega^{\Delta^c}$. Then (for $\mu_{\Delta,\beta}^{(S_{\Delta^c})} - a.e.\ S_{\lambda^c}$),

$$\mu_{\Delta,\beta}^{(S_{\Delta^c})}(\cdot|S_{\Lambda^c}) = \mu_{\Lambda,\beta}^{(S_{\Lambda^c})}(\cdot). \tag{4.2}$$

In other words, conditioning the Gibbs measure in Δ on the configuration in $\Delta \setminus \Lambda$, gives the Gibbs measure in Λ with corresponding boundary condition. This leads to the following definition.

Definition 4.1. A probability measure on $\Omega^{\mathbb{Z}^d}$ is called an *infinite volume Gibbs measure* for interaction H and inverse temperature β if for all finite $\Lambda \subset \mathbb{Z}^d$ and $\mu - a.e.\ S_{\Lambda^c}$,

$$\mu(\cdot|S_{\Lambda^c}) = \mu_{\Lambda,\beta}^{(S_{\Lambda^c})}(\cdot), \tag{4.3}$$

where $\mu^{(S_{\Lambda^c})}_{\Lambda,\beta}$ is defined using the Hamiltonian H_Λ.

Remark 4.2. The distinguishing property of Lemma 4.1 is called the DLR condition, named after Dobrushin, Lanford and Ruelle. One might wonder why we do not use Kolmogorov's extension theorem, which is the standard approach to construct infinite collections of dependent random variables, and uses marginal distributions. This is because in general there is no way to express the marginals associated to an infinite volume Gibbs measure without making explicit reference to the latter. Dobrushin, Lanford and Ruelle showed that considering conditional probabilities instead of marginals is much better suited to our needs.

The set of all infinite volume Gibbs measures at inverse temperature β is denoted by $\mathfrak{G}_\beta$. We can now define phase transitions.

Definition 4.2. The model is at *phase coexistence* (or undergoes a *first-order phase transition*) whenever the parameters are such that $|\mathfrak{G}_\beta| > 1$.

This definition essentially means that in the thermodynamic limit, providing a complete microscopical description of the system as well as well as fixing the relevant thermodynamic parameters is not sufficient to completely determine the macroscopic behaviour of the system. Since this is a rather complicated definition, it may be useful to briefly consider an example.

Example 4.1. Consider the Ising model, that on every lattice point takes the value $S_\lambda = \pm 1$, on a lattice $\Lambda_L := \{1,...,L\}^d$, with Hamiltonian $H(S) := -J\sum_{\langle x,y\rangle} S_x \cdot S_y$. Set all boundary spins to $+1$ (the *plus boundary condition*). It can be shown that the measure $\mu^+_{\Lambda_L,\beta}$ tends to a measure μ^+ as $L \to \infty$. Similarly for the *minus* boundary condition, $\mu^-_{\Lambda_L,\beta} \to \mu^-$ when $L \to \infty$. In dimensions $d \geq 2$, it turns out there exists $\beta_c(d) \in (0,\infty)$ such that

$$\beta > \beta_c(d) \Rightarrow \mu^+ \neq \mu^-, \tag{4.4}$$

which means the model is at phase coexistence, while for $\beta < \beta_c(d)$ the set of infinite volume Gibbs measures is a singleton.

This can be interpreted as that for low enough temperatures, the direction of spins in the model is influenced by the direction of spins far, far away, while for higher temperatures only spins nearby influence the direction of a spin.

4.2. Infrared bound

Consider the $O(n)$-model, which is a model on an $L \times \cdots \times L$ lattice wrapped around a torus $\mathbb{T}_L$ with Hamiltonian

$$H = -\frac{1}{2}\sum_{x,y} J_{xy} S_x \cdot S_y, \tag{4.5}$$

where the spins S_x are a priori independent and distributed according to a measure μ_0, supported in the set $\Omega := \mathbb{S}^{n-1} = \{z \in \mathbb{R}^n : |z|_2 = 1\}$. We assume the interactions are (a convex combination of)

a) Nearest-neighbour interactions:

$$J_{x,y} = \begin{cases} \frac{1}{2d}, & \text{if } |x-y| = 1, \\ 0, & \text{otherwise.} \end{cases} \tag{4.6}$$

b) Yukawa potentials:

$$J_{x,y} = Ce^{-\mu|x-y|_1}, \tag{4.7}$$

with $\mu > 0$ and $C > 0$.

c) Power-law decaying potentials:

$$J_{x,y} = \frac{C}{|x-y|_1^s}, \tag{4.8}$$

with $s > d$ and $C > 0$.

We furthermore assume the interaction constants to satisfy

1) $J_{x,x} = 0$ and $J_{x,y} = J_{0,y-x}$,
2) $\sum_x J_{0,x} = 1$.

Since all coupling constants are positive, we can interpret the coupling constants as transition probabilities of a random walk (X_n) on $\mathbb{Z}^d$. Explicitely

$$\mathsf{P}_z(X_{n+1} = y | X_n = x) := J_{x,y}, \tag{4.9}$$

where P_z is the law of a random walk started at site z. This walk can be recurrent or transient, i.e. a walk started at the origin returns there infinitely, or only finitely many times. We can formulate the following criterion.

Lemma 4.3. Let $\hat{J}(k) := \sum_x J_{0,x} e^{ikx}$, $k \in [-\pi,\pi]^d$. Then (X_n) is transient if and only if

$$\int_{[-\pi,\pi]^d} \frac{1}{(2\pi)^d} \frac{1}{1-\hat{J}(k)} dk < \infty. \tag{4.10}$$

The finiteness of this integral is sufficient for the existence of a symmetry-breaking phase transition in spin systems of the kind (4.5). This is summarized in the following theorem.

Theorem 4.4. Let (J_{xy}) be one of the 3 interactions above. Then global rotation symmetry of the $O(n)$-model is broken at low temperatures if and only if the random walk driven by (J_{xy}) is transient.

The proof relies on three theorems. For the backward direction, the principal tool is the infrared bound. To prove the infrared bound, reflection positivity is needed. The formulation of the infrared bound is the following:

Theorem 4.5. Let L be an even integer and consider the model (4.5) on a torus $\mathbb{T}_L$ with Gibbs measure $\mu_{L,\beta}$. Suppose (J_{xy}) is one of the three interactions above, and let

$$c_{L,\beta}(x) := E_{\mu_{L,\beta}}(S_0 \cdot S_x). \tag{4.11}$$

Define $\hat{c}_{L,\beta}(k) := \sum_{x\in\mathbb{T}_L} c_{L,\beta}(x) e^{ikx}$. Then

$$\hat{c}_{L,\beta}(k) \le \frac{v}{2\beta} \frac{1}{1-\hat{J}(k)}, \qquad k \in \mathbb{T}_L^* \setminus \{0\}, \tag{4.12}$$

where v is the dimension of the spin vectors and $\mathbb{T}_L^*$ is the reciprocal torus, $\mathbb{T}_L^* := \{\frac{2\pi}{L}(n_1,\dots,n_d) : n_i = 0,\dots,L-1\}$.

Using the infrared bound, the following theorem, which is the backward direction of Theorem 4.4, can be proved.

Theorem 4.6. Consider the $O(n)$-model with $n \ge 1$ and one of the three interactions above. Let

$$\beta_0 := \frac{n}{2} \int_{[-\pi,\pi]^d} \frac{1}{(2\pi)^d} \frac{1}{1-\hat{J}(k)} dk. \tag{4.13}$$

Then for any $\beta > \beta_0$ and any $\phi \in \mathbb{S}^{n-1}$ there exists $\mu_\phi \in \mathfrak{G}_\beta$ which is translation invariant and ergodic such that

$$\frac{1}{|\Lambda_L|} \sum_{x\in\Lambda_L} S_x \to m_* \phi, \qquad \mu_\phi - \text{a.s.}, \tag{4.14}$$

as $L \to \infty$ and for some $m_* = m_*(\beta) > 0$.

Note that for β_0 to exist, the random walk must be transient. The forward direction (4.4) is proved by the following theorem.

Theorem 4.7. Let $n \geq 2$ and consider the $O(n)$-model with non-negative interaction constants $(J_{x,y})$ satisfying the conditions 1) and 2). Suppose the corresponding random walk is recurrent. Then every $\mu \in \mathfrak{G}_\beta$ is invariant under any simultaneous rotation of all spins.

These theorems are all restricted to specific situations. The infrared bound is formulated for periodic boundary conditions on a torus lattice, and the coupling interactions are required to have a very specific form. There is another way to prove phase transitions, which is using the method of chessboard estimates.

4.3. Chessboard estimates

In the setting of Section 3, when a functional τ is reflection positive, we can write it as a positive semidefinite form on $\mathfrak{A}_+$. By Theorem 2.6 we know that this positive semidefinite form satisfies the Cauchy-Schwartz inequality. In terms of measures and expectations, that is

$$[E_\mu(f\theta g)]^2 \leq E_\mu(f\theta f)E_\mu(g\theta g). \tag{4.15}$$

When we work in the specific setting of a torus model, and we consider reflections through sites or through bonds, then an enhanced version of this inequality is given in the following lemma.

Lemma 4.8. Let μ be reflection positive with respect to a reflection θ and let $A, B, C_\alpha, D_\alpha \in \mathfrak{A}_+$. Then

$$[E_\mu(e^{A+\theta B+\sum_\alpha C_\alpha \theta D_\alpha})]^2 \leq [E_\mu(e^{A+\theta A+\sum_\alpha C_\alpha \theta C_\alpha})][E_\mu(e^{B+\theta B+\sum_\alpha D_\alpha \theta D_\alpha})]. \tag{4.16}$$

Note that this version of the Cauchy-Schwarz inequality is useful since we often work with Gibbs measures, where the exponent plays a major role.

We now restrict our attention further to reflections through planes of sites. Pick two integers, $B < L$, such that B divides L and L/B is even. Fixing the origin of the torus, let Λ_B the block corresponding to $\{0, 1, ..., B\}^d$, then $\mathbb{T}_L$ can be covered by translates of Λ_B,

$$\mathbb{T}_L = \bigcup_{t \in \mathbb{T}_{L/B}} (\Lambda_B + Bt), \tag{4.17}$$

where the translates are indexed by the sites in a factor torus, $\mathbb{T}_{L/B}$.

Definition 4.3. A function $f : \Omega^{\mathbb{T}_L} \to \mathbb{R}$ is called a *B-block function* if it depends only on $\{S_x : x \in \Lambda_B\}$. An event $\mathcal{A} \subset \Omega^{\mathbb{T}_L}$ is called a *B-block event* if the indicator function $1_\mathcal{A}$ is a B-block function.

Given a B-block function f, and $t \in \mathbb{T}_{L/B}$, define $\theta_t f$ the reflection of f into $\Lambda_B + Bt$, that is constructed by consecutive reflecting along a path from Λ_B to $\Lambda_B + Bt$. The result is a function that depends only on $\{S_x : x \in \Lambda_B + Bt\}$. Since reflections commute and satisfy $\theta^2 = \mathrm{Id}$, there are only 2^d distinct functions. The chessboard estimate is now given in the following theorem.

Theorem 4.9. Suppose μ is reflection positive with respect to all reflections between the neighbouring blocks of the form $\Lambda_B + Bt$, $t \in \mathbb{T}_{L/B}$. Then for any B-block functions $f_1, ..., f_m$ and any distinct $t_1, ..., t_m \in \mathbb{T}_{L/B}$,

$$E_\mu\left(\prod_{j=1}^m \theta_{t_j} f_j\right) \leq \prod_{j=1}^m \left[E_\mu\left(\prod_{t \in \mathbb{T}_{L/B}} \theta_t f_j\right)\right]^{(B/L)^d}. \tag{4.18}$$

This can be reformulated in terms of B-block events $\mathcal{A}_1, \ldots, \mathcal{A}_m$,

$$\mu\left(\bigcap_{j=1}^{m} \theta_{t_j}(\mathcal{A}_j)\right) \leq \prod_{j=1}^{m} \left[\mu\left(\bigcap_{t \in \mathbb{T}_{L/B}} \theta_t(\mathcal{A}_j)\right)\right]^{(B/L)^d}, \tag{4.19}$$

where $\theta_t(\mathcal{A}) := \{\theta_t 1_{\mathcal{A}} = 1\}$. The chessboard estimate allows to bound the probability of simultaneous occurrence of distinctly placed B-block events in terms of their disseminated versions $\bigcap_{t \in \mathbb{T}_{L/B}} \theta_t(\mathcal{A})$. The quantities to estimate are thus

$$\mathfrak{z}_L(\mathcal{A}) := \mu\left(\bigcap_{t \in \mathbb{T}_{L/B}} \theta_t(\mathcal{A})\right)^{(B/L)^d}. \tag{4.20}$$

Using the chessboard estimate it can be shown that the function $\mathcal{A} \mapsto \mathfrak{z}_L(\mathcal{A})$ is subadditive.

Lemma 4.10. Let $\mathcal{A}$ and $\mathcal{A}_1, \mathcal{A}_2, \ldots,$ be a collection of B-block events such that

$$\mathcal{A} \subset \bigcup_k \mathcal{A}_k. \tag{4.21}$$

Then

$$\mathfrak{z}_L(\mathcal{A}) \leq \sum_k \mathfrak{z}_L(\mathcal{A}_k). \tag{4.22}$$

To estimate the $\mathfrak{z}_L$-value of an event, the event is covered by the union of a collection of smaller and easier to compute event for which the $\mathfrak{z}_L$ value is calculated, and then the results are added. This gives a bound on the probability of certain events. Using these types of arguments, the idea is then to show that the set of infinite volume Gibbs measures is not a singleton for certain values of β.

The chessboard estimate is not restricted to cubic lattices. One can show that similar statements can be proved for, for instance, FCC, BCC or honeycomb lattices.

This concludes the chapter on phase transitions. We will now move on to determine whether or not certain models equipped with a reflection are reflection positive.

5

Heisenberg model

Now that we have introduced the concept of reflection positivity and have described how it can be used to prove the occurence of phase transitions, it is interesting to check whether certain models are reflection positive. We will start with the Heisenberg model, which is a physical model describing a magnet. A simplified version of the Heisenberg model is the Ising model, which is exactly solved [Bax82]. For the Heisenberg model we consider a lattice with on every lattice site a spin. This can either be a classical spin, then we call the model the classical Heisenberg model, or a quantum spin, in which case we call it the quantum Heisenberg model. In the Hamiltonian there is a free parameter J. When this parameter is negative, the model is called antiferromagnetic, otherwise it is called ferromagnetic.

We will consider the antiferromagnetic quantum Heisenberg model. In Section 5.1, we describe the model in the setting of Chapter 3, such that we can apply the developed theorems. Then, in Section 5.2, reflection positivity for the nearest neighbour Heisenberg model is evaluated. Finally, in Section 5.3, reflection positivity for the long-range Heisenberg model will be proved.

5.1. The algebra

We wish to describe the model in the setting of Chapter 3.

Consider a finite lattice $\Lambda \subseteq \mathbb{R}^n$, where $\mathbb{R}^n$ is equipped with the Euclidean metric. On every lattice site $\lambda \in \Lambda$, a spin $\frac{1}{2}$ system is located. This is described by the matrix algebra $\mathfrak{A}_\lambda = M_2$. The total system is then given by the algebra

$$\mathfrak{A} = \bigotimes_{\lambda\in\Lambda} M_2(\mathbb{C}). \tag{5.1}$$

The background functional τ is the normalized tracial state, given by

$$\tau(A_{\lambda_1} \otimes \cdots \otimes A_{\lambda_k}) = \frac{1}{2^k}\mathrm{Tr}(A_{\lambda_1}) \cdots \mathrm{Tr}(A_{\lambda_k}) \tag{5.2}$$

on the pure tensors. We only consider reflections in a reflection plane through bonds. Without loss of generality, we can thus assume the reflection $\theta : \Lambda \to \Lambda$ to be a reflection in the first coordinate, i.e. $\theta(x_1, x_2, ..., x_n) = (-x_1, x_2, ..., x_n)$. This splits the lattice Λ in two parts, Λ_+ and $\Lambda_- := \theta(\Lambda_+)$, having an empty intersection.

The reflection $\Theta : \mathfrak{A} \to \mathfrak{A}$ is the antilinear homomorphism given by

$$\Theta(A_\lambda) = \overline{\rho(A)}_{\theta(\lambda)}, \tag{5.3}$$

where ρ denotes conjugation by an arbitrary invertible operator $R \in \mathrm{GL}_n(\mathbb{C})$, namely $\rho(A) = RAR^{-1}$.

We define

$$\mathfrak{A}_\pm = \bigotimes_{\lambda\in\Lambda_\pm} M_n(\mathbb{C}), \tag{5.4}$$

then $\Theta(\mathfrak{A}_+) = \mathfrak{A}_-$, and $\mathfrak{A}$ is the linear span of $\mathfrak{A}_-\mathfrak{A}_+$. Since $\mathfrak{A} = \mathfrak{A}_- \otimes \mathfrak{A}_+$, the algebra $\mathfrak{A}$ is the double of $\mathfrak{A}_+$.

Proposition 5.1 ([JJ17])**.** The tracial state τ is faithful, factorizing, reflection invariant and reflection positive;

$$0 \le \tau(\Theta(A)A). \tag{5.5}$$

Proof. By linearity, it suffices to show reflection invariance on the tensors $A = A_{\lambda_1} \otimes \cdots \otimes A_{\lambda_k}$. This follows from

$$\tau(\Theta(A)) = \frac{1}{n^k}\mathrm{Tr}(\overline{RA_{\lambda_1}R^{-1}})\cdots\mathrm{Tr}(\overline{RA_{\lambda_k}R^{-1}}) = \frac{1}{n^k}\mathrm{Tr}(\overline{A_{\lambda_1}})\cdots\mathrm{Tr}(\overline{A_{\lambda_k}}) = \overline{\tau(A)}. \tag{5.6}$$

Factorization can be expressed as $\tau(AB) = \tau_-(A)\tau_+(B)$ for $A \in \mathfrak{A}_-$ and $B \in \mathfrak{A}_+$. The state τ is faithful since it is a finite tensor product of faithful states, and reflection positive by Proposition 3.9. □

Proposition 5.2. The tracial state τ_+ is strictly positive.

Proof. Let $A \in \mathfrak{A}_+$, then $\tau_+(A^*A) = \mathrm{Tr}(A^*A) = \sum_{i,j}\bar{A}_{ij}A_{ij} > 0$, whenever $A \neq 0$. □

We lastly need the algebra to admit a basis. For this we fix an orthonormal basis $\{c_i\}_{i\in S}$ of $M_2(\mathbb{C})$ with respect to the inner product $(X,Y) = \mathrm{Tr}(X^*Y)$ such that $c_0 = \mathbf{1}$. The basis is labelled by $i \in S = \{0,1,2,3\}$. We choose the Pauli matrices as basis. From this we obtain the tensor product basis

$$C_I = \bigotimes_{\lambda\in\Lambda_+} c_{i_\lambda},$$

for $\mathfrak{A}_+$, labelled by $I \in S^{\Lambda_+}$. This yields the basis

$$B_{IJ} = \Theta(C_I)C_J = \bigotimes_{\lambda'\in\Lambda_-} \overline{Rc_{i_{\theta(\lambda')}}R^{-1}} \bigotimes_{\lambda\in\Lambda_+} c_{j_\lambda},$$

of $\mathfrak{A}$, labelled by $(I,J) \in S^{\Lambda_+} \times S^{\Lambda_+}$.

5.2. Nearest neighbour Heisenberg model

We will turn our attention to the more specific n-dimensional $N \times N \times ... \times N$ lattice $\Lambda \subseteq \mathbb{Z}^n$ with periodic boundary conditions. On every lattice point a quantum spin at spin $\frac{1}{2}$ is located. When the distance between two lattice points is α, the Hamiltonian is given by

$$-H = \sum_{<\lambda,\lambda'>} \frac{J}{\alpha^v} \sum_{a=x,y,z} S^a_\lambda S^a_{\lambda'}, \tag{5.7}$$

where the sum is over all nearest neighbour pairs $<\lambda,\lambda'>$ and $v \ge 0$. $S^x, S^y, S^z \in M_2(\mathbb{C})$ are Hermitian spin matrices for spin $\frac{1}{2}$, the Pauli matrices. The map $X \mapsto \bar{X}$ flips the sign of S^y while leaving S^x and S^z invariant. The operator $R = \exp(i\pi S^y)$ represents a 180°-rotation around the y-axis, so the map $X \mapsto RXR^{-1}$ flips the sign of S^x and S^z, while leaving S^y invariant. Therefore the reflection Θ of the spin matrices is

$$\Theta(S^a_\lambda) = -S^a_{\theta(\lambda)}. \tag{5.8}$$

With this reflection, we see that the functional τ is continuous and factorizing on $\mathfrak{A}$, and the functional τ_+ is strictly positive. Furthermore, H is reflection invariant, thus we are in the situation to use Theorem 3.11.

Theorem 5.3. The functional $\tau_{\beta H}$ with reflections in the first component is reflection positive if and only if $J \leq 0$.

Proof. By Theorem 3.11, reflection positivity of the Boltzmann functional is equivalent to the matrix of coupling constants across the reflection plane being positive semidefinite. If we denote $\Lambda_+^P \subseteq \Lambda_+$ as the set of lattice points satisfying $|\lambda - \theta(\lambda)| = a$, then the matrix of coupling constants across the reflection plane is given by

$$J_{\lambda\lambda'}^{0ab} = -\frac{J}{\alpha^{v}}\delta^{ab}\delta_{\lambda\lambda'}, \tag{5.9}$$

where $\lambda, \lambda' \in \Lambda_+^P$ and $a, b \in \{x, y, z\}$. Note that δ is the Kronecker delta. This is a diagonal matrix, which is positive semidefinite if and only if every component is nonnegative, which proves the theorem. □

5.3. Long-range Heisenberg model

Consider a finite lattice $\Lambda \subset \mathbb{R}^n$ that is invariant for a reflection in the first coordinate. Let $\Lambda_+ \subset \Lambda$ be the set containing all lattice points with positive first component. For the long range Heisenberg model, the Hamiltonian is given by

$$-H = J \sum_{\lambda \neq \lambda'} |\lambda - \lambda'|^{-v} \sum_{a=x,y,z} S_\lambda^a S_{\lambda'}^a. \tag{5.10}$$

One might notice that, for a cubic lattice as in section 5.2, the nearest neighbour interactions are equal to the interactions in (5.7). However, we do not necessarily consider a cubic lattice.

We choose the same reflection and functional as in 5.8. Therefore we are in the situation to use Theorem 3.11. In the following theorem, we give the condition for which the Boltzmann functional is reflection positive.

Theorem 5.4. The functional $\tau_{\beta H}$ is reflection positive with respect to reflections in the first coordinate if and only if $J \leq 0$ and v is nonnegative with $v \geq n-2$.

The proof of this theorem is postponed to the end of the section, because we first need to develop some theory. Reflection positivity is equivalent to the matrix of coupling constants across the reflection plane $(J_{IJ}^0)_{\mathcal{I}\setminus\{I_0\}}$ being positive semidefinite. We therefore need to prove that this matrix is positive semidefinite. The matrix $(J_{IJ}^0)_{\mathcal{I}\setminus\{I_0\}}$ has elements

$$J_{\lambda\lambda'}^0 = -J|\theta(\lambda) - \lambda|^{-v}, \tag{5.11}$$

For the proof we need the following definition

Definition 5.1 ([JJ17])**.** Let $\theta : \mathbb{R} \to \mathbb{R}$ be an isometry of Euclidean space satisfying $\theta^2 = \mathrm{Id}$. Then a function $f : \mathbb{R}^d \to \mathbb{C}$ is called *Osterwalder-Schrader positive* (or *OS-positive*) if for all $N > 0$, for all $z_1, \dots, z_N \in \mathbb{C}$ and for all $r_1, \dots, r_N \in \mathbb{R}^d$ it holds that

$$\sum_{i,j=1}^{N} z_i \bar{z}_j f(r_i - \theta(r_j)) \geq 0. \tag{5.12}$$

We can state the following condition for the matrix of coupling constants across the reflection plane.

Proposition 5.5. The matrix of coupling constants across the reflection plane $(J_{IJ}^0)_{\mathcal{I}\setminus\{I_0\}}$ as in (5.11) is positive semidefinite if and only if the function $f : \mathbb{R}^n \to \mathbb{C}$ given by $f(x) = -J|x|^{-v}$ is OS-positive.

Proof. The proof is straightforward from the definition of Osterwalder-Schrader positive functions. If we let $\Lambda_+ = \{\lambda_1,...,\lambda_N\}$ and $z_1,...,z_N \in \mathbb{C}$, then

$$\sum_{i,j=1}^{N} z_i \bar{z}_j J^0_{\lambda_i\lambda_j} = \sum_{i,j=1}^{N} z_i \bar{z}_j (-J)|\theta(\lambda_i) - \lambda_j|^{-\upsilon}.$$

Positivity of one implies positivity of the other. □

We therefore need to show that the function $f : \mathbb{R}^n \to \mathbb{C}$ given by $f(x) = -J|x|^{-\upsilon}$ is OS-positive if and only if $J \le 0$ and $\upsilon \ge \max\{0, n-2\}$.

5.3.1. 1-dimensional lattice

Let us first focus on the case $n = 1$. Note that for our lattice we have Λ_+ the set of lattice points with positive first coordinate, which in one dimension is equal to all positive lattice points. The function $|\theta(\lambda) - \lambda'|$ is then equal to $\lambda' - \theta(\lambda)$ for all $\lambda, \lambda' \in \Lambda_+$. We formulate the following lemma.

Lemma 5.6. The function $f : \mathbb{R}_{\ge 0} \to \mathbb{C}$ given by $f(x) = x^{-\upsilon}$ is OS-positive with respect to a reflection in the first coordinate for $\upsilon \ge 0$.

Before proving this lemma, we first show that an integral of OS-positive functions over a positive measure is also OS-positive.

Theorem 5.7. Let $f_k : \mathbb{R}^d \to \mathbb{C}$ for k in some set A be OS-positive functions and let $\mu(dk)$ be a positive measure on A. Then the integral $\int_A f_k \mu(dk)$ is also OS-positive, provided that it converges.

Proof. Suppose the integral converges. Let $N \ge 0$ and choose $z_1,...,z_N \in \mathbb{C}$ and $r_1,...,r_N \in \mathbb{R}^d$. Then

$$\sum_{i,j=1}^{N} z_i \bar{z}_j \int_A f_k(r_i - \theta(r_j))\mu(dk) = \int_A \left(\sum_{i,j=1}^{N} z_i \bar{z}_j f_k(r_i - \theta(r_j)) \right) \mu(dk) \ge 0,$$

since it is an integral over a sum of positive functions. □

Proof of Lemma 5.6. For $\upsilon = 0$, we find $x^{-\upsilon} = x^0 = 1$, which is trivially OS-positive. For $\upsilon > 0$, let $x_1,...,x_N \in \mathbb{R}_{\ge 0}$ and $z_1,...,z_N \in \mathbb{C}$. Then

$$\sum_{i,j=1}^{N} z_i \bar{z}_j e^{-s|x_i - \theta(x_j)|} = \sum_{i=1}^{N} z_i e^{-sx_i} \sum_{j=1}^{N} \bar{z}_j e^{-sx_j} = |\sum_{i=1}^{N} z_i e^{-sx_i}|^2 \ge 0.$$

Now using a Laplace transform which can be found in most standard Laplace transform tables, we find

$$x^{-\upsilon} = \int_0^\infty \frac{1}{\Gamma(\upsilon)} t^{\upsilon-1} e^{-xt} dt, \tag{5.13}$$

where $\Gamma(\cdot)$ is the Gamma function. Since $t^{\upsilon-1}$ is non-negative for all $t \ge 0$, by Theorem 5.7 we conclude that $x^{-\upsilon}$ is OS-positive for all $\upsilon \ge 0$ which proves the lemma. □

5.3.2. Higher dimensional lattice

Let us now focus on the dimensions $n > 1$. We have Λ_+ the set of lattice points with positive first coordinate, and θ a reflection in the first coordinate.

Lemma 5.8. The function $f : \mathbb{R}^n \to \mathbb{C}$ given by $f(x) = |x|^{-\upsilon}$ is OS-positive with respect to the reflection θ if and only if $\upsilon \ge \max\{0, n-2\}$.

A proof based on Fourier and Laplace transformations can be found in the article by Frank and Lieb [FL09]. A proof based on harmonic analysis and Lie groups can be found in the article by Neeb and Ólafsson [NÓ14].

Proof of Theorem 5.4. Theorem 5.4 follows by Proposition 5.5 where OS-positivity of the function follows from Lemma 5.6 and Lemma 5.8. □

6
Spin ice model

A spin ice is a magnetic substance that does not have a single minimal energy state. Spin ice models are characterized by the presence of magnetic moments, that are restricted to point in two possible directions. In spin ice models magnetic monopoles emerge, which is due to the dipole moment of the underlying electronic degrees of freedom fractionalising [CMS08].

In this chapter we study whether the spin ice model described in [CMS08, Bra01] is reflection positive with respect to different reflections. The considered lattice is a pyrochlore lattice. This is a diamond lattice with halfway between each bond a spin pointing along the bond. Since every lattice point of a diamond lattice is connected with four bonds, there are four spins adjacent to a lattice point. In literature there are always two spins pointing towards a lattice point of the diamond lattice, and two pointing away. We will, however, use the slight modification that the spins can point in any direction.

In Section 6.1, we describe the model in the setting of Chapter 3, and we evaluate the symmetries of the pyrochlore lattice. Then, in Sections 6.2, 6.3 and 6.4, reflection positivity for different symmetries will be examined.

6.1. Pyrochlore lattice

Spin ice models are characterized by the presence of magnetic moments, further referred to as spins, $\boldsymbol{\mu}_i$ on the sites i of a pyrochlore lattice. This is a lattice consisting of two types of particles, the first on the sites of a diamond lattice, and the second on the midpoints of the bonds between sites on the diamond lattice. This causes the lattice of the second to consist of corner touching tetrahedra, as depicted in Figure 6.1.

The spins $\boldsymbol{\mu}_i$ point along the Ising axis of the lattice, which are the diamond lattice bonds. We can write $\boldsymbol{\mu}_i = \mu S_i \hat{e}_i$ with μ the magnitude of the magnetic moment, $S_i = \pm 1$ the Ising spin and $\hat{e}_i$ the unit vector in the direction of the Ising axis. The Hamiltonian of the system is described by a term for the nearest neighbor interaction between lattice points i and j; $< i, j >$, and a term for long-range interactions between lattice points i and j; (i, j):

$$H = \frac{J}{3} \sum_{<i,j>} S_i S_j + Da^3 \sum_{(i,j)} \left[\frac{\hat{e}_i \cdot \hat{e}_j}{|\mathbf{r}_{ij}|^3} - \frac{3(\hat{e}_i \cdot \mathbf{r}_{ij})(\hat{e}_j \cdot \mathbf{r}_{ij})}{|\mathbf{r}_{ij}|^5} \right] S_i S_j. \tag{6.1}$$

Here $\mathbf{r}_{ij}$ is the distance vector between two spins, a is the nearest neighbour distance of the pyrochlore lattice and D and J are constants, with D the fixed coupling constant of dipolar interaction and J free. We want to rewrite this Hamiltonian, so that we can use it to check reflection positivity.

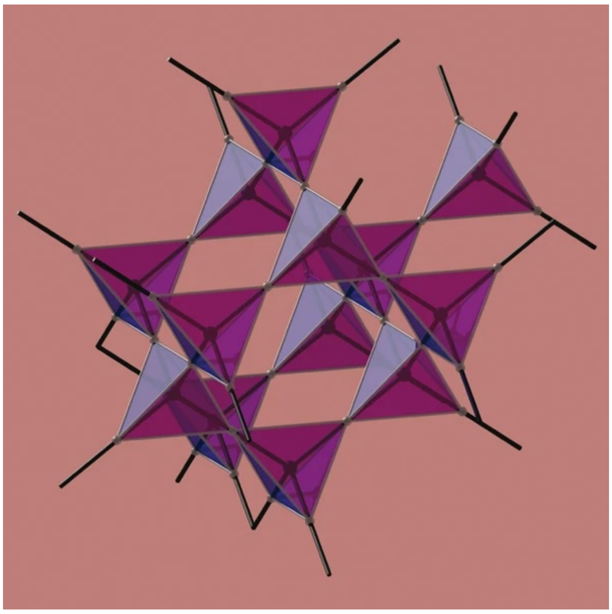

Figure 6.1: The pyrochlore lattice consisting of corner sharing tetrahedra. Black bonds represent the diamond lattice. Source: [CMS08]

6.1.1. The algebra

We wish to write the model in the setting of Chapter 3. For one spin particle, we have two possibilities for the spin vector. Therefore the probability space for one particle λ is given by $\Omega_\lambda = \{\hat{e}_\lambda, -\hat{e}_\lambda\}$, where $\hat{e}_\lambda \in T_\lambda\mathbb{R}^3$, the tangent space at λ that can be identified with $\mathbb{R}^3$. The algebra is given by all random variables on Ω_λ. A particular set of random variables is the set of spin variables S^x_λ, S^y_λ and S^z_λ, that take as argument a vector $\omega_\lambda \in \Omega_\lambda$, and returns the x, y or z component of the spin, respectively. At first, you might think that these are linearly independent, but since $\hat{e}^a_\lambda S^b_\lambda - \hat{e}^b_\lambda S^a_\lambda = 0$ for $a, b \in \{x, y, z\}$, they are, in fact, dependent.

The whole lattice Λ is countable or finite. If we choose an order of the elements of the lattice, $\Lambda = \{\lambda_1, \lambda_2, ...\}$, we construct the probability space $\Omega = \prod_i \Omega_{\lambda_i}$. The algebra is the space of random variables on Ω, so

$$\mathfrak{A} = \{F : \Omega \to \mathbb{C}\}. \tag{6.2}$$

Note that this is indeed an algebra, since random variables can be added and multiplied with each other. A special random variable is again the random variable $S^a_i : \Omega \to \mathbb{C}$, given by $S^a_i(\omega) = \omega^a_{\lambda_i}$ for $\lambda_i \in \Lambda$ and $a \in \{x, y, z\}$.

If we define the random variable $\mathbf{S}_i := \begin{bmatrix} S^x_i & S^y_i & S^z_i \end{bmatrix}^T$ and let the unit distance vector $\hat{\mathbf{r}}_{ij} = \begin{bmatrix} r^x_{ij} & r^y_{ij} & r^z_{ij} \end{bmatrix}^T$, and by using the observations made in Appendix A, we can rewrite the Hamiltonian given in (6.1) to the somewhat more practical form

$$H = \sum_{<i,j>} \langle \mathbf{S}_j, -J\mathbf{S}_i \rangle + \sum_{(i,j)} \langle \mathbf{S}_j, \frac{Da^3}{|\mathbf{r}_{ij}|^3} \left[I_3 - 3P_{\hat{\mathbf{r}}_{ij}} \right] \mathbf{S}_i \rangle, \tag{6.3}$$

where I_3 is the 3×3 identity matrix, and $P_\mathbf{u}$ is the projection matrix on a vector $\mathbf{u} \in \mathbb{R}^3$. This description is, however, not yet complete. As noted before, the elements of the random variable $\mathbf{S}_i$ are not independent. This information can be incorporated in the Hamiltonian by using the projection matrices on the Ising axes $\hat{e}_i$. So we get

$$H = \sum_{<i,j>} \langle \mathbf{S}_j, -JP_{\hat{e}_j} P_{\hat{e}_i} \mathbf{S}_i \rangle + \sum_{(i,j)} \langle \mathbf{S}_j, \frac{Da^3}{|\mathbf{r}_{ij}|^3} P_{\hat{e}_j} \left[I_3 - 3P_{\hat{\mathbf{r}}_{ij}} \right] P_{\hat{e}_i} \mathbf{S}_i \rangle. \tag{6.4}$$

This Hamiltonian is a sum of products of random variables contained in $\mathfrak{A}$, so we have $H \in \mathfrak{A}$. To shorten notation we define the matrix M_{ij} given by

$$M_{ij} = \begin{cases} (-J+D)I - 3DP_{\hat{\mathbf{r}}_{ij}}, & i,j \text{ nearest neighbours}, \\ D\frac{a^3}{|\mathbf{r}_{ij}|^3}I - 3D\frac{a^3}{|\mathbf{r}_{ij}|^3}P_{\hat{\mathbf{r}}_{ij}}, & i,j \text{ non nearest neighbours}. \end{cases} \tag{6.5}$$

Then we can write

$$H = \sum_{(i,j)} \langle \mathbf{S}_j, P_{\hat{e}_j} M_{ij} P_{\hat{e}_i} \mathbf{S}_i \rangle . \tag{6.6}$$

The used functional is the Boltzmann functional $\tau_H : \mathfrak{A} \to \mathbb{C}$, that is given by

$$\tau_H(A) = \sum_{\omega\in\Omega} A(\omega) e^{-H(\omega)}. \tag{6.7}$$

This functional has to be reflection invariant under a reflection $\Theta : \mathfrak{A} \to \mathfrak{A}$, depending on the used symmetry for the lattice. Furthermore, in order to use Theorem 3.11, the background functional needs to be factorizing and this factor has to be strictly positive, both also depending on the reflection Θ.

6.1.2. Symmetry group pyrochlore lattice

For reflection positivity, we need a reflection. There are several possibilities of reflections in the pyrochlore lattice that leave the lattice invariant. The symmetry group of the pyrochlore lattice is the $Fd\bar{3}m$ space group [GC15]. Not surprisingly, this is also the symmetry group of the diamond lattice. For the pyrochlore lattice, we are especially interested in the point group, which is a group of isometries that keep at least one point fixed. This does not necessarily have to be a lattice point. For the diamond lattice, and thus also the pyrochlore lattice, this is the group $m3m(O_h)$ [ML67, Had]. This group contains six 2-fold symmetries, nine reflection planes and an inversion. Furthermore it contains some higher fold rotations, but since our reflection θ must satisfy $\theta^2 = \mathrm{Id}$, these are not interesting for us. The symmetries of interest are shown in Figure 6.2.

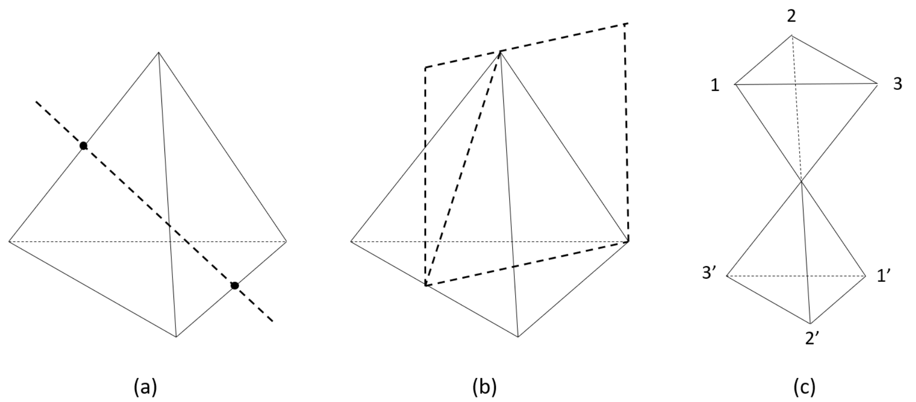

Figure 6.2: The symmetries of interest in the pyrochlore lattice. On the left, (a) is a 2-fold symmetry with rotation axis as shown. In the middle, (b) is a reflection with reflection plane. On the right (c) is an inversion where i and i' are interchanged for $i = 1,2,3$.

The 2-fold symmetries are rotations around an axis cutting through opposite sides of a tetrahedron, the reflection plane swaps two corners of a tetrahedron and leaves the other corners invariant, and the inversion swaps lattice points on opposite sides of a shared corner. We will evaluate reflection positivity for all reflections of the pyrochlore lattice, (a), (b) and (c) in Figure 6.2.

6.2. Reflection positivity for a reflection plane

We first consider a reflection plane with normal vector $\hat{\mathbf{n}}$, situation (b) in Figure 6.2. This reflection θ divides the lattice in two parts Λ_+ and $\Lambda_- := \theta(\Lambda_+)$. Their intersection $P := \Lambda_- \cap \Lambda_+$ is the fixed point set of the reflection θ. We define $\Omega_+ := \prod_j \Omega_{\lambda_j}$ where $\lambda_j \in \Lambda_+$ for all j. When the lattice Λ is finite, this product is a finite product, otherwise it is countable. From this probability space, we find the subalgebra $\mathfrak{A}_+$ of all functions in $\mathfrak{A}$ that are fully determined by their projection on Ω_+, thus

$$\mathfrak{A}_+ = \{F \in \mathfrak{A} : F(\omega) = F(\omega|_{\Omega_+}) \forall \omega \in \Omega\}. \tag{6.8}$$

Another way to describe Ω is by using functions, such that $\Omega = \{\sigma : \Lambda \to T\mathbb{R}^3 : \pi \circ \sigma(\lambda) = \lambda, \sigma(\lambda) = \pm\hat{e}_\lambda\}$. Then we can describe a reflection $\hat{\theta} : \Omega \to \Omega$ given by $\hat{\theta}\sigma(\lambda) = \theta_*\sigma(\theta\lambda)$. Now we can find a reflection $\Theta : \mathfrak{A} \to \mathfrak{A}$ that satisfies the reflection invariance property (Def 3.2). This reflection is given by

$$\Theta(A)(\omega) = \overline{A(\hat{\theta}(\omega))}. \tag{6.9}$$

If we consider the spin random variables, we have

$$\Theta(S^a_\lambda)(\sigma) = S^a_\lambda(\hat{\theta}\sigma) = ((I_3 - 2P_{\hat{\mathbf{n}}})\mathbf{S}_{\theta\lambda}(\sigma))^a, \tag{6.10}$$

for $a \in \{x, y, z\}$.

A basis for the random variables at a single lattice point is given by $\{c_{i_\lambda}\}_{i\in S}$ where $S = \{1, 2\}$ and $c_1 = \mathbf{1}_\lambda$ and $c_2 = S^x_\lambda$. From this we obtain the Schauder basis for $\mathfrak{A}_+$

$$C_I = \prod_{\lambda\in\Lambda_+} c_{i_\lambda}, \tag{6.11}$$

labelled by an index $I \in S^{\Lambda_+}$. Note that we can use any rotation of the spin random variable $\mathbf{S}$ since they are dependent, so products of random variables of the form $P_{\hat{e}_i}\mathbf{S}_i$ form a Schauder basis as well, when interpreted as one-dimensional random variables.

As stated before, the background functional τ has to be factorizing with respect to the reflection Θ. We prove this in the following lemma.

Lemma 6.1. The background functional $\tau : \mathfrak{A} \to \mathbb{C}$ given by $\tau(A) = \sum_{\omega\in\Omega} A$ is factorizing with respect to the reflection Θ of (6.9).

Proof. We use the Riesz representation theorem to switch from the functional τ to a positive measure μ, such that $\tau(A) = \mathbb{E}_\mu(A)$ for all $A \in \mathfrak{A}$. Now note that two random variables A and $\Theta(B)$ with $A, B \in \mathfrak{A}_+$ are independent conditional on the spin configuration Ω_P on the reflection plane. Invoking reflection invariance of $\mu(\cdot|\Omega_P)$, we get

$$\mathbb{E}_\mu(A\Theta(B)|\Omega_P) = \mathbb{E}_\mu(A|\Omega_P)\mathbb{E}_\mu(\Theta(B)|\Omega_P) = \mathbb{E}_\mu(A|\Omega_P)\overline{\mathbb{E}_\mu(B|\Omega_P)}. \tag{6.12}$$

We thus see that the functional $\tau_+ : \mathfrak{A}_+ \to \mathbb{C}$ is given by $\tau_+(A) = \mathbb{E}_\mu(A|\Omega_P)$, and τ is indeed factorizing. □

The functional τ_+ has to be strictly positive. We show this in Lemma 6.2

Lemma 6.2. The functional $\tau_+ : \mathfrak{A}_+ \to \mathbb{C}$ is strictly positive.

Proof. A simple calculation shows

$$\tau_+(A^*A) = \mathbb{E}_\mu(A^*A|\Omega_P) = \mathbb{E}_\mu(|A|^2|\Omega_P) > 0, \tag{6.13}$$

whenever $A \neq 0$. □

We are now in the situation of Theorem 3.11, since τ is a continuous, factorizing functional on $\mathfrak{A}$, τ_+ is strictly positive and H is a reflection invariant operator. Thus we know that the functional $\tau_{\beta H}$ is reflection positive for all $0 \leq \beta$ if and only if the matrix $(J^0_{IJ})_{\mathcal{I}}$ of coupling constants across the reflection plane is positive semidefinite. Let us first focus on a situation where we have only two spin particles.

6.2.1. Nearest neighbour interactions

We will first check reflection positivity in the case of a reflection invariant lattice with only two neighbouring spins, spin i and spin $j := \theta(i)$. Due to the geometry of the model, these spins are corner points of the same tetrahedron. The Hamiltonian of this lattice is simply

$$H = \langle P_{\hat{e}_j}\mathbf{S}_j, M_{ij}P_{\hat{e}_i}\mathbf{S}_i\rangle\,. \tag{6.14}$$

We want to write this in the form (3.15). Let us define $R := (I - 2P_{\hat{\mathbf{n}}})$ as in (6.10), then R is an idempotent matrix and we can write $H = \langle P_{\hat{e}_j}R^2\mathbf{S}_j, M_{ij}P_{\hat{e}_i}\mathbf{S}_i\rangle$. Since $R\mathbf{S}_j = \Theta(\mathbf{S}_i)$ we thus have

$$H = \langle P_{\hat{e}_j}R\Theta(\mathbf{S}_i), M_{ij}P_{\hat{e}_i}\mathbf{S}_i\rangle\,. \tag{6.15}$$

Finally, note that in general for a spin k we have $RP_{\hat{e}_{\theta(k)}} = P_{\hat{e}_k}R$. From this description we find that the matrix of coupling constants across the reflection plane is given by

$$(J^0_{IJ})_{\mathcal{I}} = -P_{\hat{e}_i}RM_{ij}P_{\hat{e}_i} = -\langle \hat{e}_i, RM_{ij}\hat{e}_i\rangle\, P_{\hat{e}_i}. \tag{6.16}$$

This matrix has eigenvalues $\lambda_{1,2} = 0$ and $\lambda_3 = -\langle \hat{e}_i, RM_{ij}\hat{e}_i\rangle$.

Since we are looking at two neighbouring spins, without loss of generality the basis can be chosen in such a way that the reflection plane is the x-z plane, and the spins are orthogonal to the x-direction. This is shown in Figure 6.3.

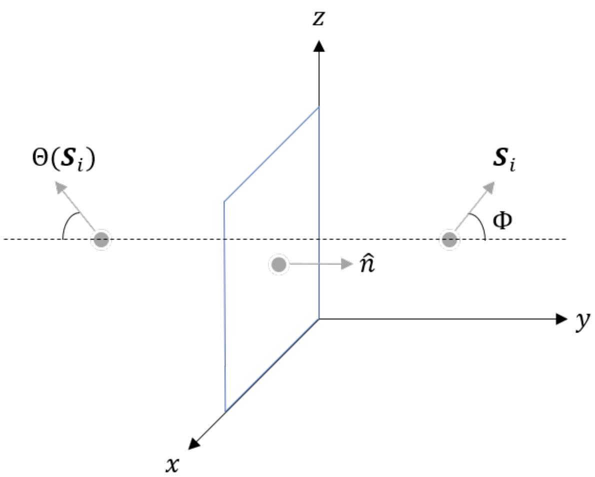

Figure 6.3: Two nearest neighbour spins with a reflection plane equal to the x-z plane, and spins in the y-z plane. Left is spin j, right spin i.

Using the description above, we can exactly calculate the matrix of coupling constants across the reflection plane. The results are summarized in the following lemma.

Lemma 6.3. The matrix of coupling constants $(J_{IJ})_{\mathcal{I}}$ given in (6.16) for the reflection through a reflection plane of two nearest neighbour spin particles is reflection positive if and only if $J \leq -5D$.

Proof. The matrix $(J_{IJ})_{\mathcal{I}}$ is positive semidefinite if and only if all eigenvalues are non-negative. We therefore need to check for which values of J we have $-\langle \hat{e}_i, RM_{ij}\hat{e}_i\rangle \geq 0$.

Note that $\hat{e}_i = \begin{bmatrix}0 & \cos\phi & \sin\phi\end{bmatrix}^T$ and thus $\hat{e}_j = \begin{bmatrix}0 & -\cos\phi & \sin\phi\end{bmatrix}^T = R\hat{e}_i$. Furthermore we know $\hat{\mathbf{r}}_{ij} = \hat{n}$. So we calculate

$$\begin{aligned} -\langle e_i, RM_{ij}e_i\rangle &= -\langle e_j, M_{ij}e_i\rangle \\ &= -\begin{bmatrix}0 & -\cos(\phi) & \sin(\phi)\end{bmatrix}\begin{bmatrix}-J+D & 0 & 0\\ 0 & -J-2D & 0\\ 0 & 0 & -J+D\end{bmatrix}\begin{bmatrix}0\\ \cos(\phi)\\ \sin(\phi)\end{bmatrix} \\ &= -\begin{bmatrix}0 & -\cos(\phi) & \sin(\phi)\end{bmatrix}\begin{bmatrix}0\\ (-J-2D)\cos(\phi)\\ (-J+D)\sin(\phi)\end{bmatrix} \\ &= -((J+2D)\cos^2(\phi)+(-J+D)\sin^2(\phi)) \geq 0. \end{aligned}$$

Rewriting gives

$$J(\cos^2(\phi)-\sin^2(\phi))+2D\cos^2(\phi)+D\sin^2(\phi) \leq 0,$$

and thus

$$J \leq D\frac{-2\cos^2(\phi)-\sin^2(\phi)}{\cos^2(\phi)-\sin^2(\phi)}.$$

Note that the two spins are part of the same tetrahedron, and thus using Appendix A we know that $\cos(\phi) = \hat{\mathbf{r}}_{ij}\cdot\hat{e}_i = \sqrt{\frac{2}{3}}$, which thus gives $J \leq -5D$. For the converse, we can make the same arguments in opposite direction. □

Remark 6.4. When we choose the reflection to be spin inverting, i.e. $\Theta(S^a_\lambda)(\sigma) = -S^a_\lambda(\hat{\theta}\sigma) = -((I_3-2P_{\hat{\mathbf{n}}})\mathbf{S}_{\theta\lambda}(\sigma))^a$, the Hamiltonian H in (6.15) changes to $H = -\langle P_{\hat{e}_j}R\Theta(\mathbf{S}_i), M_{ij}P_{\hat{e}_i}\mathbf{S}_i\rangle$. This results in a minus sign in front of the matrix of coupling constants across the reflection plane (6.16). Therefore the nonzero eigenvalue obtains a minus sign, which flips the inequality in Lemma 6.3 to $J \geq -5D$. The meaning of a spin inverting reflection can best be explained with help of a figure.

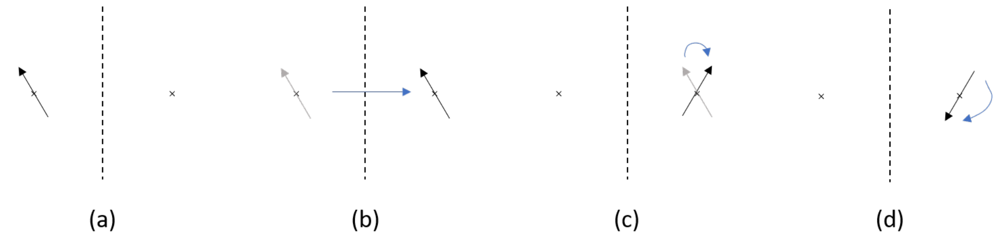

Figure 6.4: The reflection (6.10) starts with a spin on one side of the reflection plane (a), this is reflected to the other side (b) and then rotated such that it points in the direction of the Ising axis (c). A spin inverting reflection furthermore inverts the direction of the spin (d).

The reflection of (6.10) that leaves the spin invariant, starts with step (a) in Figure 6.4 and then consists of the steps (b) and (c). For a spin inverting reflection we furthermore let the spin point in the opposite direction, shown in (d).

6.2.2. Non nearest neighbour interactions

Consider the same situation as in Figure 6.3, but with the spins not being nearest neighbours. The Hamiltonian is the same as (6.15) and the matrix of coupling constants is equal to (6.16). The difference with the nearest neighbour interaction is the matrix M_{ij}, as described in (6.5).

Lemma 6.5. The matrix $(J_{IJ})_{\mathcal{I}}$ is negative semidefinite for the reflection (6.10). In particular the matrix has one negative eigenvalue.

Proof. The matrix $(J_{IJ})_{\mathcal{I}}$ is negative semidefinite if and only if the eigenvalues are nonpositive, so we need to check that $-\langle \hat{e}_i, RM_{ij}\hat{e}_i\rangle \leq 0$.

By choosing the appropriate basis, shown in Figure 6.3, we calculate

$$
\begin{aligned}
-\langle e_i, RM_{ij}e_i\rangle &= -\langle e_j, M_{ij}e_i\rangle \\
&= -D\frac{a^3}{|r_{ij}|^3}\begin{bmatrix}0 & -\cos(\phi) & \sin(\phi)\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\ 0 & -2 & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}0\\ \cos(\phi)\\ \sin(\phi)\end{bmatrix} \\
&= -D\frac{a^3}{|r_{ij}|^3}(2\cos^2(\phi)+\sin^2(\phi)) \leq 0.
\end{aligned}
$$

Since D and a are positive constants, we conclude that we must have $\cos^2(\phi)+1 \geq 0$ which is true for all ϕ. The inequality is strict as $\cos^2(\phi) \geq 0$ for all ϕ, so we indeed have one negative eigenvalue. □

Remark 6.6. When we choose the reflection to be spin inverting, i.e. $\Theta(S^a_\lambda)(\sigma) = -S^a_\lambda(\hat{\theta}\sigma) = -((I_3 - 2P_{\hat{\mathbf{n}}})\mathbf{S}_{\theta\lambda}(\sigma))^a$, the Hamiltonian obtains a minus sign. This results in a minus sign in front of the matrix of coupling constants across the reflection plane, which thus makes it a positive semidefinite matrix.

6.2.3. A larger lattice

Consider a pyrochlore lattice Λ, that is invariant under a reflection θ in a reflection plane. Assuming the lattice is big enough, that is, there is a spin which reflection is not its nearest neighbour, the Boltzmann functional τ_H is not reflection positive. This assumption is valid, since the lattice is likely to look like a bigger version of Figure 6.1, which already satisfies the assumption. The result for reflection positivity is proved in the following theorem.

Theorem 6.7. For a big enough pyrochlore lattice Λ, the Boltzmann functional $\tau_{\beta H}$ is never reflection positive with respect to the reflection (6.10).

Proof. By Theorem 3.11 reflection positivity of the Boltzmann functional is equal to the matrix of coupling constants across the reflection plane $(J^0_{IJ})_{\mathcal{I}\setminus\{I_0\}}$ being positive semidefinite.

Since we assumed the lattice to be big enough, there is a spin i which reflection $\theta(i)$ is not one of its nearest neighbours. This means somewhere on the diagonal of $(J_{IJ})_{\mathcal{I}\setminus\{I_0\}}$, we have the matrix (6.16). By Lemma 6.5 we know this matrix is negative semidefinite, with one negative eigenvalue λ. But then we can find a vector $\mathbf{q}$ such that $\sum_{I,J\in\mathcal{I}\setminus\{I_0\}}\mathbf{q}_I^* J_{IJ}\mathbf{q}_J = \lambda|\mathbf{q}|^2 < 0$, and thus the matrix of coupling constants across the reflection plane is not positive semidefinite. □

6.2.4. Spin inverting reflection

In Theorem 6.7 we have shown that, for the reflection (6.10), the Boltzmann functional is never reflection positive for a large enough lattice. However, the same proof can not be applied to the spin inverting reflection

$$\Theta(S^a_\lambda)(\sigma) = -S^a_\lambda(\hat{\theta}\sigma) = -((I_3 - 2P_{\hat{\mathbf{n}}})\mathbf{S}_{\theta\lambda}(\sigma))^a. \tag{6.17}$$

We wish to get a bit more insight in this reflection. For this, consider the lattice of Figure 6.5, composed of two corner sharing tetrahedra. The reflection through a plane then leaves the shared corner and two opposite corners invariant, and swaps the other two corners in a tetrahedron.

The Hamiltonian is given by (6.6). The reflection naturally splits the lattice in the lattice points on different sides of the plane, Λ_+ and Λ_-, with intersection being the fixed point set of the reflection. Let this fixed point set be P. We can then split the Hamiltonian in $H = H_+ + H_0 + H_-$ with

$$H_0 = \sum_{i,j\in\Lambda_+\setminus P}\langle \mathbf{S}_{\theta(j)}, P_{\hat{e}_{\theta(j)}} M_{i\theta(j)} P_{\hat{e}_i}\mathbf{S}_i\rangle. \tag{6.18}$$

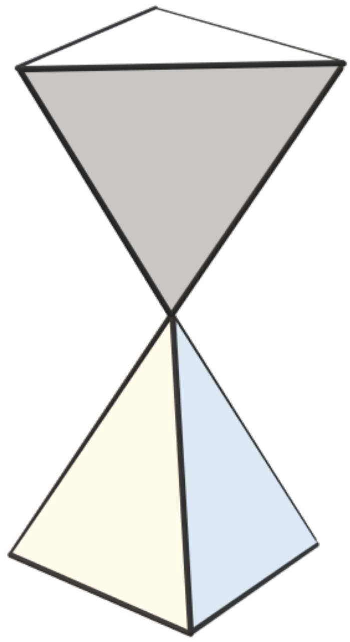

Figure 6.5: Two corner sharing tetrahedra with parallel ground planes, one of the tetrahedra is rotated π radians around the normal vector of the ground plane.

Using the same steps as in Section 6.2.1 we can rewrite this to

$$H_0 = \sum_{i,j\in\Lambda_+\setminus P} \langle \Theta(\mathbf{S}_j), -P_{\hat{e}_j} RM_{i\theta(j)} P_{\hat{e}_i} \mathbf{S}_i \rangle \,. \tag{6.19}$$

The matrix of coupling constants across the reflection plane is thus given by

$$J^0_{ij} = P_{\hat{e}_j} RM_{i\theta(j)} P_{\hat{e}_i} = \langle \hat{e}_j, RM_{i\theta(j)} \hat{e}_i \rangle \, \hat{e}_j \hat{e}_i^* = \langle \hat{e}_{\theta(j)}, M_{i\theta(j)} \hat{e}_i \rangle \, \hat{e}_j \hat{e}_i^* , \tag{6.20}$$

for $i, j \in \Lambda_+ \setminus P$.

Lemma 6.8. The matrix of coupling constants across the reflection plane (6.20) is positive semidefinite if and only if $J \geq -\frac{37}{8} D$.

Proof. We calculate the eigenvalues of J^0_{ij}. For this let $\Lambda_+ \setminus P = \{\lambda_1, \lambda_2\}$, and choose $\mathbf{u}_{\lambda_i}$, $\mathbf{v}_{\lambda_i}$ and $\mathbf{w}_{\lambda_i}$ pairwise orthogonal such that $\mathbf{u}_{\lambda_i} = \hat{e}_{\lambda_i}$ for $i = 1, 2$. Now define the basis

$$\mathcal{B} := \left\{ \begin{bmatrix} \mathbf{u}_{\lambda_1} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ \mathbf{u}_{\lambda_2} \end{bmatrix}, \begin{bmatrix} \mathbf{v}_{\lambda_1} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ \mathbf{v}_{\lambda_2} \end{bmatrix}, \begin{bmatrix} \mathbf{w}_{\lambda_1} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ \mathbf{w}_{\lambda_2} \end{bmatrix}, \right\},$$

where $\mathbf{0} \in \mathbb{R}^3$ is the zero vector. Using a change of basis we then calculate

$$J_{ij} = \langle \hat{e}_{\theta(j)}, M_{i\theta(j)} \hat{e}_i \rangle \,, \tag{6.21}$$

for $i, j = 1, 2$, and 0 otherwise. This is a square 6×6 matrix of rank 2, so we have four times the eigenvalue 0. After substituting known values as calculated in Appendix A, the left upper matrix of (6.21) becomes

$$J_{IJ} = \begin{bmatrix} \frac{J+5D}{3} & \frac{D}{8} \\ \frac{D}{8} & \frac{J+5D}{3} \end{bmatrix}. \tag{6.22}$$

This matrix has eigenvalues $\lambda_1 = \frac{8J+43D}{24}$ and $\lambda_2 = \frac{8J+37D}{24}$ and is thus positive semidefinite if and only if $J \geq -\frac{37}{8} D$. Since a change of basis does not change the eigenvalues, this proves the lemma. □

Using Lemma 6.8 we can not yet prove that the Boltzmann functional of a bigger lattice is reflection positive. However, the result for two tetrahedra does give a strong believe that there exists values of J such that the model is reflection positive using a spin inverting reflection.

Another interesting configuration are two spins on either side of the reflection plane with reflections that are not their own nearest neighbours. It is worth noting that the author numerically evaluated the situation with two spins on a line orthogonal to the reflection plane, pointing in the same direction. For that situation the matrix of coupling constants across the reflection plane stayed positive semidefinite, which further amplified the believe that the model is reflection positive with respect to a spin inverting reflection. These results are however not incorporated in this thesis.

6.3. Reflection positivity for an inversion

Consider an inversion in a lattice point, situation (c) in Figure 6.2. This inversion can be seen as a reflection θ in a point λ, that divides the lattice in two parts Λ_+ and $\Lambda_- := \theta(\Lambda_+)$, where their intersection P is the set only containing λ. Define $\Omega_+ := \prod_j \Omega_{\lambda_j}$ where $\lambda_j \in \Lambda_+$ for all j. From this probability space, we find the subalgebra $\mathfrak{A}_+$ of all random variables in $\mathfrak{A}$ that are fully determined by the projection of their argument on Ω_+, thus defined in the same way as (6.8). Similar to the reflection in a reflection plane, the reflection $\Theta : \mathfrak{A} \to \mathfrak{A}$ is given by (6.9). If we consider the spin random variables, we have for spin i

$$\Theta(S_i^a)(\sigma) = S_i^a(\hat{\theta}\sigma) = -S_{\theta i}^a(\sigma), \tag{6.23}$$

for $a \in \{x, y, z\}$. The background functional τ can be factorized as $\tau(\Theta(A)B) = \overline{\tau_+(A)}\tau_+(B)$, and this factor τ_+ is strictly positive. The proof is equal to the proof of Lemma 6.1 and Lemma 6.2. Furthermore we can construct a Schauder basis for $\mathfrak{A}_+$ in a similar way as for the reflection plane.

We are now in the situation of Theorem 3.11, so $\tau_{\beta H}$ is reflection positive for all $0 \le \beta$ if and only if the matrix $(J_{IJ}^0)_{\mathcal{I}}$ of coupling constants is positive semidefinite. Let us first focus on a situation where we only have two tetrahedra.

6.3.1. Two tetrahedra

Consider the lattice Λ as shown in Figure 6.5, composed of two corner sharing tetrahedra with parallel ground planes. One of the tetrahedra is rotated over π radians around the normal vector of the ground plane intersecting the shared corner. A spin is located on every cornerpoint of the tetrahedra as described for the pyrochlore lattice. Without loss of generality we let the shared corner be the origin.

Then we can write the Hamiltonian in the form $H = H_+ + H_0 + H_-$ with

$$H_0 = \sum_{(i,j)} \langle -\Theta(\mathbf{S}_j), P_{\hat{e}_j} M_{i\theta(j)} P_{\hat{e}_i} \mathbf{S}_i \rangle, \tag{6.24}$$

where the sum is over $i, j \in \Lambda_+ \setminus \{0\}$. From this we find the matrix of coupling constants across the reflection plane

$$J_{ij}^0 = P_{\hat{e}_j} M_{i\theta(j)} P_{\hat{e}_i} = \langle \hat{e}_j, M_{i\theta(j)} \hat{e}_i \rangle\, \hat{e}_j \hat{e}_i^* = -\langle \hat{e}_{\theta(j)}, M_{i\theta(j)} \hat{e}_i \rangle\, \hat{e}_j \hat{e}_i^*, \tag{6.25}$$

for $i, j \in \Lambda_+ \setminus \{0\}$. This matrix is indefinite, which we prove in the following lemma.

Lemma 6.9. The matrix of coupling constants across the reflection plane J_{ij}^0 as in (6.25) is indefinite.

Proof. The matrix is indefinite if and only if it has negative and positive eigenvalues, so we compute the eigenvalues. For this, let $\Lambda_+ \setminus \{0\} = \{\lambda_1, \lambda_2, \lambda_3\}$. Then choose $\mathbf{u}_{\lambda_i}$, $\mathbf{v}_{\lambda_i}$ and $\mathbf{w}_{\lambda_i}$ pairwise orthogonal such that $\mathbf{u}_{\lambda_i} = \hat{e}_{\lambda_i}$ for $i = 1, 2, 3$. Now define the basis

$$\mathcal{B} := \left\{ \begin{bmatrix} \mathbf{u}_{\lambda_1} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ \mathbf{u}_{\lambda_2} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{u}_{\lambda_3} \end{bmatrix}, \begin{bmatrix} \mathbf{v}_{\lambda_1} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ \mathbf{v}_{\lambda_2} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{v}_{\lambda_3} \end{bmatrix}, \begin{bmatrix} \mathbf{w}_{\lambda_1} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ \mathbf{w}_{\lambda_2} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{w}_{\lambda_3} \end{bmatrix} \right\}, \tag{6.26}$$

where $\mathbf{0} \in \mathbb{R}^3$ is the zero vector. After a change of basis, this reduces the matrix J^0_{ij} to

$$J_{ij} = -\langle \hat{e}_{\theta(j)}, M_{i\theta(j)}\hat{e}_i \rangle, \tag{6.27}$$

for $i, j = 1,2,3$, and 0 otherwise. Since this is a square 9×9 matrix of rank 3, we have six times the eigenvalue 0. After substituting known values as calculated in Appendix A, the left upper matrix of (6.27) becomes

$$J_{IJ} = -D \begin{bmatrix} \frac{1}{8} & \frac{1}{3\sqrt{3}} & \frac{1}{3\sqrt{3}} \\ \frac{1}{3\sqrt{3}} & \frac{1}{8} & \frac{1}{3\sqrt{3}} \\ \frac{1}{3\sqrt{3}} & \frac{1}{3\sqrt{3}} & \frac{1}{8} \end{bmatrix}. \tag{6.28}$$

This matrix has eigenvalues $\lambda_1 = -D\frac{9+16\sqrt{3}}{72} < 0$ and $\lambda_{2,3} = -D\frac{9-8\sqrt{3}}{72} > 0$, so it is indefinite. Since a change of basis does not influence the eigenvalues, this proves the lemma. □

6.3.2. A larger lattice

Consider a pyrochlore lattice Λ, that is invariant under an inversion θ in a lattice point λ. Assume the tetrahedra that contain λ are part of the lattice, which is a valid assumption since the lattice is likely to look like a bigger version of Figure 6.1. Then the Boltzmann functional $\tau_{\beta H}$ is not reflection positive with respect to the reflection (6.23), which is proved in the following theorem.

Theorem 6.10. For a finite pyrochlore lattice Λ with an inversion in a lattice point λ contained in two tetrahedra, the Boltzmann functional $\tau_{\beta H}$ is never reflection positive for the reflection (6.23).

Proof. The proof is similar to that of Theorem 6.7. Construct a vector $\mathbf{q}$ such that $\sum_{I,J\in\mathcal{I}\setminus\{I_0\}} \mathbf{q}_I (J^0_{IJ})_{\mathcal{I}\setminus\{I_0\}} \mathbf{q}_J = \lambda|\tilde{\mathbf{q}}|^2 < 0$, then $(J^0_{IJ})_{\mathcal{I}\setminus\{I_0\}}$ is not positive semidefinite, which proves the theorem. □

Remark 6.11. The result of Theorem 6.10 also holds for a spin inverting reflection, i.e. $\Theta(S^a_i)(\sigma) = -S^a_i(\hat{\theta}\sigma) = S^a_{\theta i}(\sigma))$. Using this reflection the Hamiltonian H_0 in (6.24) obtains a minus sign, and thus the matrix of coupling constants across the reflection plane obtains a minus sign. This however still results in an indefinite matrix, for which the same proof holds.

6.4. Reflection positivity for a 2-fold symmetry

The method for a 2-fold symmetry is very similar to the method for a reflection in a plane. Consider a rotation around an axis through a tetrahedron, situation (a) in Figure 6.2. This rotation is a 2-fold symmetry that can be seen as a reflection θ in an axis $\mathbf{u}$, that divides the lattice in two parts Λ_+ and $\Lambda_- := \theta(\Lambda_+)$, with empty intersection. Define $\Omega_+ := \prod_j \Omega_{\lambda_j}$ where $\lambda_j \in \Lambda_+$ for all j. From this probability space, we find the subalgebra $\mathfrak{A}_+$ of all random variables in $\mathfrak{A}$ that are fully determined by the projection of their argument on Λ_+, thus defined in the same way as (6.8). Similar to the reflection in a reflection plane, the reflection $\Theta : \mathfrak{A} \to \mathfrak{A}$ is given by (6.9). If we consider the spin random variables, we have for spin i

$$\Theta(S^a_i)(\sigma) = S^a_i(\hat{\theta}\sigma) = (R_{\mathbf{u}}\mathbf{S}_{\theta i}(\sigma))^a, \tag{6.29}$$

for $a \in \{x, y, z\}$. Here $R_{\mathbf{u}}$ is the rotation matrix around the axis $\mathbf{u}$. The background functional τ can be factorized as $\tau(\Theta(A)B) = \overline{\tau_+(A)}\tau_+(B)$, and this factor τ_+ is strictly positive. The proof is equal to the proof of Lemma 6.1 and Lemma 6.2, except we do not need to condition on the spin configuration of the fixed point set of the reflection, since that is empty. Furthermore we can construct a Schauder basis for $\mathfrak{A}_+$ in a similar way as for the reflection plane.

We are now in the situation of Theorem 3.11, so $\tau_{\beta H}$ is reflection positive for all $0 \leq \beta$ if and only if the matrix $(J^0_{IJ})_{\mathcal{I}}$ of coupling constants across the reflection plane is positive semidefinite. Let us first focus on a situation where we have two spins that lie in the plane through their lattice point and rotation axis.

6.4.1. Two spins

Consider the lattice Λ as shown in Figure 6.6, consisting of two lattice points that are not nearest neighbours with spin vector that lies in a plane through the lattice point and the rotation axis. Suppose furthermore that $j = \theta(i)$

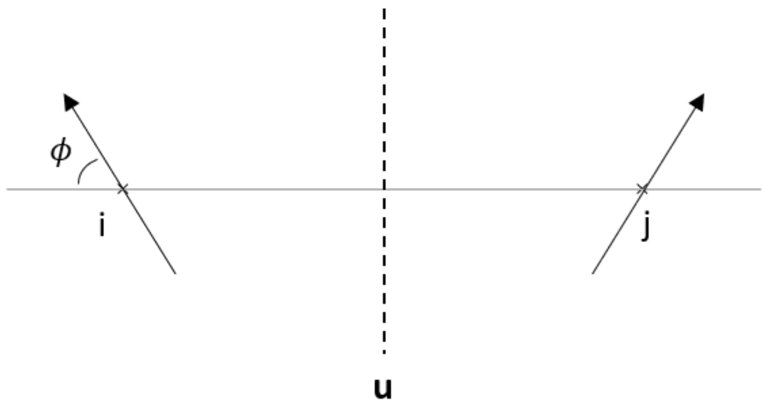

Figure 6.6: Two lattice points with spin vector that lies in a plane through the lattice point and the rotation axis, and is rotated over ϕ degrees.

The Hamiltonian of this situation is given by

$$H = \langle P_{\hat{e}_j}\mathbf{S}_j, M_{ij}P_{\hat{e}_i}\mathbf{S}_i\rangle\,. \tag{6.30}$$

We want to write this in the form (3.15). Since $R_{\mathbf{u}}$ is idempotent, we can write $H = \langle P_{\hat{e}_j}R^2\mathbf{S}_j, M_{ij}P_{\hat{e}_i}\mathbf{S}_i\rangle$. Since we have $R_{\mathbf{u}}\mathbf{S}_j = \Theta(S_{\theta(j)}) = \Theta(S_i)$ and, for a general spin k, $R_{\mathbf{u}}P_{\hat{e}_{\theta(k)}} = P_{\hat{e}_k}R_{\mathbf{u}}$, the Hamiltonian can be rewritten to

$$H = \langle\Theta(\mathbf{S}_i), P_{\hat{e}_i}R_{\mathbf{u}}M_{ij}P_{\hat{e}_i}\mathbf{S}_i\rangle\,. \tag{6.31}$$

This gives the matrix of coupling constants across the reflection plane

$$(J^0_{IJ})_{\mathcal{I}} = -P_{\hat{e}_i}R_{\mathbf{u}}M_{ij}P_{\hat{e}_i} = -\langle\hat{e}_i, R_{\mathbf{u}}M_{ij}\hat{e}_i\rangle\,P_{\hat{e}_i}\,. \tag{6.32}$$

We now formulate the following lemma.

Lemma 6.12. The matrix $(J^0_{IJ})_{\mathcal{I}}$ is negative semidefinite for the reflection (6.29). In particular the matrix has one negative eigenvalue.

Proof. The proof is an exact copy of the proof of Lemma 6.5. □

Remark 6.13. Similar to the reflection plane in Section 6.2, the matrix $(J^0_{IJ})_{\mathcal{I}}$ for the situation in Figure 6.6 is positive semidefinite for a spin inverting reflection, i.e. $\Theta(S^a_i)(\sigma) = -S^a_i(\hat{\theta}\sigma) = -(R_{\mathbf{u}}\mathbf{S}_{\theta i}(\sigma))^a$.

6.4.2. A larger lattice

Consider a pyrochlore lattice Λ, which is invariant under a rotation θ in an axis $\mathbf{u}$. Assuming the lattice contains the situation of Figure 6.6, and the rotation is given by (6.29), the Boltzmann functional τ_H is not reflection positive. This assumption for the lattice is valid, since the lattice is likely to look like a bigger version of Figure 6.1, which satisfies the assumption. The result is proved in the following theorem.

Theorem 6.14. For a big enough pyrochlore lattice Λ, the Boltzmann functional $\tau_{\beta H}$ is never reflection positive with respect to the reflection (6.29).

Proof. The proof is similar to the proof of Theorem 6.7, and uses Lemma 6.12. □

Remark 6.15. The proof of Theorem 6.14 can not be applied to the spin inverting reflection

$$\Theta(S_i^a)(\sigma) = -S_i^a(\hat{\theta}\sigma) = -(R_{\mathbf{u}}\mathbf{S}_{\theta i}(\sigma))^a, \tag{6.33}$$

since the matrix of Lemma 6.12 is positive semidefinite for this reflection. There is reason to believe that this reflection will result in a reflection positive Boltzmann functional. This believe is supported similar to the believe in Section 6.2, for the reflection plane with spin inverting reflection.

7

6-vertex model

The 6-vertex model is an example of an ice type model. It is a two dimensional version of the spin ice model considered in the previous chapter. We consider a square lattice where on every edge a spin is located. For every lattice point there are two spins pointing towards the vertex, and two pointing away. To every configuration an energy is assigned. The model is based on the one described in [Bax73].

In this chapter we evaluate reflection positivity with respect to diagonal reflections. In Section 7.1, the model is translated to the framework developed in Chapter 3. Then, in Section 7.2, the energy values for which the model is reflection positive will be calculated.

7.1. A description of the model

Consider a square $N \times N$ lattice $\Lambda \subseteq \mathbb{Z} \times \mathbb{Z}$ wrapped around a torus, and place an arrow on each bond such that at every vertex two arrows are pointing outwards, and two are pointing inwards. There are $\binom{4}{2} = 6$ possible configurations, as shown in Figure 7.1.

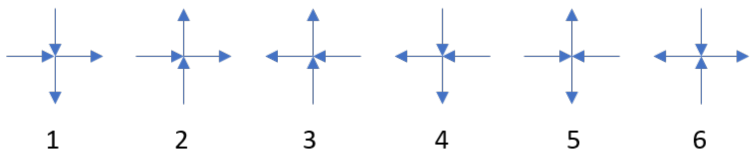

Figure 7.1: The six possible configurations in the 6-vertex model.

To every configuration, we assign the energy $\epsilon_i \in \mathbb{R}$, such that the Hamiltonian of the system is given by

$$H = \sum_{i=1}^{6} N_i \epsilon_i, \tag{7.1}$$

where N_i is the number of times that the specific configuration is found.

7.1.1. The algebra

We wish to translate the model to the setting of Chapter 3. For this, consider the reciprocal lattice of Λ, which we call Λ'. This is the $N \times N$ lattice with lattice points $\{\frac{2\pi}{N}(i,j) : i,j \in \{0,\ldots,N-1\}\}$. Now consider functions $\omega : \Lambda' \to \mathbb{Z}$, satisfying $|\omega(\lambda) - \omega(\lambda')| = 1$ for nearest neighbour $\lambda, \lambda' \in \Lambda'$. If we then look at a plaquette in the reciprocal lattice, there are, up to an additional constant, six possible configurations, as depicted in Figure 7.2.

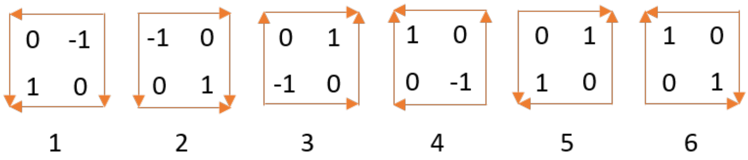

Figure 7.2: The six possible configurations in the reciprocal lattice of the 6-vertex model.

These configurations are the same as the configurations in 7.1. If we interpret the configurations in 7.2 as a 'mountain scenery', or in other words, a solid on solid model, and we want to walk a path with the mountain always on our right hand, then we walk exactly in the direction of the arrows in Figure 7.1. For instance, when we walk between a '0' and a '1', we need a path in the upper direction; $0 \uparrow 1$, such that the mountain (the '1') is to our right hand. The similarity of the configurations is shown in Figure 7.3.

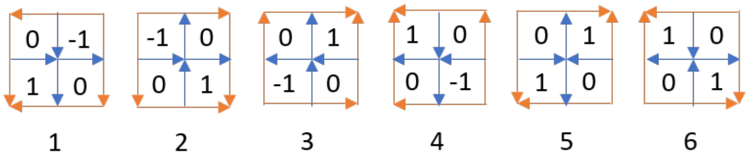

Figure 7.3: The six configurations are equal, and we can interpret them as a 'mountain scenery' and paths with the mountain to our right hand.

Another way of interpreting the arrows in Figure 7.3 is as the divergence and rotation of a vector field. We thus see that we can describe the probability space of possible configurations as

$$\Omega = \{\omega : \Lambda' \to \mathbb{Z} : |\omega(\lambda) - \omega(\lambda')| = 1 \text{ for nearest neighbour } \lambda, \lambda' \in \Lambda'\}/\mathbb{Z}, \tag{7.2}$$

where $[\omega] = [\bar{\omega}]$ whenever $\bar{\omega} - \omega \in \mathbb{Z}$. Now we define the algebra as all random variables acting on the probability space, i.e.

$$\mathfrak{A} = \{F : \Omega \to \mathbb{C}\}. \tag{7.3}$$

This is indeed an algebra, since we can add and multiply random variables. A special random variable in this algebra is the Hamiltonian, which we can write as

$$H([\omega]) = \sum_p h([\omega]|_p), \tag{7.4}$$

where the sum is over all plaquettes in the lattice, and $h([\omega]|_p)$ is the Hamiltonian restricted to a plaquette p. This restriction is one of the configurations shown in Figure 7.2, so we have $h([\omega]|_p) = \epsilon_i$ depending on the configuration of $[\omega]|_p$.

7.1.2. The reflection

There are several possible lattice invariant reflections in the torus lattice. We choose to look at the diagonal reflections, as depicted in Figure 7.4. The reason for this is that the plaquettes on the reflection line of a diagonal reflection do not influence each other. Such a reflection θ splits the lattice into two parts Λ_+ and $\Lambda_- := \theta(\Lambda_+)$. Their intersection is the fixed point set P of the reflection plane.

We can now define the probability space Ω_+ by using the reciprocal lattice Λ'_+ of Λ_+. This reciprocal lattice contains exactly all points on one side of the reflection plane, including the point on the reflection plane, as indicated with black bullet points in Figure 7.4. For Ω_+, we then have

$$\Omega_+ := \{\omega : \Lambda'_+ \to \mathbb{Z} : |\omega(\lambda) - \omega(\lambda')| = 1 \text{ for nearest neighbour } \lambda, \lambda' \in \Lambda'_+\}/\mathbb{Z}. \tag{7.5}$$

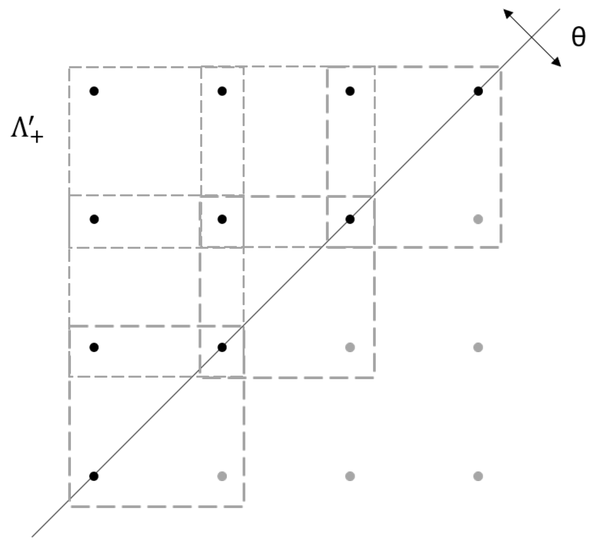

Figure 7.4: The diagonal reflection in the 6-vertex model on the reciprocal lattice. The reflection θ and some plaquettes are shown.

From this we find the subalgebra $\mathfrak{A}_+$ of all functions in $\mathfrak{A}$ that are fully determined by their value on Ω_+, thus

$$\mathfrak{A}_+ = \{F \in \mathfrak{A} : F([\omega]) = F([\omega]|_{\Lambda'_+})\}. \tag{7.6}$$

Since Ω is finite, there exists a basis for the subalgebra $\mathfrak{A}_+$.

7.1.3. The functional

The functional we use is the Boltzmann functional $\tau_H : \mathfrak{A} \to \mathbb{C}$. Since our lattice is discrete and finite, it is given by

$$\tau_H(A) = \sum_{[\omega]\in\Omega} \frac{A([\omega])e^{-H([\omega])}}{Z}, \tag{7.7}$$

where $Z \geq 0$ is the partition function. Since τ_H has to be reflection invariant under the reflection $\Theta : \mathfrak{A} \to \mathfrak{A}$, we choose the reflection to be given by

$$\Theta(A)([\omega]) = \overline{A(\hat{\theta}([\omega]))}, \tag{7.8}$$

where $\hat{\theta} : \Omega \to \Omega$ is given by $\hat{\theta}(\omega)(\lambda) = \omega(\theta(\lambda))$.

From the reflection invariance property we can furthermore conclude that the following condition on the energies of the six configurations must be satisfied,

$$\begin{aligned} \epsilon_1 = \epsilon_3 = a, \qquad \epsilon_5 = c, \\ \epsilon_2 = \epsilon_4 = b, \qquad \epsilon_6 = d, \end{aligned} \tag{7.9}$$

where $a, b, c, d \in \mathbb{R}$. We have equality of ϵ_1 and ϵ_3, and equality of ϵ_2 and ϵ_4, since these are diagonal reflections of each other, and we want reflection invariance in both diagonal directions.

We furthermore need the background functional τ to be factorizing and strictly positive, which can be proved similar to Lemma 6.1 and Lemma 6.2.

7.2. Reflection positivity of the 6-vertex model

We want the functional to be reflection positive, which will likely further restrict the values of the energies. Since the functional τ is continuous and factorizing on $\mathfrak{A}$, τ_+ is strictly positive, and the

Hamiltonian $H \in \mathfrak{A}$ is a reflection invariant operator, by Theorem 3.11 we know that the Boltzmann functional $\tau_{\beta H}$ is reflection positive for all $\beta \geq 0$ if and only if there is a decomposition $H = H_- + H_0 + H_+$ with $H_+ \in \mathfrak{A}_+$, $H_- = \Theta(H_+)$ and $-H_0 \in \overline{\text{co}}(\mathcal{K}_+)$.

If we let H_+ be the sum over all plaquettes above the reflection line, as indicated with the small dashed lines in Figure 7.4, then indeed $H_- = \Theta(H_+)$ regarding the energy values in (7.9). We thus need to check that the negative sum over all plaquettes on top of the reflection line, $-H_0$, is contained in the reflection positive cone. This we will prove in Theorem 7.1. The plaquettes in H_0 are indicated with the bigger dashed lines in Figure 7.4. The reflection positive cone is the closure of the convex hull of $\mathcal{K}_+ = \{\Theta(A)A : A \in \mathfrak{A}_+\}$. Note that for every $A \in \mathfrak{A}_+$, we also have $cA \in \mathfrak{A}_+$ for every $c \in \mathbb{C}$. Therefore for any $B \in \mathcal{K}_+$, we have $kB \in \mathcal{K}_+$ where $k \in \mathbb{R}_{\geq 0}$.

Theorem 7.1. The Hamiltonian $-H_0$ is contained in $\overline{\text{co}}(\mathcal{K}_+)$ for both diagonal reflections if and only if the energies assigned to the different configurations as in (7.9) satisfy $c, d \leq 0$ and $-\sqrt{cd} \leq a, b \leq 0$.

We will prove Theorem 7.1 with help of a lemma, in which we consider only one plaquette.

Lemma 7.2. Let $-B$ be a random variable acting on a single plaquette, taking values as in (7.9) on the different configurations. Then $-B \in \overline{\text{co}}(\mathcal{K}_+)$ for both diagonal reflections if and only if $c, d \leq 0$ and $-\sqrt{cd} \leq a, b \leq 0$.

Proof. "$\Rightarrow$" Suppose $-B \in \overline{\text{co}}(\mathcal{K}_+)$, then we can write $-B$ as a convex sum of elements in $\mathcal{K}_+$. First consider only one of the diagonal reflections. Let us focus on a random variable in $\mathfrak{A}_+$ and the restriction of its argument to the plaquette on the reflection plane. There are, up to a constant, four possible configurations for the argument, as shown in Figure 7.5.

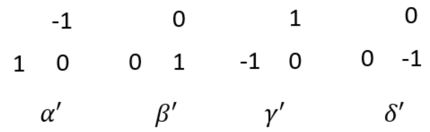

Figure 7.5: The four possible configurations when restricting the argument of an element in $\mathfrak{A}_+$ to a plaquette on the reflection plane.

Define a random variable $A \in \mathfrak{A}_+$ that on this plaquette takes the values

$$A = \begin{cases} \alpha & \text{if the restriction to the plaquette has configuration } \alpha', \\ \beta & \text{if the restriction to the plaquette has configuration } \beta', \\ \gamma & \text{if the restriction to the plaquette has configuration } \gamma', \\ \delta & \text{if the restriction to the plaquette has configuration } \delta', \end{cases} \tag{7.10}$$

and zero elsewhere. Then for $\Theta(A)A$ we find for the configurations of Figure 7.2,

$$\Theta(A)A = \begin{cases} \bar{\alpha}\alpha & \text{if the plaquette has configuration 1,} \\ \bar{\delta}\beta & \text{if the plaquette has configuration 2,} \\ \bar{\gamma}\gamma & \text{if the plaquette has configuration 3,} \\ \bar{\beta}\delta & \text{if the plaquette has configuration 4,} \\ \bar{\delta}\delta & \text{if the plaquette has configuration 5,} \\ \bar{\beta}\beta & \text{if the plaquette has configuration 6.} \end{cases} \tag{7.11}$$

Since we can write $-B$ as a sum with positive coefficients of random variables of the form (7.11), we infer that a, c and d are nonpositive. To determine the restriction on b, observe that we can write

$$\begin{bmatrix} \beta\bar{\beta} & \beta\bar{\delta} \\ \gamma\bar{\beta} & \gamma\bar{\gamma} \end{bmatrix} = \begin{bmatrix} \beta \\ \gamma \end{bmatrix} \begin{bmatrix} \bar{\beta} & \bar{\gamma} \end{bmatrix}, \tag{7.12}$$

which is the projection matrix on the vector $\begin{bmatrix}\beta & \gamma\end{bmatrix}^T$. Then we can write the matrix

$$M = \begin{bmatrix}-d & -\bar{b}\\ -b & -c\end{bmatrix}, \tag{7.13}$$

as a sum with positive coefficients of matrices of the form (7.12). Now using Theorem 2.3, we know that M must be positive semidefinite, so it has a nonnegative determinant. This gives the restriction $|b| \leq \sqrt{cd}$.

Reflection positivity for a reflection in the other diagonal switches the roles of a and b, and will thus yield the restrictions $b, c, d \leq 0$ and $|a| \leq \sqrt{cd}$. This proves the right implication.

"$\Leftarrow$" Suppose a, b, c and d satisfy the restrictions of the lemma. Then for both reflections, we want to construct a random variable in $\overline{\text{co}}(\mathcal{K}_+)$ that is exactly equal to B. First consider the reflection in the lower-left to upper-right diagonal. Then using Theorem 2.3 we can write the matrix $M = \lambda_1 \mathbf{q}_1 \mathbf{q}_1^* + \lambda_2 \mathbf{q}_2 \mathbf{q}_2^*$, where M as in (7.13) and λ_1 and λ_2 the eigenvalues of M. This is a sum with positive coefficients of projection matrices. Now let $A_1, A_2 \in \mathfrak{A}_+$ be as in (7.10) with coefficients satisfying $|\alpha| = |\gamma| = \sqrt{\frac{-a}{\lambda_i}}$, β the first component of $\mathbf{q}_i$ and δ the second component of $\mathbf{q}_i$ for $i = 1, 2$. Then $-B = \lambda_1 \Theta(A_1) A_1 + \lambda_2 \Theta(A_2) A_2$. For the other reflection we do the same but with the roles of a and b swapped. Then indeed $-B \in \overline{\text{co}}(\mathcal{K}_+)$ for both diagonal reflections, which proves the left implication. □

Proof of Theorem 7.1. "$\Leftarrow$" We want to write $-H_0$ as a sum with positive coefficients of elements in $\mathcal{K}_+$. Since we consider a finite $N \times N$ lattice and due to periodic boundary conditions, H_0 is the sum over N plaquettes. Using Lemma 7.2 we know that there exist random variables in $-B \in \overline{\text{co}}(\mathcal{K}_+)$ such that we have reflection positivity for one plaquette. If we label the plaquettes in H_0 by $p_1, \ldots, p_N$, we can construct a random variable B_{p_i} on every plaquette, taking the values of $-B$ on that plaquette. Then we have $B_{p_i} \in \overline{\text{co}}(\mathcal{K}_+)$ and $-H_0 = \sum_{i=1}^N B_{p_i}$, so $-H_0$ is a sum with positive coefficient of elements in $\mathcal{K}_+$, thus $-H_0 \in \overline{\text{co}}(\mathcal{K}_+)$. This proves the left implication.

"$\Rightarrow$" Now suppose $-H_0 \in \overline{\text{co}}(\mathcal{K}_+)$. Since different plaquettes in H_0 overlap in only one corner, they don't interact, so $-H_0$ can be written as a sum of random variables acting only on a single plaquette. Lemma 7.2 now proves the right implication. □

We conclude that the 6-vertex model on an $N \times N$ lattice with diagonal reflections, is reflection positive whenever the energy values satisfy $c, d \leq 0$ and $-\sqrt{cd} \leq a, b \leq 0$.

7.3. Infinite lattice

Although we will not look at phase transitions in the 6-vertex model, it is interesting to evaluate reflection positivity of the Boltzmann functional for infinite lattices. For this the proof of Theorem 7.1 does not apply, because H_0 is infinite for almost all possible spin configurations. We can however show that reflection positivity is preserved when taking limits of functionals.

Theorem 7.3. Let $\mathfrak{A}$ be an algebra with a reflection $\Theta : \mathfrak{A} \to \mathfrak{A}$, such that $\mathfrak{A}$ is the double of $\mathfrak{A}_+ \mathfrak{A}_-$. For $N \in \mathbb{N}$, let $\tau_N : \mathfrak{A} \to \mathbb{C}$ be reflection positive functionals converging to a neutral and linear functional $\tau : \mathfrak{A} \to \mathbb{C}$ in the sense that $\lim_{N\to\infty} \tau_N(A) = \tau(A)$ for all $A \in \mathfrak{A}$. Then τ is also reflection positive.

Proof. Choose $A \in \mathfrak{A}_+$. Then $\tau(\Theta(A)A) = \lim_{N\to\infty} \tau_N(\Theta(A)A) \geq 0$. □

Since the Boltzmann functionals that we constructed for the $N \times N$ lattices are also functionals on the algebra $\mathfrak{A}$ for an infinite lattice, we can directly apply Theorem 7.3 to show that the Boltzmann functional on the infinite lattice is reflection positive.

8

16-vertex model

The 16-vertex model is a modification of the 6-vertex model described in the previous chapter. In this model there is no requirement on the number of spins allowed to point towards a vertex. It has great resemblance to the spin ice model described in Chapter 6, where the spins were also allowed to point in every direction. The difference being the dimension of the two models, and the formulation of the Hamiltonian. In the case of the 16-vertex model an energy is assigned to every possible configuration of a vertex with neighbouring spins, which is based on the model described in [Bax73]. The goal of this section is to find values of the energy such that the model is reflection positive with respect to diagonal reflections.

In Section 8.1, the model is described in the setting of Chapter 3. Then, in Section 8.2, the values for which the model is reflection positive are calculated. Finally in Section 8.3, reflection positivity for the model with energy values that allow for the existence of magnetic monopoles is evaluated.

8.1. A description of the model

The 16-vertex model is an extension of the 6-vertex model. Consider a square $N \times N$ lattice $\Lambda \subseteq \mathbb{Z} \times \mathbb{Z}$ wrapped around a torus. On every bond we place an arrow, with no condition on the number of arrows pointing inside or outside of the vertex. There are $2^4 = 16$ possible configurations. To every configuration we assign the energy $\epsilon_i \in \mathbb{R}$, as depicted in Figure 8.1. The configurations are ordered in orbits under the elements of the reflection group generated by reflections in both diagonals, labeled a to g. We will refer to this later.

The Hamiltonian is given by

$$H = \sum_{i=1}^{16} N_i \epsilon_i, \tag{8.1}$$

where N_i is the number of times the specific configuration with energy ϵ_i is found.

8.1.1. The setting

We wish to translate the model to the setting of Chapter 3. The probability space of the model can be described by all directed graphs on the $N \times N$ lattice wrapped around a torus, i.e.

$$\Omega = \{\text{all graphs } G = (V, A) : V \text{ vertex set } \Lambda \text{ , } A \text{ directed edges between nearest neighbours}\}. \tag{8.2}$$

We then define the algebra as all random variables acting on the probability space,

$$\mathfrak{A} := \{F : \Omega \to \mathbb{C}\}. \tag{8.3}$$

A special random variable in this algebra is the Hamiltonian.

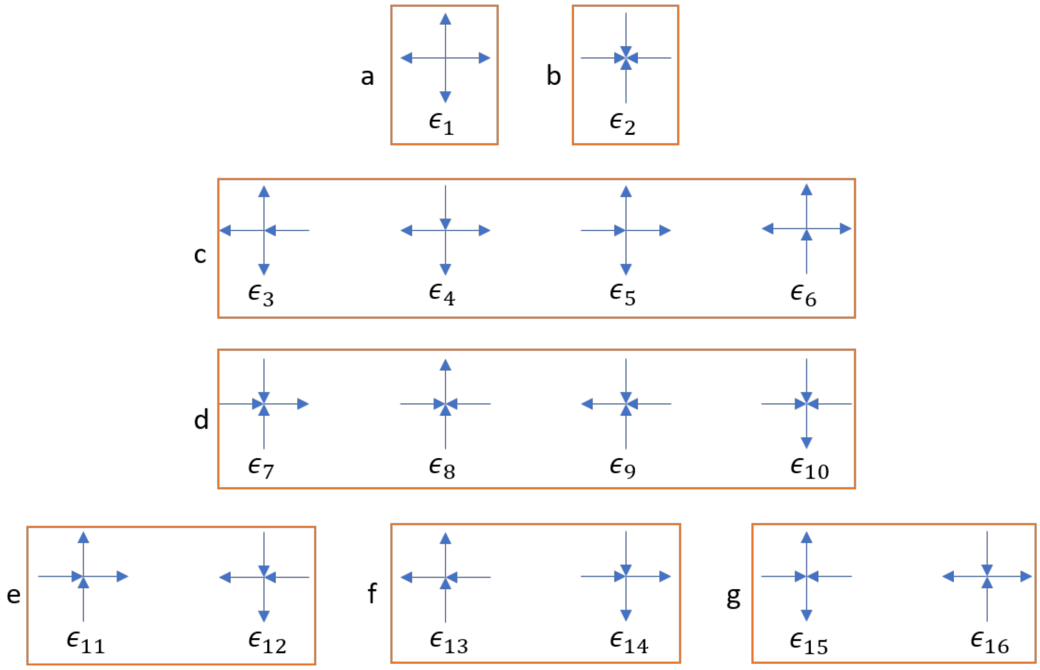

Figure 8.1: The sixteen possible configuration in the 16-vertex model, with energy ϵ_i for $i = 1, ..., 16$. The orbits of configurations under the elements of the reflection group generated by reflections in both diagonals, labelled a to g, is also shown.

Just as in the 6-vertex model, we choose to look at diagonal reflections. The reason for this, is that different vertices that are located on top of the reflection plane don't influence each other, thus making it easier to use Theorem 3.11. The reflection θ splits the lattice in two parts, Λ_+ and $\Lambda_- := \theta(\Lambda_+)$. Their intersection is the fixed point set P of the reflection plane. The probability space Ω_+ is the set of all directed graphs on Λ_+. The subalgebra $\mathfrak{A}_+$ then contains all functions in $\mathfrak{A}$ that are fully determined by their value on Ω_+. Since Ω is finite, there exists a basis for this subalgebra.

We use the Boltzmann functional $\tau_H : \mathfrak{A} \to \mathbb{C}$. Since our Ω is finite, it is given by

$$\tau_H(A) = \sum_{\omega\in\Omega} \frac{A(\omega)e^{-H(\omega)}}{Z}, \tag{8.4}$$

where Z is the partition function. Since τ_H has to be reflection invariant under the reflection Θ, we infer that the reflection is given by

$$\Theta(A)(\omega) = \overline{A(\hat{\theta}\omega)}, \tag{8.5}$$

where $\hat{\theta} : \Omega \to \Omega$ mirrors the graph in the reflection plane.

From the reflection invariance property already a few conclusions can be drawn on the allowed values of the energy of the vertices. We look at the actions of the Klein-four group $K_4 = \{I, \sigma_1, \sigma_2, \sigma_1\sigma_2\}$ where σ_1 and σ_2 are reflection in the different diagonals. All configurations that are in the same orbit need to take the same energy value. The orbits are depicted in Figure 8.1. We conclude that

$$\begin{aligned} \epsilon_1 &= -a & \epsilon_2 &= -b \\ \epsilon_3 = \epsilon_4 = \epsilon_5 = \epsilon_6 &= -c & \epsilon_7 = \epsilon_8 = \epsilon_9 = \epsilon_{10} &= -d \\ \epsilon_{11} = \epsilon_{12} &= -e & \epsilon_{13} = \epsilon_{14} &= -f \\ \epsilon_{15} = \epsilon_{16} &= -g. \end{aligned} \tag{8.6}$$

The functional τ is factorizing and its factor τ_+ is strictly positive. The proof of this is similar to the proof of Lemma 6.1 and Lemma 6.2.

Remark 8.1. Note that the reflection Θ in (8.5) is different from the one in (7.8). In the 6-vertex model we formulated the algebra as a 'mountain scenery', reflecting this scenery in a diagonal simply reflects the values of the scenery to the other side of the plane. In the 16-vertex model, however, the reflection changes the direction of the arrows. This difference is visualized in Figure 8.2.

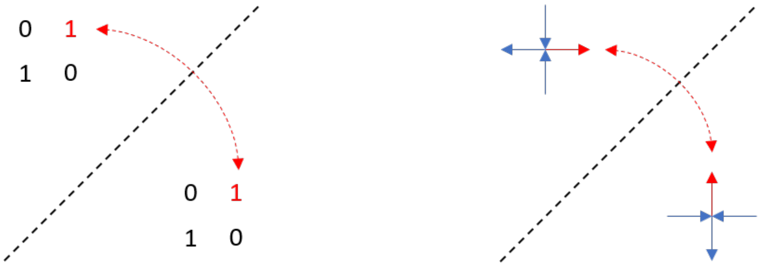

Figure 8.2: On the left a reflection in the 6-vertex model, where the values of the 'mountain scenery' are reflected. On the right a reflection in the 16-vertex model, where an arrow is reflected and its direction changes.

8.2. Reflection positivity of the 16-vertex model

We want the function to be reflection positive. Since the functional τ is continuous and factorizing on $\mathfrak{A}$, τ_+ is strictly positive, and $H \in \mathfrak{A}$ is a reflection invariant operator, by Theorem 3.11 we know that the Boltzmann functional $\tau_{\beta H}$ is reflection positive for all $\beta \geq 0$ if and only if there is a decomposition $H = H_- + H_0 + H_+$ with $H_+ \in \mathfrak{A}_+$, $H_- = \Theta(H_+)$ and $-H_0 \in \overline{\text{co}}(\mathcal{K}_+)$.

If we let H_+ be the sum over all vertices above the reflection line, then indeed $H_- = \Theta(H_+)$. We thus need to check if $-H_0$ is contained in the reflection positive cone. Let us first consider a random variable acting on only one vertex, then we can formulate the following lemma.

Lemma 8.2. Let $-B$ be a random variable that depends on a single vertex on the reflection line, taking the values of (8.6). Then $-B \in \overline{\text{co}}(\mathcal{K}_+)$ for reflections in both diagonals if and only if the matrices

$$M_1 = \begin{bmatrix} a & c & c & f \\ c & e & g & d \\ c & g & e & d \\ f & d & d & b \end{bmatrix}, \quad M_2 = \begin{bmatrix} a & c & c & e \\ c & f & g & d \\ c & g & f & d \\ e & d & d & b \end{bmatrix} \tag{8.7}$$

are positive semidefinite.

Proof. Let us first consider the reflection in only one diagonal, and focus on a vertex on the reflection line. The possible configurations of the edges are as given in Figure 8.3.

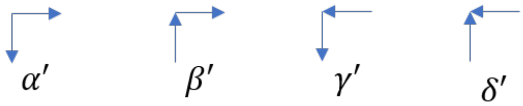

Figure 8.3: The four possible configurations of the edges for a vertex on the reflection plane.

We define a random variable $A \in \mathfrak{A}_+$ that on this vertex takes the values

$$A = \begin{cases} \alpha & \text{if the restriction to the vertex has configuration } \alpha', \\ \beta & \text{if the restriction to the vertex has configuration } \beta', \\ \gamma & \text{if the restriction to the vertex has configuration } \gamma', \\ \delta & \text{if the restriction to the vertex has configuration } \delta'. \end{cases} \tag{8.8}$$

The random variable $\Theta(A)A$ then acts on the configurations of Figure 8.1, and for a vertex p we have $\Theta(A)A(p) = \rho\bar{\sigma}$ if p is of the form $\rho'\theta(\sigma')$ for $\rho, \sigma = \alpha, \beta, \gamma, \delta$. This result can be written as a projection matrix on the vector $\begin{bmatrix}\alpha & \beta & \gamma & \delta\end{bmatrix}^T$, i.e.

$$\begin{bmatrix} \alpha\bar{\alpha} & \alpha\bar{\beta} & \alpha\bar{\gamma} & \alpha\bar{\delta} \\ \beta\bar{\alpha} & \beta\bar{\beta} & \beta\bar{\gamma} & \beta\bar{\delta} \\ \gamma\bar{\alpha} & \gamma\bar{\beta} & \gamma\bar{\gamma} & \gamma\bar{\delta} \\ \delta\bar{\alpha} & \delta\bar{\beta} & \delta\bar{\gamma} & \delta\bar{\delta} \end{bmatrix}. \tag{8.9}$$

We have $-B \in \overline{\text{co}}(\mathcal{K}_+)$ for this reflection if and only if the matrix M_1 of (8.7) is a sum of matrices of the form (8.9). By Theorem 2.3, we thus know that M_1 is positive semidefinite. For the reflection in the other diagonal, a similar result is obtained for the matrix M_2 of (8.7). To prove the converse direction, we can decompose the matrices M_1 and M_2 in a positive sum of projection matrices, which are contained in the reflection positive cone of the considered diagonal reflection. This proves the lemma. □

Using Lemma 8.2, we can find a condition for reflection positivity of the whole model.

Theorem 8.3. The 16-vertex model with energy taking the values of (8.6) is reflection positive with respect to reflections in the diagonal if and only if the matrices M_1 and M_2 of (8.7) are positive semidefinite.

Proof. By Theorem 3.11, the first statement is equivalent to having $-H_0 \in \overline{\text{co}}(\mathcal{K}_+)$. Equivalence of the latter with the second statement can be proved in a similar way as in the proof of Theorem 7.1. □

Remark 8.4. The result can be extended to an infinite lattice using Theorem 7.3.

8.3. Magnetic monopoles

A special feature of spin ice models, is their allowance for the existence of magnetic monopoles. Castelnovo, Moessner and Sondhi proposed that the spins in spin ice models can be thought of as two separated and oppositely charged magnetic monopoles [CMS08]. In the spin ice model of Section 6, there are then four charges at the center of every tetrahedron. In the ice type models of Section 7 and 8 there are four charges at every vertex. This results in a local magnetic charge neutrality. At finite temperature, spin fluctuations create pairs of defects breaking the 2 in, 2 out rule, which creates the 16 configurations in the 16-vertex model, and is also the reason that we looked at spins pointing in a random direction in Section 6. The result is that every tetrahedron/vertex carries a net magnetic charge, depending on the configuration.

The easiest way in which the 16-vertex model allows for monopoles, is by assigning an energy of $n-2$ (or a scaled version of these energies) to every vertex, where n is the number of arrows pointing inside of the vertex. That means that for the energy values of (8.6) we find $-a = -2$, $-b = 2 - c = -1$, $-d = 1$ and $-e = -f = -g = 0$. The question that arises is if this model is reflection positive with respect to reflections in the diagonal. This question is easy to answer, because the Hamiltonian is not reflection invariant.

We could consider to, instead of an energy $n-2$, look at the absolute value of these energies, i.e. $\mu|n-2|$ with $\mu > 0$. By Theorem 8.3 we have a concrete way of checking reflection positivity. Substituting the new values of a, b, c, d, e, f, g in the matrix M_1 (or M_2), gives

$$M_{1,2} = \mu \begin{bmatrix} -2 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & -2 \end{bmatrix}. \tag{8.10}$$

Since $\mathbf{e}_1^* \mu M_{1,2} \mathbf{e}_1 = -2\mu$ with $\mathbf{e}_1$ being the first unit vector, the matrix $M_{1,2}$ is not positive semidefinite. Therefore the model with these energies is not reflection positive.

Remark 8.5. If we let the energies take values $a = b = 2$, $c = d = 1$ and $e = f = g = 0$ (or scaled by a factor $\mu > 0$, then the matrix $M_{1,2}$ is still not positive semidefinite. This can be shown by calculating the inner product $\langle \mathbf{a}, M_{1,2}\mathbf{a} \rangle$, which will give a negative value for $a = \begin{bmatrix} 1-\sqrt{2} & 1 & 0 & 0 \end{bmatrix}^T$.

Since we thus do not have reflection positivity with respect to a reflection in the diagonal, this shows that we can not prove phase transitions using the developed methods of Section 4 in the 16-vertex model, with energy values that allow for the existence of magnetic monopoles. It may, however, be possible using vertical and horizontal reflections, but that reflection is not evaluated in this thesis.

9

Conclusion

In this thesis, reflection positivity was studied. Reflection positivity is a mathematical tool with applications in constructive quantum field theory and statistical physics. In statistical physics, reflection positivity is used to prove phase transitions in physical models. A brief explanation of different methods to prove phase transitions was given, based on the description in [Bis09]. An overview of reflection positivity was given, based on the work 'reflection positive doubles' by Jaffe and Janssens [JJ17]. In this overview, the proof of a theorem regarding tractable conditions on a Hamiltonian, to show reflection positivity of the Boltzmann functional, was given for the more specific case of bosonic algebras.

The theorem was then applied to prove or disprove reflection positivity in four different physical models. The first model treated was the antiferromagnetic quantum Heisenberg model, where reflection positivity of the Boltzmann functional was shown regarding reflections in a reflection plane. For both the nearest neighbour and the long-range model, this was done by proving that the so-called matrix of coupling constants across the reflection plane is positive semidefinite. The result was obtained by proving that a specific function only depending on the distance between two lattice points is Osterwald-Schrader positive.

The second model treated was the spin ice model. For this model a pyrochlore lattice with spins located on the midpoints of the bonds of a diamond lattice was considered. There are three possible symmetries in this lattice, a reflection in a plane, an inversion and a rotational symmetry. It was shown that, for these symmetries, the Boltzmann functional with respect to a spin invariant reflection is never reflection positive, which is a new result. Furthermore, for the inversion it was shown that the Boltzmann functional is also not reflection positive for a spin inverting reflection. However, a similar result is not rigorously proved for the reflection plane and rotational symmetry.

The third and fourth models we treated were the 6-vertex and 16-vertex model. These are both two-dimensional versions of the spin ice model, and are classified as 'ice-type' models. Using diagonal reflections, a restriction on the allowed energy values was given for both models, such that the Boltzmann functional is reflection positive. These were both new results. Specifically, regarding the condition for reflection positivity of the 16-vertex model, we formulated and proved a theorem such that one only needs to check whether a matrix is positive semidefinite to prove reflection positivity of the model. Furthermore, for the 16-vertex model, we showed that the energy values that allow for the existence of magnetic monopoles do not give a reflection positive Boltzmann functional.

A topic for further research is proving the occurrence of phase transitions in the models that were shown to be reflection positive. This is believed to be possible using chessboard estimates, by showing that the set of Gibbs measures on an infinite lattice is non-singular for certain values of the inverse temperature. Furthermore, it is interesting to further investigate reflection positivity of the

Boltzmann functional for the spin ice model, considering spin inverting reflections in a plane or for a rotational symmetry. This could require computational methods.

9.1. Acknowledgements

First and foremost I would like to thank Dr. B. Janssens and Dr. A.R. Akhmerov for their supervision and guidance during the project. Their comments and explanation were of great value for the obtained results in this thesis. Furthermore, I would like to thank Sarah Jansen, Jan Bosma, Sándor Mahieu and Sammy Go for their unconditional support during the project, and pre-reading the report to find grammatical errors. Their support was highly appreciated, especially considering the strange Covid-19 times during which the research was conducted. Lastly, I would like to thank my family and other close friends for supporting me during the whole course of my bachelor.

Bibliography

[Bax73] Rodney Baxter. Eight-vertex model in lattice statistics and one-dimensional anisotropic heisenberg chain. i. some fundamental eigenvectors. *Annals of Physics*, 76(1):1–24, March 1973.

[Bax82] Rodney Baxter. *Exactly solved models in statistical mechanics.* Academic Press, London New York, 1982.

[Bis09] Marek Biskup. Reflection positivity and phase transitions in lattice spin models. *Lecture Notes in Mathematics Methods of Contemporary Mathematical Statistical Physics*, page 1–86, 2009.

[Bra01] S. T. Bramwell. Spin ice state in frustrated magnetic pyrochlore materials. *Science*, 294(5546):1495–1501, November 2001.

[CMS08] C. Castelnovo, R. Moessner, and S. L. Sondhi. Magnetic monopoles in spin ice. *Nature*, 451(7174):42–45, 2008.

[DLS76] Freeman J. Dyson, Elliott H. Lieb, and Barry Simon. Phase transitions in the quantum heisenberg model. *Physical Review Letters*, 37(3):120–123, July 1976.

[DLS78] Freeman J. Dyson, Elliott H. Lieb, and Barry Simon. Phase transitions in quantum spin systems with isotropic and nonisotropic interactions. *Journal of Statistical Physics*, 18(4):335–383, April 1978.

[Dud02] Richard M. Dudley. *Real analysis and probability.* Cambridge Univ. Press, 2002.

[FILS78] Jürg Fröhlich, Robert Israel, Elliot H. Lieb, and Barry Simon. Phase transitions and reflection positivity. i. general theory and long range lattice models. *Communications in Mathematical Physics*, 62(1):1–34, August 1978.

[FL09] Rupert L. Frank and Elliott H. Lieb. Inversion positivity and the sharp hardy–littlewood–sobolev inequality. *Calculus of Variations and Partial Differential Equations*, 39(1-2):85–99, December 2009.

[FSS76] J. Fröhlich, B. Simon, and T. Spencer. Infrared bounds, phase transitions and continuous symmetry breaking. *Communications in Mathematical Physics*, 50(1):79–95, February 1976.

[FV17] Sacha Friedli and Yvan Velenik. *Statistical Mechanics of Lattice Systems.* Cambridge University Press, November 2017.

[GC15] V. Ovidiu Garlea and Bryan C. Chakoumakos. Magnetic structures. In *Experimental Methods in the Physical Sciences*, pages 203–290. Elsevier, 2015.

[Gij17] D.C. Gijswijt. *Algebra 1.* TU Delft, 2017.

[GJS74] James Glimm, Arthur Jaffe, and Thomas Spencer. The wightman axioms and particle structure in the $\mathsf{P}(\varphi)_2$ quantum field model. *The Annals of Mathematics*, 100(3):585, November 1974.

[GJS75] James Glimm, Arthur Jaffe, and Thomas Spencer. Phase transitions for φ_2^4 quantum fields. *Communications in Mathematical Physics*, 45(3):203–216, October 1975.

[Had] Peter Hadley. Diamond crystal structure.

[HGK04] Michiel Hazewinkel, Nadiya Gubareni, and Vladimir V. Kirichenko. *Algebras, rings and modules*. Springer, 2004.

[JJ17] Arthur Jaffe and Bas Janssens. Reflection positive doubles. *Journal of Functional Analysis*, 272(8):3506–3557, April 2017.

[ML67] S.C. Miller and W.F. Love. *Tables of irreducible representations of space groups and co-representations of magnetic space groups*. Pruett Press, Boulder, Col., 1967.

[NÓ14] Karl-Hermann Neeb and Gestur Ólafsson. Reflection positivity and conformal symmetry. *Journal of Functional Analysis*, 266(4):2174–2224, February 2014.

[OS73a] K. Osterwalder and R. Schrader. Euclidean fermi fields and a feynman-kac formula for boson-fermion models. *Helv. Phys. Acta*, 46:277–302, 1973.

[OS73b] Konrad Osterwalder and Robert Schrader. Axioms for euclidean green's functions. *Comm. Math. Phys.*, 31(2):83–112, 1973.

[OS75] Konrad Osterwalder and Robert Schrader. Axioms for euclidean green's functions II. *Communications in Mathematical Physics*, 42(3):281–305, October 1975.

[Rud86] Walter Rudin. *Real and Complex Analysis (Higher Mathematics Series)*. McGraw-Hill Education, may 1986.

[Sim13] Steven H. Simon. *The Oxford Solid State Basics*. Oxford University Press, 2013.

[Thi19] J.M. Thijssen. *Lecture notes statistical physics*. TU Delft, 2019.

[Ver17] Johannes Vermeer. *Lineaire Algebra, deel 2 voor Technische Natuurkunde*. TU Delft, 2017.

A

Tetrahedra

The corner points of a regular tetrahedon in 3 dimensions (Figure A.1) can be described by the euclidean space coordinates $a = (1,0,0)$, $b = (0,1,0)$, $c = (0,0,1)$, $d = (1,1,1)$ with midpoint $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

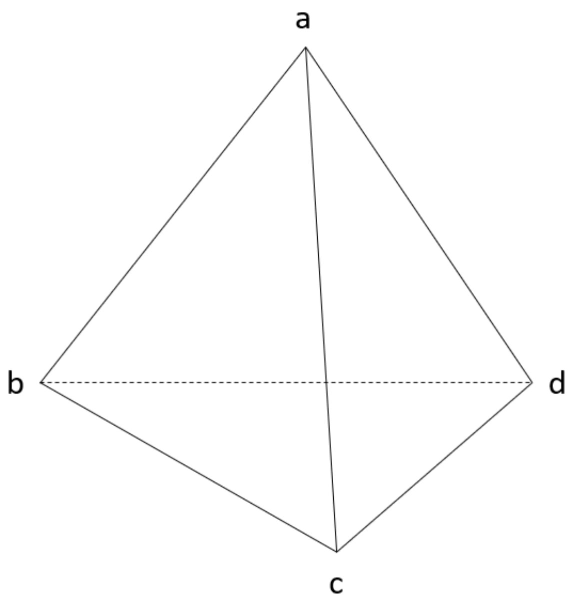

Figure A.1: A regular tetrahedron with corner points a, b, c and d.

The normalized vectors pointing from the corner points to the midpoints are given by $\hat{e}_a = \frac{2}{\sqrt{3}}(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $\hat{e}_b = \frac{2}{\sqrt{3}}(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})$, $\hat{e}_c = \frac{2}{\sqrt{3}}(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$ and $\hat{e}_d = \frac{2}{\sqrt{3}}(-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})$. From this we find the inner product between two of those vector to be

$$\hat{e}_i \cdot \hat{e}_j = \begin{cases} 1 & \text{if } i = j, \\ -\frac{1}{3} & \text{otherwise,} \end{cases} \tag{A.1}$$

where $i, j \in \{a, b, c, d\}$. We furthermore would like to know the inner products between a vector pointing from corner to corner and a vector pointing from corner to midpoint, i.e. $\hat{e}_i \cdot \hat{\mathbf{r}}_{ij}$ and $\hat{e}_j \cdot \hat{\mathbf{r}}_{ij}$ in the tetrahedron. Using the convention that $\hat{\mathbf{r}}_{ij}$ is the unit vector from i to j, we calculate for a

and b; $\hat{\mathbf{r}}_{ab} = \frac{1}{\sqrt{2}}(-1,1,0)$. Thus we find

$$\begin{aligned} \hat{e}_a \cdot \hat{\mathbf{r}}_{ab} &= \sqrt{\frac{2}{3}}, \\ \hat{e}_b \cdot \hat{\mathbf{r}}_{ab} &= -\sqrt{\frac{2}{3}}. \end{aligned} \tag{A.2}$$

We can put another tetrahedron on top of the one in Figure A.1, such that they have one shared corner and their ground plane is rotated π radians. This second tetrahedron has cornerpoints $d = (1,1,1)$, $a' = (1,2,2)$, $b' = (2,1,2)$ and $c' = (2,2,1)$ with midpoint $(\frac{3}{2},\frac{3}{2},\frac{3}{2})$. We then wist to calculate the inner product $\hat{e}_a \cdot \hat{r}_{ab'}$ and $\hat{e}_{b'} \cdot \hat{r}_{ab'}$. Now $\hat{r}_{ab'} = \frac{1}{\sqrt{6}}(1,1,2)$ and $\hat{e}_{b'} = \hat{e}_b = \frac{2}{\sqrt{3}}(\frac{1}{2},-\frac{1}{2},\frac{1}{2})$, so we find

$$\begin{aligned} \hat{e}_a \cdot \hat{r}_{ab'} &= \frac{\sqrt{2}}{3}, \\ \hat{e}_{b'} \cdot \hat{r}_{ab'} &= \frac{\sqrt{2}}{3}. \end{aligned} \tag{A.3}$$

As the inner product is preserved under isometries of the euclidean space, (A.1), (A.2) and (A.3) are invariant of our basis. This means for instance that we can replace A and B in A.2 with i and j where $i, j \in \{A,B,C,D\}$ and $i \neq j$. We prove this in the following theorem.

Theorem A.1. Let $T : \mathbb{R}^n \to \mathbb{R}^n$ be an isometry with $x \mapsto Ax$, then the inner product is preserved under T.

Proof. T is an isometry, so A is an orthogonal matrix. Now let $u, v \in \mathbb{R}^n$. Then $T(u) \cdot T(v) = (Au)^T Av = u^T A^T Av = u^T v = u \cdot v$. So indeed the inner product is preserved. □