CHARACTERIZATION OF REFLECTION POSITIVITY: MAJORANAS AND SPINS

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Abstract. We study linear functionals on a Clifford algebra (algebra of Majoranas) equipped with a reflection automorphism. For Hamiltonians that are functions of Majoranas or of spins, we find necessary and sufficient conditions on the coupling constants for reflection positivity to hold. One can easily check these conditions in concrete models. We illustrate this by discussing a number of spin systems with nearest-neighbor and long-range interactions.

Contents

I. Introduction

We consider a finite-dimensional $\mathbb{Z}_2$-graded $*$-algebra $\mathfrak{A}$. The algebra $\mathfrak{A}$ is a graded (super) tensor product of two algebras $\mathfrak{A}_\pm$, related by an anti-linear automorphism $\Theta\colon \mathfrak{A} \to \mathfrak{A}$, satisfying $\Theta(\mathfrak{A}_\mp) = \mathfrak{A}_\pm$ and $\Theta^2 = I$. In this sense, $\mathfrak{A}$ is the *double* of $\mathfrak{A}_+$. Such automorphisms often arise from geometric reflections on an underlying manifold, so we refer to Θ as the *reflection automorphism.* The main results summarized in Theorem I.1 do not refer to an underlying geometry–while in the examples of §VII this becomes relevant.

In the context of the present work, we introduce a twisted product on the algebra $\circ : \mathfrak{A} \times \mathfrak{A} \mapsto \mathfrak{A}$. Let ω denote a linear functional on $\mathfrak{A}$. One says that the functional ω is *reflection positive* on $\mathfrak{A}_+$ with respect to the reflection Θ, in case that

$$0 \leqslant \omega(\Theta(A) \circ A) , \quad \text{for all} \quad A \in \mathfrak{A}_+ . \tag{I.1}$$

We consider in detail the case that $\omega = \omega_H$ is a *Boltzmann functional.* By this we mean that there is an element $H \in \mathfrak{A}$ called the Hamiltonian, such that

$$\omega_H(A) = \operatorname{Tr}(A\, e^{-H}) ,$$

where Tr is a tracial state on $\mathfrak{A}$. If the *partition sum* $Z_H := \operatorname{Tr}(e^{-H})$ is nonzero, define the *Gibbs functional* ρ_H as the normalized Boltzmann functional,

$$\rho_H(A) = Z_H^{-1} \operatorname{Tr}(A\, e^{-H}) . \tag{I.2}$$

In many applications $H \in \mathfrak{A}$ is self-adjoint. In this case $Z_H > 0$, and ρ_H is a state, meaning that ρ_H is positive and normalized. Furthermore, it has the KMS property with respect to the the automorphisms of $\mathfrak{A}$ induced by e^{itH}.

Here we specialize to two types of algebras $\mathfrak{A}$. In the first part of the paper, §I–§IV, $\mathfrak{A}$ will be an algebra of Majoranas, whereas in the second part §V–§VII, $\mathfrak{A}$ will generally be an algebra of spins.

An algebra of Majoranas is a $*$-algebra generated by self-adjoint operators c_i. They are labeled by indices i running over a finite set Λ, and satisfy the Clifford relations

$$c_i c_j + c_j c_i = 2\delta_{ij} I\,, \quad i, j \in \Lambda\,. \tag{I.3}$$

The $\mathbb{Z}_2$ grading of $\mathfrak{A}$ is defined as $+1$ on the even and -1 on the odd monomials in the c_i. Even elements of $\mathfrak{A}$ are often called *globally gauge invariant*.

The reflection automorphism Θ of the Majorana algebra $\mathfrak{A}$ comes from a fixed point free reflection $\vartheta\colon \Lambda \to \Lambda$. If Λ is the disjoint union of Λ_+ and Λ_- with $\vartheta(\Lambda_\pm) = \Lambda_\mp$, then the algebras $\mathfrak{A}_\pm$ are generated by the Majoranas c_i with $i \in \Lambda_\pm$. In many applications, Λ will be a finite lattice in Euclidean space, and ϑ the reflection in a hyperplane which does not intersect Λ.

We give necessary and sufficient conditions such that the functionals ω_H and ρ_H are reflection positive on $\mathfrak{A}_+$. Every Hamiltonian $H \in \mathfrak{A}$ is defined by a coupling-constant matrix J as

$$H = -\sum J_{i_1,\ldots,i_k\,;\,i'_1,\ldots,i'_{k'}}\, \Theta(c_{i_1}\cdots c_{i_k}) \circ (c_{i'_1}\cdots c_{i'_{k'}})\,, \tag{I.4}$$

where k and k' range over $\mathbb{N}$, and $i_1, \ldots, i_k$ and $i'_1, \ldots, i'_{k'}$ range over Λ_+. In fact one restricts the set over which one sums, in order to make the expansion unique, as explained in §I.3–§I.5. The conditions on reflection positivity are expressed in terms of the submatrix J^0 of J for which $k \neq 0$ and $k' \neq 0$. If ϑ comes from a reflection in Euclidean space, J^0 describes the *couplings across the reflection plane*. We use this terminology even if a geometric interpretation is lacking.

The central result in this paper, which also holds with $\rho_{\beta H}$ replaced by $\omega_{\beta H}$, is the following:

Theorem I.1. *Let H be reflection invariant and globally gauge invariant. Then $\rho_{\beta H}$ is reflection positive for all $0 < \beta$, if and only if $0 \leqslant J^0$.*

In the second part of the paper, we focus on spin algebras $\mathfrak{A}^{\mathrm{spin}}$, generated by the Pauli matrices σ^1_j, σ^2_j, σ^3_j associated to each lattice site $j \in \Lambda$. In §V we study Hamiltonians of the form

$$H^{\mathrm{spin}} = -\sum J^{a_1,\ldots,a_k}_{i_1,\ldots,i_k}\, \sigma^{a_1}_{i_1} \cdots \sigma^{a_k}_{i_k}\ . \tag{I.5}$$

By expressing the spins σ^a_j as even polynomials in the Majoranas, we translate Theorem I.1 to the spin context. This yields necessary and sufficient conditions on reflection positivity in terms of the coupling constants $J^{a_1,\ldots,a_k}_{i_1,\ldots,i_k}$. Again, the condition involves only the couplings across the reflection plane.

In §VI we analyze different reflections Θ and $\Theta' = \alpha\Theta\alpha^{-1}$, both of which interchange the same $\mathfrak{A}_\pm$. If they are related by a reflection-invariant gauge automorphism α, then our characterization of reflection positivity applies to to Θ' as well as Θ.

In §VII we illustrate the main results by showing that a number of spin Hamiltonians with nearest neighbor as well as long-range interactions fit naturally into our general framework.

Reflection positivity of functionals has a long history in physics, as well as mathematics. Some earlier work can be found in [OS73, OS75, GJS75, FSS76, DLS78, FILS78, KL81, FOS83, Lie94, MN96, NÓ14, NÓ15]. The present work was inspired by [JP15a, JP15b], and generalizes it in the following way: we obtain reflection positivity for couplings that are not necessarily diagonal (including long-range interactions), for observables that are not necessarily even, and with hypotheses that are not only sufficient, but also necessary.

I.1. **Reflections.** Here we study a finite set Λ which is an index set for the generators c_i of our algebra. We assume that Λ is invariant under an involution $\vartheta\colon \Lambda \to \Lambda$ that we call a *reflection*. We assume that ϑ exchanges two subsets $\Lambda_\pm$ whose union is Λ, and that ϑ has no fixed points.

In specific models, Λ is often a finite subset of a manifold $\mathcal{M}$, and ϑ is the restriction to $\Lambda \subset \mathcal{M}$ of a reflection $\vartheta_{\mathcal{M}}\colon \mathcal{M} \to \mathcal{M}$. In the examples of interest, $\mathcal{M}$ is a disjoint union $\mathcal{M} = \mathcal{M}_+ \sqcup \mathcal{M}_0 \sqcup \mathcal{M}_-$, where $\vartheta_{\mathcal{M}}$ interchanges $\mathcal{M}_+$ and $\mathcal{M}_-$, and leaves the hypersurface $\mathcal{M}_0$ invariant. The set Λ_+ is then a finite set of points in $\mathcal{M}_+$, and Λ_- is its reflection.

We give a number of examples of this situation, where $\mathcal{M}$ is the Eucidean space $\mathbb{R}^d$, a torus $\mathbb{T}^d$, or a Riemann surface.

If $\mathcal{M} = \mathbb{R}^d$, the reflection $\vartheta_{\mathbb{R}^d}\colon \mathbb{R}^d \to \mathbb{R}^d$ is given in suitable coordinates by

$$\vartheta(x_0, x_1, \ldots, x_{d-1}) = (-x_0, x_1, \ldots, x_{d-1})\,.$$

The half-spaces $\mathbb{R}^d_\pm$ have as a common boundary the reflection plane $\mathbb{R}^d_0 = \{x \in \mathbb{R}^d \,:\, x_0 = 0\}$. Then $\Lambda_+ \subset \mathbb{R}^d_+$ is a finite set of points on one side of the reflection plane $\mathbb{R}^d_0$, the set Λ_- is its reflection, and $\Lambda = \Lambda_+ \sqcup \Lambda_-$. Note that Λ contains no points in the reflection hyperplane.

An important example is the d-dimensional simple cubic lattice

$$\Lambda^{\text{cubic}} = \{-L - \tfrac{1}{2}, L + \tfrac{1}{2}, \ldots, L - \tfrac{1}{2}, L + \tfrac{1}{2}\}^d\,,$$

with the reflection plane illustrated by the dashed line in Figure 1.

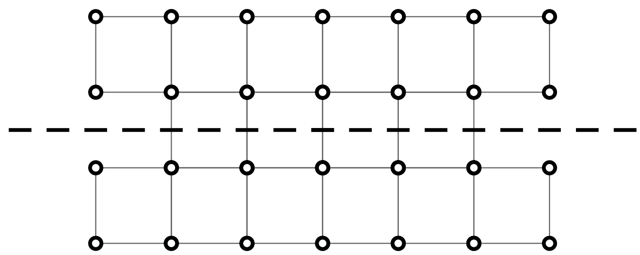

FIGURE 1. Reflection in a cubic lattice.

Another example, with $\mathcal{M} = \mathbb{R}^2$, is the honeycomb lattice in Figure 2.

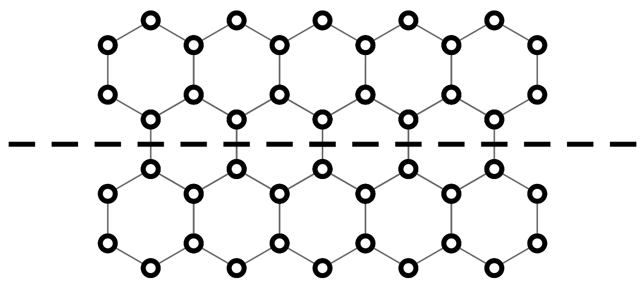

FIGURE 2. Reflection in the 2-dimensional honeycomb lattice.

One often has periodic boundary conditions, in which case $\mathcal{M}$ is the torus $\mathbb{T}^d$ instead of $\mathbb{R}^d$. The invariant hypersurface $\mathcal{M}_0$ is then the union of two $(d-1)$-tori.

Examples where $\mathcal{M}$ is a Riemann surface of arbitrary genus arise from considering the conformal inversion ϑ of a Schottky double of an open Riemann surface T, with Λ_+ a finite set of points in T.

In §I–§V, including the main Theorems III.4, IV.2, IV.3, and V.2, we only need Λ to be an abstract set with a fixed point free involution ϑ. In the discussion of examples in §VII, we require additional structure for Λ, involving its geometric significance as a subset of a manifold $\mathcal{M}$, as explained later.

I.2. **Majoranas.** One defines an algebra of Majoranas on the lattice Λ as the $*$-algebra $\mathfrak{A}$ with self-adjoint generators $c_i = c_i^*$ that satisfy the Clifford relations (I.3). For any subset $\Gamma \subset \Lambda$, let $\mathfrak{A}(\Gamma)$ denote the algebra generated by the c_j's with $j \in \Gamma$. In particular, $\mathfrak{A} = \mathfrak{A}(\Lambda)$, and we define $\mathfrak{A}_\pm := \mathfrak{A}(\Lambda_\pm)$.

We call the automorphism $\alpha\colon \mathfrak{A} \to \mathfrak{A}$ that implements the $\mathbb{Z}_2$ grading a *global gauge automorphism.* On the generators, it satisfies

$$c_j \mapsto \alpha(c_j) = -c_j \ . \tag{I.6}$$

The algebra $\mathfrak{A}$ decomposes into the spaces $\mathfrak{A}^{\mathrm{even}}$ and $\mathfrak{A}^{\mathrm{odd}}$ of elements that are even and odd for the $\mathbb{Z}_2$-grading,

$$\mathfrak{A} = \mathfrak{A}^{\mathrm{even}} \oplus \mathfrak{A}^{\mathrm{odd}} \, .$$

In the same vein, $\mathfrak{A}(\Gamma) = \mathfrak{A}(\Gamma)^{\mathrm{even}} \oplus \mathfrak{A}(\Gamma)^{\mathrm{odd}}$. An element $A \in \mathfrak{A}$ that is either even or odd is called *homogeneous.* Since $A \in \mathfrak{A}$ is even if $\alpha(A) = A$ and odd if $\alpha(A) = -A$, the even elements are also called *globally gauge invariant.*

Define the *degree* $|A|$ of A as $|A| = 0$ for $A \in \mathfrak{A}^{\mathrm{even}}$, and $|A| = 1$ for $A \in \mathfrak{A}^{\mathrm{odd}}$. The algebra $\mathfrak{A}(\Gamma)$ commutes with $\mathfrak{A}^{\mathrm{even}}(\Gamma')$ when $\Gamma \cap \Gamma' = \varnothing$. More generally, if $A \in \mathfrak{A}(\Gamma)$ and $B \in \mathfrak{A}(\Gamma')$ are both eigenvectors of α, then

$$AB = (-1)^{|A||B|} BA \ , \quad \text{when} \quad \Gamma \cap \Gamma' = \varnothing \ .$$

One says that $\mathfrak{A}(\Gamma)$ and $\mathfrak{A}(\Gamma')$ supercommute if Γ and Γ' are disjoint.

I.3. **Reflections and Invariant Bases.** The reflection $\vartheta\colon \Lambda \to \Lambda$ defines an *anti-linear* *-automorphism $\Theta\colon \mathfrak{A} \to \mathfrak{A}$ given by

$$\Theta(c_{i_1} \cdots c_{i_k}) := c_{\vartheta(i_1)} \cdots c_{\vartheta(i_k)} \, . \tag{I.7}$$

Note that Θ exchanges $\mathfrak{A}_+$ with $\mathfrak{A}_-$, namely $\Theta(\mathfrak{A}_\pm) = \mathfrak{A}_\mp$, and satisfies $\Theta^2 = \mathrm{Id}$. We construct bases of $\mathfrak{A}$ that are adapted to this reflection.

For $\Gamma \subseteq \Lambda$, let $\mathcal{S}_\Gamma$ denote the set of sequences $\mathfrak{I} = (i_1, \ldots, i_k)$ of *distinct* lattice points $i_1, \ldots, i_k \in \Gamma$. For the important choices $\Gamma = \Lambda$, $\Gamma = \Lambda_+$ and $\Gamma = \Lambda_-$, we denote $\mathcal{S}_\Gamma$ by $\mathcal{S}$, $\mathcal{S}_+$, and $\mathcal{S}_-$, respectively. For $\mathfrak{I} \in \mathcal{S}_\Gamma$, define the monomial

$$C_\mathfrak{I} := c_{i_1} \cdots c_{i_k} \, ,$$

and define $C_\mathfrak{I} := I$ for $\mathfrak{I} = \varnothing$. Each $C_\mathfrak{I}$ is an eigenvector of the gauge automorphism α, and we denote its degree by

$$|\mathfrak{I}| := |C_\mathfrak{I}| \, . \tag{I.8}$$

Then $|\mathfrak{I}| = 0$ if k is even, and $|\mathfrak{I}| = 1$ if k is odd. Also

$$C_\mathfrak{I}^* = (-1)^{\frac{1}{2}k(k-1)} C_\mathfrak{I} \ . \tag{I.9}$$

The algebra $\mathfrak{A}(\Gamma)$ is spanned by the operators $C_\mathfrak{I}$ with $\mathfrak{I} \in \mathcal{S}_\Gamma$, but they are linearly dependent. In fact, $C_\mathfrak{I} = \pm C_{\mathfrak{I}'}$ if the sets $\{i_1, \ldots, i_k\}$ and $\{i'_1, \ldots, i'_{k'}\}$ are the same. A choice $\mathcal{P}_+ \subseteq \mathcal{S}_+$ such that every set

$\{i_1, \ldots, i_k\}$ of distinct lattice points corresponds to precisely one tuple $(i_1, \ldots, i_k)$ in $\mathcal{P}_+$ yields a basis

$$\mathcal{B}_+ = \{C_{\mathfrak{I}}\,;\, \mathfrak{I} \in \mathcal{P}_+\}$$

of $\mathfrak{A}_+$. This, in turn, yields a basis $\mathcal{B}_- = \Theta(\mathcal{B}_+)$ of $\mathfrak{A}_-$.

I.4. **The Twist.** From the two bases $\mathcal{B}_+$ and $\mathcal{B}_-$, we construct a basis $\mathcal{B}$ of $\mathfrak{A}$, that is adapted to the reflection Θ. For this, fix a square root of minus one, $\zeta = \pm\sqrt{-1}$, and define a basis for $\mathfrak{A}$ by

$$\mathcal{B} := \{\zeta^{|\mathfrak{I}||\mathfrak{I}'|}\Theta(C_{\mathfrak{I}})C_{\mathfrak{I}'}\,;\; C_{\mathfrak{I}}, C_{\mathfrak{I}'} \in \mathcal{B}_+\}\,.$$

Although the main results on reflection positivity will hold for both twists $\zeta = \sqrt{-1}$ and $\zeta = -\sqrt{-1}$, the class of allowed Hamiltonians will *not* be the same.

Note that, in a sense, the basis elements in $\mathcal{B}$ are the geometric mean of the operators $\Theta(C_{\mathfrak{I}})C_{\mathfrak{I}'}$ and $C_{\mathfrak{I}'}\Theta(C_{\mathfrak{I}})$, which differ by a factor $(-1)^{|\mathfrak{I}||\mathfrak{I}'|}$. The identity $I = C_{\varnothing} = \Theta(C_{\varnothing}) = \Theta(C_{\varnothing})C_{\varnothing}$ is a basis element in all three bases $\mathcal{B}_+$, $\mathcal{B}_-$ and $\mathcal{B}$. Every $A \in \mathfrak{A}$ has an expansion

$$A = \sum_{\mathfrak{I},\mathfrak{I}'} a_{\mathfrak{I}\mathfrak{I}'}\, \zeta^{|\mathfrak{I}||\mathfrak{I}'|}\Theta(C_{\mathfrak{I}})C_{\mathfrak{I}'}\,, \tag{I.10}$$

which is unique if the $\mathfrak{I}, \mathfrak{I}'$ are restricted to be in $\mathcal{P}_+$.

I.5. **Twisted Product.** In order to streamline notation, introduce the following (non-associative) twisted product

$$\circ :\; \mathfrak{A} \times \mathfrak{A} \to \mathfrak{A}\,. \tag{I.11}$$

Definition I.2. *Let $A \in \mathfrak{A}$ be of the form $A = A_-A_+$ with $A_\pm \in \mathfrak{A}_\pm$, and similarly $B = B_-B_+$ with $B_\pm \in \mathfrak{A}_\pm$. If $A_\pm$ and $B_\pm$ are homogeneous, then $A \circ B$ is defined by*

$$A \circ B := \zeta^{|A_-||B_+|-|A_+||B_-|}AB\,.$$

This extends bilinearly to the product $\circ :\; \mathfrak{A} \times \mathfrak{A} \to \mathfrak{A}$.

Note that the formula $A \circ B := \zeta^{|A_-||B_+|-|A_+||B_-|}AB$ also holds for $A = A_+A_-$ and $B = B_+B_-$. One finds

$$X_{\mathfrak{I}_1\mathfrak{I}_1'} \circ X_{\mathfrak{I}_2\mathfrak{I}_2'} = \zeta^{|\mathfrak{I}_1|\,|\mathfrak{I}_2'|-|\mathfrak{I}_1'|\,|\mathfrak{I}_2|}X_{\mathfrak{I}_1\mathfrak{I}_1'}X_{\mathfrak{I}_2\mathfrak{I}_2'} \tag{I.12}$$

for twisted products of elements of the form $X_{\mathfrak{I}\mathfrak{I}'} = \Theta(C_{\mathfrak{I}})C_{\mathfrak{I}'}$ or $X_{\mathfrak{I}\mathfrak{I}'} = C_{\mathfrak{I}'}\Theta(C_{\mathfrak{I}})$.

In terms of the twisted product, the basis $\mathcal{B}$ can be written

$$\mathcal{B} = \{\Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'} \;:\; \mathfrak{I}, \mathfrak{I}' \in \mathcal{P}_+\}\,. \tag{I.13}$$

Correspondingly we can rewrite the expansion (I.10) of a general element $A \in \mathfrak{A}$ in basis elements as

$$A = \sum_{\mathfrak{I},\mathfrak{I}' \in \mathcal{P}_+} a_{\mathfrak{I}\mathfrak{I}'}\, \Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'}\ . \tag{I.14}$$

The twisted product has a number of useful properties. For example $\mathfrak{A}_+$ and $\mathfrak{A}_-$ commute with respect to the twisted product.

Proposition I.3. *If $A_+ \in \mathfrak{A}_+$ and $B_- \in \mathfrak{A}_-$, then $A_+ \circ B_- = B_- \circ A_+$.*

Proof. It suffices to prove this for homogeneous elements, in which case the result follows from $A_+ \circ B_- = \zeta^{-|A_+||B_-|} A_+ B_-$, $B_- \circ A_+ = \zeta^{|A_+||B_-|} B_+ A_-$, and $A_+ B_- = (-1)^{|A_+||B_-|} B_+ A_-$. □

The twisted product respects the reflection;

Proposition I.4. *For all $A, B \in \mathfrak{A}$, one has $\Theta(A \circ B) = \Theta(A) \circ \Theta(B)$.*

Proof. It suffices to check this for $A = A_- A_+$ and $B = B_- B_+$ as in Definition I.2. By antilinearity of Θ, one then finds

$$\Theta(A \circ B) = \Theta(\zeta^{|A_-||B_+| - |A_+||B_-|} AB) = \zeta^{-|A_-||B_+| + |A_+||B_-|} \Theta(A)\Theta(B)$$

for the left side of the equation. For the right side, one finds the same expression

$$\begin{aligned} \Theta(A) \circ \Theta(B) &= \Theta(A_-)\Theta(A_+) \circ \Theta(B_-)\Theta(B_+) \\ &= \zeta^{|A_+||B_-| - |A_-||B_+|} \Theta(A)\Theta(B)\,, \end{aligned}$$

since $\Theta(A_\pm), \Theta(B_\pm) \in \mathfrak{A}_\mp$. □

It follows that the reflection permutes the basis $\mathcal{B}$.

Corollary I.5. *The twisted product satisfies*

$$\Theta\big(\Theta(A) \circ B\big) = \Theta(B) \circ A\,, \quad \textit{for} \quad A, B \in \mathfrak{A}_+\ , \ \textit{or}\ A, B \in \mathfrak{A}_-\ . \tag{I.15}$$

In particular, the basis $\mathcal{B}$ is permuted by Θ,

$$\Theta(\Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'}) = \Theta(C_{\mathfrak{I}'}) \circ C_{\mathfrak{I}}\ . \tag{I.16}$$

Proof. By Proposition I.4, one has $\Theta(\Theta(A) \circ B) = A \circ \Theta(B)$, which equals $\Theta(B) \circ A$ by Proposition I.3. □

Proposition I.6. *Let $A \in \mathfrak{A}$ have the expansion (I.14). Then A is reflection invariant, namely $\Theta(A) = A$, if and only if the matrix $a_{\mathfrak{I}\mathfrak{I}'}$ is hermitian, namely $a_{\mathfrak{I}'\mathfrak{I}} = \overline{a_{\mathfrak{I}\mathfrak{I}'}}$.*

Proof. This follows from anti-linearity of Θ and Corollary I.5. □

Define $k\colon \Lambda \to \mathbb{N}$ by $k_{\mathfrak{I}} = r$ for $\mathfrak{I} = (i_1, \ldots, i_r)$. When dealing with adjoint operators, one frequently encounters the derived expressions

$$q_{\mathfrak{I}} := (-1)^{\frac{1}{2}k_{\mathfrak{I}}(k_{\mathfrak{I}}-1)} \quad \text{and} \quad s_{\mathfrak{I}} := \zeta^{\frac{1}{2}k_{\mathfrak{I}}(k_{\mathfrak{I}}-1)} . \tag{I.17}$$

Note that $q_{\mathfrak{I}}$ is 4-periodic in k, and $s_{\mathfrak{I}}$ is 8-periodic.

Proposition I.7. *Let $\mathfrak{I}, \mathfrak{I}' \in \mathcal{P}_+$. Then*

$$(\Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'})^* \;=\; q_{\mathfrak{I}}\, q_{\mathfrak{I}'}\, \Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'} \, . \tag{I.18}$$

Proof. As Θ is a $*$-automorphism,

$$(\Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'})^* = \zeta^{-|\mathfrak{I}||\mathfrak{I}'|}(\Theta(C_{\mathfrak{I}})C_{\mathfrak{I}'})^* = \zeta^{-|\mathfrak{I}||\mathfrak{I}'|}C_{\mathfrak{I}'}^*\Theta(C_{\mathfrak{I}}^*) \, .$$

Inserting (I.9) gives

$$\begin{aligned}(\Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'})^* &= \zeta^{-|\mathfrak{I}||\mathfrak{I}'|}\, q_{\mathfrak{I}}\, q_{\mathfrak{I}'}\, C_{\mathfrak{I}'}\Theta(C_{\mathfrak{I}}) \\ &= q_{\mathfrak{I}}\, q_{\mathfrak{I}'}\, \Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'} \, .\end{aligned}$$

In the last equality we use $C_{\mathfrak{I}'}\Theta(C_{\mathfrak{I}}) = \zeta^{2|\mathfrak{I}||\mathfrak{I}'|}\Theta(C_{\mathfrak{I}})C_{\mathfrak{I}'}$ and the definition of the circle product to give the desired relation (I.18). □

Using this, one derives the following characterization of hermiticity.

Corollary I.8. *If $A \in \mathfrak{A}$ has an expansion (I.14) with coefficients $a_{\mathfrak{I}\mathfrak{I}'}$, then A^* has coefficients $q_{\mathfrak{I}}\, q_{\mathfrak{I}'}\, \overline{a_{\mathfrak{I}\mathfrak{I}'}}$. The operator A is hermitian if and only if $s_{\mathfrak{I}}\, s_{\mathfrak{I}'}\, a_{\mathfrak{I}\mathfrak{I}'}$ is real for all $\mathfrak{I}, \mathfrak{I}' \in \mathcal{P}_+$.*

Proof. The first statement follows from

$$\begin{aligned}A^* &= \sum_{\mathfrak{I},\mathfrak{I}' \in \mathcal{P}_+} \overline{a_{\mathfrak{I}\mathfrak{I}'}}\, (\Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'})^* \\ &= \sum_{\mathfrak{I},\mathfrak{I}' \in \mathcal{P}_+} \overline{a_{\mathfrak{I}\mathfrak{I}'}}\, q_{\mathfrak{I}}\, q_{\mathfrak{I}'}\, \Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'} \, .\end{aligned} \tag{I.19}$$

Therefore, A is hermitian if and only if $a_{\mathfrak{I}\mathfrak{I}'} = \overline{a_{\mathfrak{I}\mathfrak{I}'}}\, q_{\mathfrak{I}}\, q_{\mathfrak{I}'}$. Since $s_{\mathfrak{I}}^2 = s_{\mathfrak{I}}^{-2} = q_{\mathfrak{I}}$, this is equivalent to $s_{\mathfrak{I}}\, s_{\mathfrak{I}'}\, a_{\mathfrak{I}\mathfrak{I}'} = \overline{s_{\mathfrak{I}}\, s_{\mathfrak{I}'}\, a_{\mathfrak{I}\mathfrak{I}'}}$. □

I.6. **The Tracial State.** Define the functional $\mathrm{Tr} : \mathfrak{A} \to \mathbb{C}$ by

$$\mathrm{Tr}(A) = a_{\varnothing\varnothing} \, , \tag{I.20}$$

where $a_{\mathfrak{I}\mathfrak{I}'}$ are the coefficients in (I.14).

Proposition I.9. *Let $\mathfrak{I}_0$ and $\mathfrak{I}_0'$ be elements of $\mathcal{P}_+$. Then*

$$\mathrm{Tr}\Big(\big(\Theta(C_{\mathfrak{I}_0}) \circ C_{\mathfrak{I}_0'}\big)^* \,\Theta(C_{\mathfrak{I}_1}) \circ C_{\mathfrak{I}_1'}\Big) = \delta_{\mathfrak{I}_0\mathfrak{I}_1}\delta_{\mathfrak{I}_0'\mathfrak{I}_1'} \, . \tag{I.21}$$

Also

$$\mathrm{Tr}\left(\big(\Theta(C_{\mathfrak{I}_0}) \circ C_{\mathfrak{I}_0'}\big)\, \big(\Theta(C_{\mathfrak{I}_1}) \circ C_{\mathfrak{I}_1'}\big)\right) = q_{\mathfrak{I}_0}\, q_{\mathfrak{I}_0'}\, \delta_{\mathfrak{I}_0\mathfrak{I}_1}\delta_{\mathfrak{I}_0'\mathfrak{I}_1'} \, . \tag{I.22}$$

Proof. The identity (I.22) is equivalent to (I.21) as a consequence of (I.18). The left hand side of (I.21) vanishes unless $\mathfrak{I}_0 = \mathfrak{I}_1$ and $\mathfrak{I}'_0 = \mathfrak{I}'_1$, in which case (I.18) along with $C^*_{\mathfrak{I}_1} C_{\mathfrak{I}_1} = C^*_{\mathfrak{I}'_1} C_{\mathfrak{I}'_1} = I$ yields

$$\begin{aligned}(\Theta(C_{\mathfrak{I}_0}) \circ C_{\mathfrak{I}'_0})^* \cdot \Theta(C_{\mathfrak{I}_1}) \circ C_{\mathfrak{I}'_1} \\ &= \zeta^{-|\mathfrak{I}_0||\mathfrak{I}'_0| + |\mathfrak{I}_1||\mathfrak{I}'_1|} C^*_{\mathfrak{I}'_0} \Theta(C^*_{\mathfrak{I}_0}) \Theta(C_{\mathfrak{I}_1}) C_{\mathfrak{I}'_1} \\ &= C^*_{\mathfrak{I}'_1} \Theta(C^*_{\mathfrak{I}_1} C_{\mathfrak{I}_1}) C_{\mathfrak{I}'_1} = I\,. \end{aligned} \tag{I.23}$$

This proves equation (I.21). □

Proposition I.10 (**The Normalized Trace).** *The functional* Tr *is a tracial, factorizing, reflection-invariant state. Namely*

(a) *It is normalized,* $\mathrm{Tr}(I) = 1$.
(b) *It is positive definite,* $\mathrm{Tr}(A^*A) \geqslant 0$ *for all* $A \in \mathfrak{A}$*, with equality only for* $A = 0$.
(c) *It is cyclic,*
$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA) \quad \text{for all} \quad A, B \in \mathfrak{A}\,. \tag{I.24}$$
(d) *It satisfies*
$$\mathrm{Tr}(\Theta(A)) = \overline{\mathrm{Tr}(A)} \quad \text{for all} \quad A \in \mathfrak{A}\,. \tag{I.25}$$
(e) *It factorizes,*
$$\mathrm{Tr}(A_- A_+) = \mathrm{Tr}(A_-)\,\mathrm{Tr}(A_+)\,, \quad \text{for} \quad A_\pm \in \mathfrak{A}_\pm\,. \tag{I.26}$$

Proof. (a) As $I = \Theta(C_\varnothing) \circ C_\varnothing$, one has $\mathrm{Tr}(I) = 1$.

(b) From (I.21) and the expansion (I.14), one finds

$$\mathrm{Tr}(A^*A) = \sum_{\mathfrak{I}, \mathfrak{I}' \in \mathcal{P}_+} |a_{\mathfrak{I}\mathfrak{I}'}|^2 \geqslant 0\,.$$

Furthermore $\mathrm{Tr}(A^*A) = 0$ only if all the $a_{\mathfrak{I}\mathfrak{I}'} = 0$. As the $\Theta(C_\mathfrak{I}) \circ C_{\mathfrak{I}'}$ are a basis, the vanishing of $a_{\mathfrak{I}\mathfrak{I}'}$ ensures that $A = 0$. Hence Tr is positive definite.

(c) From equation (I.22), one obtains

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA) = \sum_{\mathfrak{I}, \mathfrak{I}' \in \mathcal{P}_+} q_\mathfrak{I} q_{\mathfrak{I}'} a_{\mathfrak{I}\mathfrak{I}'} b_{\mathfrak{I}\mathfrak{I}'}\,. \tag{I.27}$$

Hence the state Tr is cyclic.

(d) As Θ is antilinear and the basis elements satisfy (I.16), it follows that Tr satisfies (I.25).

(e) To demonstrate factorization, consider $A_- = \sum_{\mathfrak{I} \in \mathcal{P}_+} a_{\mathfrak{I}\varnothing}\,\Theta(C_\mathfrak{I})$ and $B_+ = \sum_{\mathfrak{K}' \in \mathcal{P}_+} b_{\varnothing\mathfrak{K}'}\,C_{\mathfrak{K}'}$. The identity (I.27) reads $\mathrm{Tr}(A_- B_+) = a_{\varnothing\varnothing} b_{\varnothing\varnothing}$, so the factorization property follows.

□

Corollary I.11. *If $H \in \mathfrak{A}$ is reflection invariant, $\Theta(H) = H$, then the partition sum $Z_H = \mathrm{T}(e^{-H})$ is real.*

Proof. Since Θ is an automorphism, it follows from $\Theta(H) = H$ that $\Theta(e^{-H}) = e^{-H}$. Using Proposition I.10.d, one then finds

$$Z_H = \mathrm{Tr}(e^{-H}) = \mathrm{Tr}(\Theta(e^{-H})) = \overline{\mathrm{Tr}(e^{-H})} = \overline{Z_H}\,,$$

so that Z_H is real. □

II. Reflection Positive Functionals

In this section, we characterize reflection invariance and reflection positivity of linear functionals in terms of their density matrix.

II.1. **Reflection Invariance.** Let $\omega\colon \mathfrak{A} \to \mathbb{C}$ be a linear functional on $\mathfrak{A}$. From Proposition I.10.b, we infer that every functional can be written

$$\omega(A) = \mathrm{Tr}(AR) \tag{II.1}$$

for a unique *density matrix* $R \in \mathfrak{A}$. If ω is a state, then R is a positive operator with trace 1.

Consider the sesquilinear form $\langle\,\cdot\,,\,\cdot\,\rangle_{R,\Theta}$ on $\mathfrak{A}$ given as

$$\langle A, B\rangle_{R,\Theta} := \omega(\Theta(A) \circ B) = \mathrm{Tr}((\Theta(A) \circ B)R)\,. \tag{II.2}$$

If we expand R in terms of matrix elements $r_{\mathfrak{I}\mathfrak{I}'}$ as

$$R = \sum_{\mathfrak{I},\mathfrak{I}' \in \mathcal{P}_+} r_{\mathfrak{I}\mathfrak{I}'}\, \Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'}\,, \tag{II.3}$$

then (I.9) and Proposition I.9 ensure that

$$r_{\mathfrak{I}\mathfrak{I}'} = \langle C_{\mathfrak{I}}^*, C_{\mathfrak{I}'}^*\rangle_{R,\Theta}\,, \quad \text{where} \quad C_{\mathfrak{I}}, C_{\mathfrak{I}'} \in \mathcal{B}_+\,. \tag{II.4}$$

Definition II.1 (Reflection Invariance). *The linear functional ω is reflection invariant on $\mathfrak{A}$ if $\omega(\Theta(A)) = \overline{\omega(A)}$ for all $A \in \mathfrak{A}$.*

Proposition II.2 (Reflection-Invariant Functionals). *The following conditions are equivalent:*

(a) *The functional $\omega(A) = \mathrm{Tr}(AR)$ is reflection invariant on $\mathfrak{A}$.*
(b) *The operator R is reflection invariant, $\Theta(R) = R$.*
(c) *The matrix $r_{\mathfrak{I}\mathfrak{I}'}$ is hermitian, $r_{\mathfrak{I}'\mathfrak{I}} = \overline{r_{\mathfrak{I}\mathfrak{I}'}}$.*
(d) *The sesquilinear form $\langle\,\cdot\,,\,\cdot\,\rangle_{R,\Theta}$ is hermitian on $\mathfrak{A}_+$,*

$$\langle A, B\rangle_{R,\Theta} = \overline{\langle B, A\rangle}_{R,\Theta}\,, \quad \textit{for all} \quad A, B \in \mathfrak{A}_+\,.$$

Proof. (b)⇒(a): By Proposition I.10.d, the trace is reflection invariant, $\mathrm{Tr}(\Theta(X)) = \overline{\mathrm{Tr}(X)}$. If $\Theta(R) = R$, one finds

$$\overline{\mathrm{Tr}(AR)} = \mathrm{Tr}(\Theta(AR)) = \mathrm{Tr}(\Theta(A)\Theta(R)) = \mathrm{Tr}(\Theta(A)R)\,.$$

Thus $\overline{\omega(A)} = \omega(\Theta(A))$, and ω is reflection invariant.

(a)⇒(d): If ω is reflection invariant, then

$$\overline{\omega(\Theta(B) \circ A)} = \omega(\Theta(\Theta(B) \circ A)) = \omega(\Theta(A) \circ (B))\,,$$

where the second equality follows from Proposition I.5.

(d)⇒(b): Since $\overline{\langle B, A\rangle}_{R,\Theta} = \overline{\mathrm{Tr}((\Theta(A) \circ B)R)}$, reflection invariance of the trace and Proposition I.5 yield

$$\overline{\langle B, A\rangle}_{R,\Theta} = \mathrm{Tr}(\Theta(\Theta(B) \circ A)\Theta(R)) = \mathrm{Tr}((\Theta(A) \circ B)\Theta(R))\,,$$

for all $A, B \in \mathfrak{A}_+$. Since $\langle A, B\rangle_{R,\Theta} = \mathrm{Tr}((\Theta(A) \circ B)R)$, we infer from $\langle A, B\rangle_{R,\Theta} = \overline{\langle B, A\rangle}_{R,\Theta}$ that

$$\mathrm{Tr}((\Theta(A) \circ B)R) = \mathrm{Tr}((\Theta(A) \circ B)\Theta(R))\,.$$

Since $\mathfrak{A}$ is spanned by elements of the form $\Theta(A) \circ B$ with $A, B \in \mathfrak{A}_+$, nondegeneracy of the trace implies $\Theta(R) = R$.

We conclude that (a)⇔(b)⇔(d). The equivalence (b)⇔(c) was already proven in Proposition I.6. □

II.2. **Reflection Positivity.** In this section, we characterize reflection positive functionals in terms of their density matrix.

Definition II.3. *The linear functional ω in (II.1) is reflection positive on $\mathfrak{A}_+$ with respect to Θ, if the form $\langle\,\cdot\,,\,\cdot\,\rangle_{R,\Theta}$ in (II.2) is positive, semidefinite on $\mathfrak{A}_+$.*

Proposition II.4. *The functional ω in (II.1) is reflection positive on $\mathfrak{A}_+$, if and only if it is reflection invariant on $\mathfrak{A}_-$. In fact*

$$\langle\Theta(A), \Theta(B)\rangle_{R,\Theta} = \langle B, A\rangle_{R,\Theta}\,, \quad \textit{for} \quad A, B \in \mathfrak{A}_+\,. \tag{II.5}$$

Proof. For $A, B \in \mathfrak{A}_+$, we infer from Corollary I.5 that

$$\omega(\Theta(\Theta(A)) \circ \Theta(B)) = \omega(A \circ \Theta(B)) = \omega(\Theta(B) \circ A)\,.$$

The first term equals $\langle\Theta(A), \Theta(B)\rangle_{R,\Theta}$ and the last one $\langle B, A\rangle_{R,\Theta}$. □

Theorem II.5 (**Basic Reflection Positivity).** *The linear functional ω in (II.1) is reflection positive on $\mathfrak{A}_+$, if and only if the matrix $r_{\mathfrak{I}\mathfrak{I}'}$ defined in (II.3) is positive semidefinite.*

Proof. Expand $A, B \in \mathfrak{A}_+$ as $A = \sum_{\mathfrak{I}\in\mathcal{P}_+} a_{\mathfrak{I}}\, C_{\mathfrak{I}}$ and $B = \sum_{\mathfrak{I}\in\mathcal{P}_+} b_{\mathfrak{I}}\, C_{\mathfrak{I}}$. Using (I.9) and (II.4) we obtain

$$\begin{aligned}
\langle A, B\rangle_{R,\Theta} &= \mathrm{Tr}((\Theta(A)\circ B)R) \\
&= \sum_{\substack{\mathfrak{I}_0,\mathfrak{I}_0'\in\mathcal{P}_+\\ \mathfrak{I}_1,\mathfrak{I}_1'\in\mathcal{P}_+}} \overline{a_{\mathfrak{I}_0}}\, b_{\mathfrak{I}_0'}, r_{\mathfrak{I}_1\mathfrak{I}_1'}\, \mathrm{Tr}\Big(\big(\Theta(C_{\mathfrak{I}_0})\circ C_{\mathfrak{I}_0'}\big)\,\big(\Theta(C_{\mathfrak{I}_1})\circ C_{\mathfrak{I}_1'}\big)\Big) \\
&= \sum_{\mathfrak{I},\mathfrak{I}'} \overline{a_{\mathfrak{I}}}\, q_{\mathfrak{I}}\, b_{\mathfrak{I}'} q_{\mathfrak{I}'}\, r_{\mathfrak{I}\mathfrak{I}'}\,.
\end{aligned}$$

It follows that $\langle A, A\rangle_{R,\Theta} \geqslant 0$ for all $A \in \mathfrak{A}_+$ if and only if the matrix $r_{\mathfrak{I}\mathfrak{I}'}$ is is positive semidefinite. □

III. Sufficient Conditions for Reflection Positivity

In statistical physics, Gibbs states are defined in terms of a Hamiltonian H, which in turn is given by a matrix J of coupling constants. In this section, we provide a sufficient condition on J for the associated Gibbs state to be reflection positive. This will be further refined to a necessary and sufficient condition in Section IV.

III.1. **Density Matrices and Hamiltonians.** For a (not necessarily hermitian) Hamiltonian $H \in \mathfrak{A}$, consider the unnormalized density matrix $R = e^{-H}$. We now focus on the Hamiltonian H rather than R, and define the *Boltzmann functional* $\omega_H : \mathfrak{A} \to \mathbb{C}$ by

$$\omega_H(A) = \mathrm{Tr}(A\, e^{-H})\,. \tag{III.1}$$

If the partition function $Z_H := \mathrm{Tr}(e^{-H})$ is nonzero, then define the *Gibbs functional* $\rho_H : \mathfrak{A} \to \mathbb{C}$ as the normalization of ω_H,

$$\rho_H(A) := \frac{\omega_H(A)}{Z_H} = \frac{\mathrm{Tr}(Ae^{-H})}{\mathrm{Tr}(e^{-H})}\,. \tag{III.2}$$

Using equation II.2, the (unnormalized) Boltzmann functional ω_H yields the sesquilinear form

$$\langle A, B\rangle^0_{H,\Theta} := \mathrm{Tr}((\Theta(A)\circ B)\, e^{-H}) \tag{III.3}$$

on $\mathfrak{A}_+$. Similarly, the the (normalized) Gibbs functional ρ_H yields the form

$$\langle A, B\rangle_{H,\Theta} := \frac{\mathrm{Tr}((\Theta(A)\circ B)\, e^{-H})}{\mathrm{Tr}(e^{-H})}\,. \tag{III.4}$$

Remark III.1. The functional ω_H in (III.1) is reflection positive on $\mathfrak{A}_+$ if $\langle A, B\rangle^0_{H,\Theta}$ in (III.3) is positive semidefinite on $\mathfrak{A}_+$. The functional ρ_H defined in (III.2) is reflection positive on $\mathfrak{A}_+$ if the form $\langle A, B\rangle_{H,\Theta}$ in (III.4) is positive semidefinite on $\mathfrak{A}_+$.

In §IV.2 we show reflection positivity of the Boltzmann functional ω_H for a large class of reflection symmetric, globally gauge invariant Hamiltonians H, namely all those for which the matrix of coupling constants is positive semidefinite. For such Hamiltonians $Z_H \geqslant 1$.

We use this result to prove reflection positivity for an even wider class of Hamiltonians, namely those for which the matrix of coupling constants *across the reflection plane* is positive semidefinite.

Neither result will require H to be hermitian, but if this happens to be the case, Z_H is automatically nonzero, and ρ_H is the Gibbs state with respect to the Hamiltonian H.

III.2. **Hamiltonians.** The class of Hamiltonians for which these reflection positivity results hold, is defined in terms of the matrix of coupling constants,

$$J = (J_{\mathfrak{I}\mathfrak{I}'}) \ , \quad \text{where} \quad \mathfrak{I}, \mathfrak{I}' \in \mathcal{P}_+ \ . \tag{III.5}$$

By definition, these are the coefficients $J_{\mathfrak{I}\mathfrak{I}'} \in \mathbb{C}$ of the Hamiltonian H in its expansion with respect to the basis $\mathcal{B}$,

$$H = - \sum_{\mathfrak{I}, \mathfrak{I}' \in \mathcal{P}_+} J_{\mathfrak{I}\mathfrak{I}'} \, \Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'} \ . \tag{III.6}$$

The following proposition expresses some relevant properties of H in terms of the matrix J. Recall that H is called reflection invariant if $\Theta(H) = H$, and globally gauge invariant if $\alpha(H) = H$, where α is the global gauge automorphism defined in (I.6).

Proposition III.2. *The Hamiltonian H in (III.6) is*

- **RI:** *reflection-invariant if and only if J is hermitian, $J_{\mathfrak{I}'\mathfrak{I}} = \overline{J_{\mathfrak{I}\mathfrak{I}'}}$.*
- **GI:** *globally gauge-invariant if and only if $J_{\mathfrak{I}\mathfrak{I}'} = 0$ for $|\mathfrak{I}| \neq |\mathfrak{I}'|$.*
- **H:** *hermitian if and only if $q_{\mathfrak{I}} q_{\mathfrak{I}'} J_{\mathfrak{I}\mathfrak{I}'}$ is real.*

Proof. The first statement is Proposition I.6. For the second statement, note that the global gauge transformation α leaves the basis element $\Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'}$ fixed if $|\mathfrak{I}| = |\mathfrak{I}'|$, and otherwise multiplies it by -1. Linear independence of the basis $\mathcal{B}$ ensures that each term in the expansion of H must be gauge invariant. The third statement is a consequence of Proposition I.7. □

Proposition III.3. *If H is reflection invariant, then the sesquilinear form $\langle A, B \rangle^0_{H,\Theta}$ on $\mathfrak{A}_+$ given by (III.3) is hermitian, and $Z_H = \mathrm{Tr}(e^{-H})$ is real:*

$$\Theta(H) = H \quad \Rightarrow \quad \langle A, B \rangle^0_{H,\Theta} = \overline{\langle B, A \rangle^0_{H,\Theta}} \ , \quad \textit{and} \quad \overline{Z_H} = Z_H \ .$$

If both H is reflection invariant and $Z_H \neq 0$, then the form $\langle A, B \rangle_{H,\Theta}$ is defined in (III.4) and is hermitian.

Proof. The operator R of §II equals e^{-H} here. So $\Theta(R) = e^{-\Theta(H)}$, and if H is reflection invariant, then so is R. By the implication (b)⇒(d) of Proposition II.2, the form $\langle\,\cdot\,,\,\cdot\,\rangle_{R,\Theta}$ is hermitian. Also (b)⇒(a) ensures that $Z_H = \mathrm{Tr}(e^{-H}) = \mathrm{Tr}(\Theta(e^{-H})) = \overline{Z_H}$ is real. Hence if $Z_H \neq 0$, the form $\langle A, B\rangle_{H,\Theta}$ is also hermitian. □

III.3. **Reflection Positivity: Preliminary Results.** We now prove reflection positivity of the Bolzmann functional ω_H for Hamiltonians H that arise from a positive semidefinite matrix J of coupling constants.

Theorem III.4 (Reflection Positivity of ω_H, Part I). *Let $H \in \mathfrak{A}$ be reflection symmetric and globally gauge invariant. If the matrix J of coupling constants for H, defined in equation (III.6), is positive semidefinite, then ω_H is reflection positive on $\mathfrak{A}_+$.*

We give some preliminary results before proving the theorem.

Lemma III.5. *Let $\mathfrak{I}_1, \ldots, \mathfrak{I}_k, \mathfrak{I}'_1, \ldots \mathfrak{I}'_k \in \mathcal{S}_+$ and $|\mathfrak{I}_j| = |\mathfrak{I}'_j|$ for $j \geqslant 1$. Then for all $\mathfrak{I}_0, \mathfrak{I}'_0 \in \mathcal{S}_+$,*

$$\overline{\mathrm{Tr}(C_{\mathfrak{I}_0} \cdots C_{\mathfrak{I}_k})}\, \mathrm{Tr}(C_{\mathfrak{I}'_0} \cdots C_{\mathfrak{I}'_k})\,. \tag{III.7}$$

is nonzero only if $|\mathfrak{I}_0| = |\mathfrak{I}'_0|$.

Proof. For every lattice point $i \in \Lambda$, let $k_i(\mathfrak{I})$ be 1 if i occurs in $\mathfrak{I} = (i_1, \ldots, i_s)$, and 0 otherwise. Then $s = k_{\mathfrak{I}} = \sum_{i\in\Lambda} k_i(\mathfrak{I})$. If $\mathrm{Tr}(C_{\mathfrak{I}_0} \cdots C_{\mathfrak{I}_k})$ is nonzero, then $\sum_{j=0}^{k} k_i(\mathfrak{I}_j)$ is even, as every $i \in \Lambda$ must occur an even number of times. Therefore,

$$\sum_{i\in\Lambda} \sum_{j=0}^{k} k_i(\mathfrak{I}_j) = \sum_{j=0}^{k} \left(\sum_{i\in\Lambda} k_i(\mathfrak{I}_j) \right) = \sum_{j=0}^{k} k_{\mathfrak{I}_j}$$

is even. Since $|\mathfrak{I}| = k_{\mathfrak{I}} \bmod 2$, the sum $\sum_{j=0}^{k} |\mathfrak{I}_j|$ is even.

Similarly, one finds that $\sum_{j=0}^{k} |\mathfrak{I}'_j|$ is even if $\mathrm{Tr}(C_{\mathfrak{I}'_0} \cdots C_{\mathfrak{I}'_k})$ is nonzero. Since $|\mathfrak{I}_j| = |\mathfrak{I}'_j|$ for $j \geqslant 1$ by assumption, we infer that $|\mathfrak{I}_0| = |\mathfrak{I}'_0|$ if III.7 is nonzero. □

Lemma III.6. *Under the hypotheses of Lemma III.5,*

$$\begin{aligned} &\mathrm{Tr}\left((\Theta(C_{\mathfrak{I}_0}) \circ C_{\mathfrak{I}'_0}) \cdots (\Theta(C_{\mathfrak{I}_k}) \circ C_{\mathfrak{I}'_k}) \right) \\ &\qquad = \overline{\mathrm{Tr}(C_{\mathfrak{I}_0} \cdots C_{\mathfrak{I}_k})}\, \mathrm{Tr}(C_{\mathfrak{I}'_0} \cdots C_{\mathfrak{I}'_k})\,. \end{aligned} \tag{III.8}$$

Proof. Use the definition of $\circ$ to write

$$\begin{aligned} &\mathrm{Tr}((\Theta(C_{\mathfrak{I}_0}) \circ C_{\mathfrak{I}'_0}) \cdots (\Theta(C_{\mathfrak{I}_k}) \circ C_{\mathfrak{I}'_k})) \\ &\qquad = \zeta^{\sum_{j=0}^{k} |\mathfrak{I}_j||\mathfrak{I}'_j|}\, \mathrm{Tr}\left(\Theta(C_{\mathfrak{I}_0}) C_{\mathfrak{I}'_0} \cdots \Theta(C_{\mathfrak{I}_k}) C_{\mathfrak{I}'_k} \right), \end{aligned} \tag{III.9}$$

and bring the terms of the form $\Theta(C_{\mathfrak{I}_j})$ to the left. In doing so, one has to exchange $\Theta(C_{\mathfrak{I}_j})$ with $C_{\mathfrak{I}'_{j'}}$ for each $j' < j$, yielding a factor

$$(-1)^{\sum_{j'=0}^{j} |\mathfrak{I}'_{j'}||\mathfrak{I}_j|} = \zeta^{2\sum_{j'=0}^{j} |\mathfrak{I}'_{j'}||\mathfrak{I}_j|} .$$

The right hand side in equation III.9 can thus be written

$$\zeta^{\sum_{j=0}^{k} |\mathfrak{I}_j||\mathfrak{I}'_j| + 2\sum_{0\leqslant j'<j\leqslant k} |\mathfrak{I}_j||\mathfrak{I}'_{j'}|} \operatorname{Tr}(\Theta(C_{\mathfrak{I}_0}\cdots C_{\mathfrak{I}_k})C_{\mathfrak{I}'_0}\cdots C_{\mathfrak{I}'_k}) , \quad \text{(III.10)}$$

where we used that $\Theta(C_{\mathfrak{I}_0})\cdots\Theta(C_{\mathfrak{I}_k})$ equals $\Theta(C_{\mathfrak{I}_0}\cdots C_{\mathfrak{I}_k})$.

Using the factorization of the trace, $\operatorname{Tr}(X_- X_+) = \operatorname{Tr}(X_-)\operatorname{Tr}(X_+)$ for $X_\pm \in \mathfrak{A}_\pm$, and reflection invariance, $\operatorname{Tr}(\Theta(X)) = \overline{\operatorname{Tr}(X)}$, given in Proposition I.10.d and e, (III.10) becomes

$$\zeta^{\sum_{j=0}^{k} |\mathfrak{I}_j||\mathfrak{I}'_j| + 2\sum_{0\leqslant j'<j\leqslant k} |\mathfrak{I}_j||\mathfrak{I}'_{j'}|} \overline{\operatorname{Tr}(C_{\mathfrak{I}_0}\cdots C_{\mathfrak{I}_k})}\operatorname{Tr}(C_{\mathfrak{I}'_0}\cdots C_{\mathfrak{I}'_k}) . \quad \text{(III.11)}$$

Using Lemma III.5, we rewrite the phase in (III.10)

$$\zeta^{\sum_{j=0}^{k} |\mathfrak{I}_j||\mathfrak{I}'_j| + 2\sum_{0\leqslant j'<j\leqslant k} |\mathfrak{I}_j||\mathfrak{I}'_{j'}|} = \zeta^{\left(\sum_{j=0}^{k} |\mathfrak{I}_j|\right)^2} = 1 . \quad \text{(III.12)}$$

The last equality holds as $\sum_{j=0}^{k} |\mathfrak{I}_j|$ must be even, so its square is 0 mod 4, and the phase vanishes. Combining (III.12) with (III.11), the proof is complete. $\square$

Proof of Theorem III.4. Expand $A, B \in \mathfrak{A}_+$ as

$$A = \sum_{\mathfrak{I}\in\mathcal{P}_+} a_{\mathfrak{I}}\, C_{\mathfrak{I}} \quad \text{and} \quad B = \sum_{\mathfrak{I}\in\mathcal{P}_+} b_{\mathfrak{I}}\, C_{\mathfrak{I}} , \quad \text{with} \quad C_{\mathfrak{I}} \in \mathcal{B}_+ .$$

We claim that the sesquilinear form $\langle A, B\rangle^0_{H,\Theta} = \operatorname{Tr}(\Theta(A)\circ B\, e^{-H})$ can then be written in the form

$$\begin{aligned} \langle A, B\rangle^0_{H,\Theta} \;&=\; \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\mathfrak{I}_0,\ldots\mathfrak{I}_k} \sum_{\mathfrak{I}'_0,\ldots,\mathfrak{I}'_k} \overline{a_{\mathfrak{I}_0}} b_{\mathfrak{I}'_0} J_{\mathfrak{I}_1,\mathfrak{I}'_1}\cdots J_{\mathfrak{I}_k,\mathfrak{I}'_k} \\ &\qquad \times \overline{\operatorname{Tr}(C_{\mathfrak{I}_0}\cdots C_{\mathfrak{I}_k})}\; \operatorname{Tr}(C_{\mathfrak{I}'_0}\cdots C_{\mathfrak{I}'_k}) . \quad \text{(III.13)} \end{aligned}$$

From the power series for e^{-H} with H given by (III.6), one obtains the expansion

$$\begin{aligned} \langle A, B\rangle^0_{H,\Theta} \;&=\; \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\mathfrak{I}_0,\ldots\mathfrak{I}_k\in\mathcal{P}_+} \; \sum_{\mathfrak{I}'_0,\ldots,\mathfrak{I}'_k\in\mathcal{P}_+} \overline{a_{\mathfrak{I}_0}}\, b_{\mathfrak{I}'_0} J_{\mathfrak{I}_1\mathfrak{I}'_1}\cdots J_{\mathfrak{I}_k\mathfrak{I}'_k} \\ &\qquad \times\; \operatorname{Tr}((\Theta(C_{\mathfrak{I}_0})\circ C_{\mathfrak{I}'_0})\;\cdots\;(\Theta(C_{\mathfrak{I}_k})\circ C_{\mathfrak{I}'_k})) . \quad \text{(III.14)} \end{aligned}$$

The terms with $\mathfrak{I}_0$ and $\mathfrak{I}'_0$ arise from A and B, while the remaining $\mathfrak{I}_j$, $\mathfrak{I}'_j$ come from powers of H. By Proposition III.2, global gauge invariance of H ensures that $|\mathfrak{I}_j| = |\mathfrak{I}'_j|$ for all $j \geqslant 1$. From Lemma III.6, we conclude that

$$\begin{aligned}\mathrm{Tr}((\Theta(C_{\mathfrak{I}_0}) \circ C_{\mathfrak{I}'_0}) \cdots (\Theta(C_{\mathfrak{I}_k}) \circ C_{\mathfrak{I}'_k}))& \\ = \overline{\mathrm{Tr}(C_{\mathfrak{I}_0} \cdots C_{\mathfrak{I}_k})}\, \mathrm{Tr}(C_{\mathfrak{I}'_0} \cdots C_{\mathfrak{I}'_k})\,.& \qquad \text{(III.15)}\end{aligned}$$

So by Lemma III.5, $|\mathfrak{I}_0| = |\mathfrak{I}'_0|$ unless (III.15) vanishes. Using this and the expansion III.14, one obtains III.13.

Let χ^k, ψ^k denote vectors with components

$$\chi^k_{\mathfrak{I}_1,\ldots,\mathfrak{I}_k} = \sum_{\mathfrak{I}_0 \in \mathcal{P}_+} a_{\mathfrak{I}_0}\, \mathrm{Tr}(C_{\mathfrak{I}_0} \cdots C_{\mathfrak{I}_k})\ ,$$

and

$$\psi^k_{\mathfrak{I}_1,\ldots,\mathfrak{I}_k} = \sum_{\mathfrak{I}_0 \in \mathcal{P}_+} b_{\mathfrak{I}_0}\, \mathrm{Tr}(C_{\mathfrak{I}_0} \cdots C_{\mathfrak{I}_k})\ ,$$

labelled by $\mathcal{P}^k_+$. Let $J^{\otimes k}_{\mathfrak{I}_1,\ldots,\mathfrak{I}_k;\mathfrak{I}'_1,\ldots,\mathfrak{I}'_k} := J_{\mathfrak{I}_1\mathfrak{I}'_1} \cdots J_{\mathfrak{I}_k\mathfrak{I}'_k}$ be the k^{th} tensor power of the matrix $J_{\mathfrak{I}\mathfrak{I}'}$. Since $J_{\mathfrak{I}\mathfrak{I}'}$ is a positive semidefinite matrix, $J^{\otimes k}$ is also positive semidefinite. Then

$$\langle A, B\rangle^0_{H,\Theta} = \sum_{k=0}^{\infty} \frac{1}{k!}\, \langle \chi^k, J^{\otimes k}\psi^k\rangle\ , \qquad \text{(III.16)}$$

with the inner product

$$\langle \chi^k, \psi^k\rangle := \sum_{\mathfrak{I}_1,\ldots\mathfrak{I}_k \in \mathcal{P}_+} \overline{\chi^k_{\mathfrak{I}_1\ldots\mathfrak{I}_k}}\, \psi^k_{\mathfrak{I}_1\ldots\mathfrak{I}_k}\,.$$

Setting $B = A$ one has $\psi^k = \chi^k$. Since each term in the sum (III.16) is non-negative, the theorem follows. □

Corollary III.7. *If $A \in \mathfrak{A}_+$ has the expansion (I.14), then under the conditions of Theorem III.4, one has*

$$\langle A, A\rangle^0_{H,\Theta} \geqslant |a_{\varnothing\varnothing}|^2\ . \qquad \text{(III.17)}$$

Proof. The right side of III.17 is the $k = 0$ term in III.13. This yields a lower bound, as all the other terms are nonnegative by the proof of Theorem III.4. □

Proposition III.8. *Suppose that the matrix J of coupling constants for H, defined in (III.6), is positive semidefinite. Then $Z_{\beta H}$ is a non-decreasing function of $0 \leqslant \beta$ with $Z_0 = 1$. In particular, $1 \leqslant Z_{\beta H}$ for all $0 \leqslant \beta$.*

Proof. Let $R = e^{-\beta H}$ and consider $Z_{\beta H} = \mathrm{Tr}(e^{-\beta H}) = \mathrm{Tr}(R)$ for $\beta \geqslant 0$. Note that $Z_0 = 1$ by Proposition I.10.a. Using Proposition I.9 to evaluate the trace, one obtains

$$\frac{dZ_{\beta H}}{d\beta} = -\,\mathrm{Tr}(He^{-\beta H}) = -\,\mathrm{Tr}(HR) = \sum_{\mathfrak{I},\mathfrak{I}' \in \mathcal{P}_+} q_{\mathfrak{I}}\, J_{\mathfrak{I}\mathfrak{I}'}\, r_{\mathfrak{I}\mathfrak{I}'}\, q_{\mathfrak{I}'}\ , \tag{III.18}$$

with $q_{\mathfrak{I}} = (-1)^{k_{\mathfrak{I}}(k_{\mathfrak{I}}-1)}$ as defined in equation (I.17). Since the matrix $J_{\mathfrak{I}\mathfrak{I}'}$ is positive semidefinite, the Bolzmann functional ω_H is reflection positive by Theorem III.8. The matrix $r_{\mathfrak{I}\mathfrak{I}'}$ of coefficients of $R = e^{-\beta H}$ is positive semidefinite, as a consequence of Theorem II.5. It follows that the Hadamard product matrix K, with matrix elements $K_{\mathfrak{I}\mathfrak{I}'} = J_{\mathfrak{I}\mathfrak{I}'}\, r_{\mathfrak{I}\mathfrak{I}'}$, is also positive semidefinite. From III.18, we infer that

$$\frac{dZ_{\beta H}}{d\beta} = \sum_{\mathfrak{I},\mathfrak{I}' \in \mathcal{P}+} q_{\mathfrak{I}}\, K_{\mathfrak{I}\mathfrak{I}'}\, q_{\mathfrak{I}'} = \langle q, Kq \rangle_{\ell^2} \geqslant 0\ . \tag{III.19}$$

It follows that $Z_{\beta H}$ is a non-decreasing function of β. □

IV. Necessary and Sufficient Conditions

In Theorem III.4 we have given sufficient conditions for reflection positivity of the Bolzmann functional ω_H; it is reflection positive if $J \geqslant 0$, where J is the matrix (III.5) of couplings by which H is defined.

Now we establish a stronger result, providing necessary and sufficient conditions in terms of the submatrix J^0 of J that contains only the couplings between Majoranas on different sides of the reflection plane. If J is positive semidefinite, then J^0 is positive semidefinite, but the converse does not hold.

In Section IV.2 we prove that ω_H is reflection positive if and only if $J^0 \geqslant 0$. Using this, we prove the analogous statement for Gibbs functional ρ_H in Section IV.3.

IV.1. **Coupling Constants Across the Reflection Plane.** Let H be reflection invariant, so that the coupling-constant matrix J is hermitian. Order the basis elements in $\mathcal{B}_+$ so $C_\varnothing = I$ is the first one, and consider the decomposition of J,

$$J = \begin{pmatrix} J_{\varnothing\varnothing} & J_{\varnothing\mathfrak{I}'} \\ J_{\mathfrak{I}\varnothing} & J_{\mathfrak{I}\mathfrak{I}'} \end{pmatrix} = \begin{pmatrix} E & V^* \\ V & J^0 \end{pmatrix}\ . \tag{IV.1}$$

Here $E = J_{\varnothing\varnothing}$ yields the additive constant $-E$ in H. Reflection invariance of H ensures that E is real.

In fact E is not of physical relevance. It does not affect whether the functional ω_H is reflection positive. Furthermore it does not even enter the normalized Gibbs functional. The energy shift $H \mapsto H - E$

multiplies both ω_H and Z_H by e^E, so it it does not affect their quotient ρ_H. The column vector $V_{\mathfrak{I}} = J_{\mathfrak{I}\varnothing}$ has indices labelled by $\mathfrak{I} \in \mathcal{P}_+ - \{\varnothing\}$, as does its hermitian adjoint V^*. The hermitian matrix

$$J^0 = (J^0_{\mathfrak{I},\mathfrak{I}'}) \;, \quad \text{with indices} \quad \mathfrak{I}, \mathfrak{I}' \in \mathcal{P}_+ - \{\varnothing\} \tag{IV.2}$$

is called the matrix of *coupling constants across the reflection plane.*

The matrix decomposition (IV.1) corresponds to the four terms in the decomposition

$$H = H_- + H_0 + H_+ - E \,, \tag{IV.3}$$

where

$$-H_- = \sum_{\mathfrak{I} \in \mathcal{P}_+ - \{\varnothing\}} J_{\mathfrak{I}\varnothing}\, \Theta(C_{\mathfrak{I}}) = \sum_{\mathfrak{I} \in \mathcal{P}_+ - \{\varnothing\}} V_{\mathfrak{I}}\, \Theta(C_{\mathfrak{I}}) \in \mathfrak{A}_- \tag{IV.4}$$

is the sum of the interactions on one side of the reflection plane, namely on sites in Λ_-. The reflection H_+ of H_- is the interaction within Λ_+,

$$-H_+ = \Theta(-H_-) = \sum_{\mathfrak{I} \in \mathcal{P}_+ - \{\varnothing\}} \overline{V_{\mathfrak{I}}}\, C_{\mathfrak{I}} \in \mathfrak{A}_+ \;. \tag{IV.5}$$

The interaction across the reflection plane is

$$-H_0 = \sum_{\mathfrak{I},\mathfrak{I}' \in \mathcal{P}_+ - \{\varnothing\}} J^0_{\mathfrak{I}\mathfrak{I}'}\, \Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'} \;. \tag{IV.6}$$

IV.2. **Characterization of Reflection Positivity.** We give necessary and sufficient conditions on the Hamiltonian $H \in \mathfrak{A}$ for the Bolzmann functional

$$\omega_H(A) = \mathrm{Tr}(Ae^{-H})$$

to be reflection positive on $\mathfrak{A}_+$.

Remark IV.1. Reflection positivity of ω_H means that the hermitian form on $\mathfrak{A}_+$ defined by

$$\langle A, B\rangle^0_{H,\Theta} = \mathrm{Tr}(\vartheta(A) \circ B \cdot e^{-H})$$

is positive semidefinite; $0 \leqslant \langle A, A\rangle^0_{H,\Theta}$ for $A \in \mathfrak{A}_+$. In particular,

$$Z_H = \mathrm{Tr}(e^{-H}) = \langle I, I\,\rangle^0_{H,\Theta} \geqslant 0\,. \tag{IV.7}$$

If $Z_H \neq 0$, reflection positivity of the Bolzmann functional ω_H therefore implies reflection positivity of the (physically relevant) Gibbs functional $\rho_H = Z_H^{-1}\omega_H$.

Theorem IV.2 (Reflection Positivity of $\boldsymbol{\omega_H}$, Part II). *Let $H \in \mathfrak{A}$ be reflection symmetric and globally gauge invariant. Let J^0 be the matrix of coupling constants across the reflection plane, defined in (IV.1)–(IV.2). Then:*

(a) *If J^0 is positive semidefinite, the functional ω_H is reflection positive on $\mathfrak{A}_+$.*
(b) *Conversely, if there exists an $\varepsilon > 0$ such that $\omega_{\beta H}$ is reflection positive on $\mathfrak{A}_+$ for all $\beta \in [0, \varepsilon)$, then the matrix J^0 is positive semidefinite.*

Proof. (a) Since H is reflection invariant, we infer from Proposition III.2 that J is hermitian. Writing J as in (IV.1), recall that reflection positivity of ω_H is independent of the value of E. So for simplicity we can add a constant to H so that $E = 0$. Now we approximate J by J_ε defined as the matrix

$$J_\varepsilon := \begin{pmatrix} 0 & V^* \\ V & J^0 \end{pmatrix} + \varepsilon \begin{pmatrix} 0 & 0 \\ 0 & VV^* \end{pmatrix} , \qquad \text{(IV.8)}$$

where $0 \leqslant \varepsilon$ is a small parameter. Here VV^* denotes the matrix with elements $(VV^*)_{\mathfrak{I}\mathfrak{I}'} = V_{\mathfrak{I}} \overline{V_{\mathfrak{I}'}}$ with $\mathfrak{I}, \mathfrak{I}' \in \mathcal{P} - \varnothing$. Clearly $J_\epsilon \to J$ as $\varepsilon \to 0$, so that $H_\varepsilon \to H$ as $\varepsilon \to 0$. Hence $\omega_{H_\epsilon} \to \omega_H$ as $\varepsilon \to 0$.

Assume that the functional ω_{H_ε} satisfies reflection positivity on $\mathfrak{A}_+$ for every $\varepsilon > 0$. Then the convergence explained above means that for $A \in \mathfrak{A}_+$, the expectations $\omega_{H_\varepsilon}(\Theta(A) \circ A) \geqslant 0$ converge to $\omega_H(\Theta(A) \circ A) \geqslant 0$ as $\varepsilon \to 0$. We infer that ω_H is reflection positive.

Now we show that ω_{H_ε} does satisfy reflection positivity for every $\varepsilon > 0$. In order to see this, we make a second modification to J, by adding the constant ε^{-1} to H_ϵ. Thus we obtain a new matrix of couplings $\widetilde{J}_\varepsilon$ defined as

$$\widetilde{J}_\varepsilon = J_\varepsilon + \frac{1}{\varepsilon} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & J^0 \end{pmatrix} + \begin{pmatrix} \varepsilon^{-1} & V^* \\ V & \varepsilon VV^* \end{pmatrix} . \qquad \text{(IV.9)}$$

The couplings $\widetilde{J}_\varepsilon$ correspond to a Hamiltonian $\widetilde{H}_\varepsilon$, that differs from H_ε only by an additive constant. So $\omega_{\widetilde{H}_\varepsilon}$ satisfies reflection positivity if and only if ω_{H_ε} does. Furthermore we can appeal to Theorem III.4, so it is sufficient to show that the matrix $\widetilde{J}_\varepsilon$ is positive semidefinite for every $\varepsilon > 0$.

We claim that $\widetilde{J}_\varepsilon$ is positive semidefinite, since each of the two matrices on the right of (IV.9) are positive semidefinite, as is the sum of two positive semidefinite matrices. The first matrix on the right is positive semidefinite by the assumption that J^0 is positive semidefinite. The second matrix is also positive semidefinite, as it is a positive multiple $(\varepsilon^{-1} + \varepsilon V^* V)$ of the orthogonal projection in $\ell^2(\mathcal{P}_+)$ onto the vector W with components $W_{\mathfrak{I}} = \delta_{\mathfrak{I}\varnothing}\, \varepsilon^{-1} + (1 - \delta_{\mathfrak{I}\varnothing})\, V_{\mathfrak{I}}$. This concludes the proof that ω_H is reflection positive on $\mathfrak{A}_+$.

(b). Suppose that $\omega_{\beta H}$ is reflection positive on $\mathfrak{A}_+$ for $\beta \in [0, \varepsilon)$. Choose $A = \sum_{\mathfrak{I} \in \mathcal{P}_+} a_{\mathfrak{I}} C_{\mathfrak{I}}$ with $a_\varnothing = 0$, so A is in the null space of the form $\langle A, A \rangle^0_{0,\Theta}$, as $\mathrm{Tr}(\Theta(A) \circ A) = |a_\varnothing|^2 = 0$. Reflection positivity then ensures that the first derivative cannot be negative,

$$0 \leqslant \frac{d}{d\beta} \langle A, A \rangle^0_{\beta H, \Theta} \bigg|_{\beta = 0} = -\,\mathrm{Tr}((\Theta(A) \circ A) H)\,, \qquad \text{(IV.10)}$$

for otherwise reflection positivity would be violated for small β. One can evaluate (IV.10) in a fashion similar to the computation of (III.18), but with $\Theta(A) \circ A$ replacing R.

Expanding $\Theta(A) \circ A$ as $\sum_{\mathfrak{I}, \mathfrak{I}'} \overline{a_{\mathfrak{I}}} a_{\mathfrak{I}'} \Theta(C_{\mathfrak{I}}) \circ C_{\mathfrak{I}'}$, and using Proposition I.9 to evaluate the trace, one obtains

$$0 \leqslant -\,\mathrm{Tr}(\Theta(A) \circ AH) = \sum_{\mathfrak{I}, \mathfrak{I}' \in \mathcal{P}_+ - \varnothing} \overline{(q_{\mathfrak{I}} a_{\mathfrak{I}})}\, J^0_{\mathfrak{I}\mathfrak{I}'}\, (q_{\mathfrak{I}'} a_{\mathfrak{I}'}), \qquad \text{(IV.11)}$$

with $q_{\mathfrak{I}} = (-1)^{k_{\mathfrak{I}}(k_{\mathfrak{I}} - 1)}$ as in (I.17). As $a_\varnothing = 0$, the sum restricts to $\mathcal{P}_+ - \varnothing$, and only J^0 contributes. From equation IV.11, one then obtains

$$0 \leqslant \langle f, J^0 f \rangle\,. \qquad \text{(IV.12)}$$

Since this holds for all $f \in \ell^2(\mathcal{P}_+)$ with $f_\varnothing = 0$, this assures that the matrix J^0 is positive semidefinite. □

IV.3. **Reflection Positive Gibbs Functionals.** Using Theorem IV.2, we obtain the following necessary and sufficient conditions on H for the Gibbs functional

$$\rho_H(A) = Z_H^{-1}\, \mathrm{Tr}(A e^{-H})\,,$$

to be reflection positive on $\mathfrak{A}_+$. In this expression, $Z_H = \mathrm{Tr}(e^{-H})$ denotes the partition sum.

Theorem IV.3 (Reflection Positivity of Gibbs Functionals). *Let $H \in \mathfrak{A}$ be a reflection symmetric, globally gauge invariant Hamiltonian.*

(a) *Suppose that $Z_H \neq 0$, and that the matrix J^0 of coupling constants across the reflection plane is positive semidefinite. Then ρ_H is reflection positive, and $Z_H > 0$.*

(b) *If there exists an $\varepsilon > 0$ such that $\rho_{\beta H}$ is reflection positive for all $\beta \in [0, \varepsilon)$, then the matrix J^0 of coupling constants across the reflection plane is positive semidefinite.*

Remark IV.4. In many applications, $H \in \mathfrak{A}^{\mathrm{even}}$ is self-adjoint, so that the condition $Z_{\beta H} \neq 0$ is automatically satisfied for all $\beta \geqslant 0$.

Proof. (a) If J^0 is positive semidefinite, then ω_H is reflection positive by Theorem IV.2. Reflection positivity of the Gibbs functional ρ_H then follows by Remark IV.1.

(b) The partition function $Z_{\beta H} = \mathrm{Tr}(e^{-\beta H})$ is analytic in β, and real by Corollary I.11. Since $Z_0 = 1$, the expression

$$\rho_{\beta H}(X) = Z_{\beta H}^{-1}\,\mathrm{Tr}(Xe^{-\beta H})$$

is well defined and analytic in a neighborhood U of $\beta = 0$. The inequality $0 \leqslant \rho_{\beta H}(\Theta(A) \circ A)$ for $\beta \in U$ thus yields

$$0 \leqslant Z_{\beta H}\ \rho_{\beta H}(\Theta(A) \circ A) = \omega_{\beta H}(\Theta(A) \circ A)\,.$$

Since this holds for all $A \in \mathfrak{A}_+$ and $\beta \in U$, the Bolzmann functional $\omega_{\beta H}$ is reflection positive for all $\beta \in U$, and J^0 is positive semidefinite by Theorem IV.2. □

V. Reflection Positivity for Spin Systems

From the corresponding result for Majoranas, we now derive necessary and sufficient conditions for reflection positivity in the context of spin systems. As in the case of Majoranas, these will be formulated in terms of the matix of coupling constants across the reflection plane.

V.1. **Spin Algebras.** In spin models, the algebra of observables for a lattice site $j \in \Lambda$ is $M_2(\mathbb{C})$, spanned by I and the Pauli spin matrices $\sigma_j^1, \sigma_j^2, \sigma_j^3$. The operators σ_j^a and $\sigma_{j'}^b$ commute for $j \neq j'$, and otherwise satisfy the familiar relations $\sigma_j^a \sigma_j^b = \delta^{ab} I + i \sum_c \epsilon_{abc} \sigma_j^c$. In this context, the full algebra of observables is

$$\mathfrak{A}^{\mathrm{spin}} = \bigoplus_{j \in \Lambda} M_j^2(\mathbb{C})\,,$$

and the algebra of observables on the $\pm$ side of the reflection plane is

$$\mathfrak{A}_{\pm}^{\mathrm{spin}} = \bigoplus_{j \in \Lambda_{\pm}} M_j^2(\mathbb{C})\,.$$

Define the operators $\Sigma_{(\mathfrak{I},A)}$ as the product of spins

$$\Sigma_{(\mathfrak{I},A)} = \sigma_{j_1}^{a_1} \ldots \sigma_{j_k}^{a_k}\,.$$

They are labelled by sets of the form

$$(\mathfrak{I}, A) := \{(i_1, a_1), \ldots, (i_k, a_k)\}\,, \tag{V.1}$$

where i_s is a lattice point in Λ, a_s is a spin label in $\{1, 2, 3\}$, and $i_s \neq i_t$ for $s \neq t$. Together with the identity $\Sigma_{\varnothing} := I$, the operators $\Sigma_{(\mathfrak{I},A)}$

constitute an orthonormal basis of $\mathfrak{A}$ with respect to the bilinear trace pairing,

$$\mathrm{Tr}_{\mathrm{spin}}(\Sigma_{(\mathfrak{I},A)}\Sigma_{(\mathfrak{I}',A')}) = \delta_{AA'}\delta_{\mathfrak{I}\mathfrak{I}'} \,. \tag{V.2}$$

Definition V.1 (Standard Reflection). *The standard reflection* Θ *on* $\mathfrak{A}^{\mathrm{spin}}$ *is defined by* $\Theta(\sigma_j^a) = -\sigma_{\vartheta(j)}^a$, *for* $j \in \Lambda$ *and* $a \in \{1,2,3\}$.

The standard reflection satisfies

$$\Theta(\Sigma_{(\mathfrak{I},A)}) = (-1)^{k_{\mathfrak{I}}}\Sigma_{\vartheta(\mathfrak{I},A)} \,. \tag{V.3}$$

V.2. **Spin Hamiltonians.** Any Hamiltonian $H^{\mathrm{spin}} \in \mathfrak{A}^{\mathrm{spin}}$, not necessarily Hermitian, takes the form

$$H^{\mathrm{spin}} = -\sum_k \sum_{j_1,\ldots,j_k} \sum_{a_1,\ldots,a_k} J_{j_1}^{a_1} \,\cdots\, {}_{j_k}^{a_k}\, \sigma_{j_1}^{a_1} \cdots \sigma_{j_k}^{a_k} \,. \tag{V.4}$$

Partition $j_1 \ldots j_k$ into the sets $\vartheta(\mathfrak{I}) \subseteq \Lambda_-$ and $\mathfrak{I}' \subseteq \Lambda_+$, where both $\mathfrak{I}$ and $\mathfrak{I}'$ are subsets of Λ_+. Using (V.3) and setting

$$J_{\vartheta(\mathfrak{I})\mathfrak{I}'}^{AA'} = J_{j_1}^{a_1} \,\cdots\, {}_{j_k}^{a_k} \,, \tag{V.5}$$

equation (V.4) can be expressed as

$$\begin{aligned} H^{\mathrm{spin}} &= -\sum_{\substack{(\mathfrak{I},A)\\(\mathfrak{I}',A')}} J_{\vartheta(\mathfrak{I})\mathfrak{I}'}^{AA'}\, \Sigma_{(\vartheta(\mathfrak{I}),A)}\Sigma_{(\mathfrak{I}',A')} && \text{(V.6)}\\ &= -\sum_{\substack{(\mathfrak{I},A)\\(\mathfrak{I}',A')}} (-1)^{k_{\mathfrak{I}}} J_{\vartheta(\mathfrak{I})\mathfrak{I}'}^{AA'}\, \Theta(\Sigma_{(\mathfrak{I},A)})\Sigma_{(\mathfrak{I}',A')} \,. && \text{(V.7)} \end{aligned}$$

V.3. **Mapping Spins to Majoranas.** Spin models map to Majorana models by a well-known transformation. For a single site, this is similar to the infinitesimal rotation written in terms of Dirac matrices. The tensor product construction, projected to a chiral subspace, is known in the condensed matter literature as the Kitaev transformation. This map $X \mapsto \widehat{X}$ from the algebra $\mathfrak{A}^{\mathrm{spin}}$ of spins to the algebra $\mathfrak{A}$ of Majoranas is constructed as follows.

Choose four Majoranas at site j denoted c_j^α, for $\alpha = 1,2,3,4$. (The superscripts denote labels, not powers.) The Majoranas satisfy the Clifford relations $\{c_j^\alpha, c_{j'}^\beta\} = 2\delta^{\alpha\beta}\delta_{jj'}I$ and $c_j^{\alpha *} = c_j^\alpha$. They generate the Majorana algebra $\mathfrak{A}$ indexed by $\widehat{\Lambda} = \Lambda \times \{1,2,3,4\}$.

The product $\gamma_j^5 = c_j^1 c_j^2 c_j^3 c_j^4$ is both self adjoint and unitary, so $P_j^5 = \frac{1}{2}(I + \gamma_j^5)$ is the projection corresponding to the $+1$ eigenvalue. The projections P_j^5 mutually commute, and also commute with all even elements of $\mathfrak{A}$. Their product $P^5 := \prod_j P_j^5$ is called the *chiral pojection.* It can be written as a product

$$P^5 = P_-^5 P_+^5 \tag{V.8}$$

of the two commuting projections $P_\pm^5 = \prod_{j \in \Lambda_\pm} P_j^5$ in $\mathfrak{A}_\pm$.

The map from spins to Majoranas is given by

$$\widehat{\sigma}_j^a := i c_j^a c_j^4 \tag{V.9}$$

on single spins σ_j^a, and extends to a linear map $\mathfrak{A}^{\mathrm{spin}} \to \mathfrak{A}$ by

$$\widehat{\Sigma}_{(\mathfrak{I},A)} := \widehat{\sigma}_{j_1}^{a_1} \cdots \widehat{\sigma}_{j_k}^{a_k} .$$

The resulting linear map $X \mapsto \widehat{X}$ is a homomorphism when restricted to P^5, in the sense that for all $X, Y \in \mathfrak{A}^{\mathrm{spin}}$, one has

$$\widehat{XY}\, P_5 = \widehat{X}\widehat{Y}\, P_5 . \tag{V.10}$$

V.4. **Reflection Positivity for Spin Hamiltonians.** Recall that for a (not necessarily Hermitian) Hamiltonian $H \in H^{\mathrm{spin}}$, the Bolzmann functional $\omega_H(X) = \mathrm{Tr}_{\mathrm{spin}}(X e^{-H})$ is is called refection positive on $\mathfrak{A}_+$ if

$$0 \leqslant \omega_H(\Theta(X)X) = \mathrm{Tr}_{\mathrm{spin}}(\Theta(X)X\, e^{-H}) . \tag{V.11}$$

If the partition sum $Z_H = \mathrm{Tr}_{\mathrm{spin}}(e^{-H})$ is nonzero, then the Gibbs functional is defined by $\rho_H(X) := Z_H^{-1}\omega_H(X)$. Reflection positivity of ρ_H is equivalent to

$$0 \leqslant \rho_H(\Theta(X)X) = Z_H^{-1}\mathrm{Tr}_{\mathrm{spin}}(\Theta(X)X\, e^{-H}) . \tag{V.12}$$

From Theorem IV.2 for Majoranas, one derives the following characterization of reflection positivity for spin systems. It is given in terms of the matrix $J^{0\,AA'}_{\mathfrak{I}\mathfrak{I}'}$ of coupling constants across the reflection plane. This is the submatrix of the matrix $J^{AA'}_{\mathfrak{I}\mathfrak{I}'}$ of coupling constants (V.5) with $\mathfrak{I} \neq \varnothing$ and $\mathfrak{I}' \neq \varnothing$.

Theorem V.2 (**Reflection Positivity for Spins**). *Let $H \in \mathfrak{A}^{\mathrm{spin}}$ be a (not necessarily Hermitian) reflection invariant Hamiltonian.*

(a) *If the matrix $i^{k_{\mathfrak{I}}+k_{\mathfrak{I}'}} J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ is positive semidefinite, then the Bolzmann functional ω_H is reflection positive. If $Z_H \neq 0$, then $Z_H > 0$, and the Gibbs state ρ_H is reflection positive.*

(b) *If there exists an $\varepsilon > 0$ such that either $\omega_{\beta H}$ or $\rho_{\beta H}$ is reflection positive on $\mathfrak{A}_+^{\mathrm{spin}}$ for all $\beta \in [0, \varepsilon)$, then the matrix $i^{k_{\mathfrak{I}}+k_{\mathfrak{I}'}} J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ is positive semidefinite.*

Remark V.3. The requirement that H is reflection invariant is equivalent to Hermiticity of the matrix $i^{k_{\mathfrak{I}}+k'_{\mathfrak{I}}}J^{AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$. Furthermore, the requirement that $Z_H \neq 0$ is automatically fulfilled if H is Hermitian, which is the case in many applications.

Proof. It suffices to prove (a) and (b) for the Bolzmann functional ω_H. Statement (a) for the Gibbs functional ρ_H then follows from Remark IV.1. Following word by word the proof of Theorem IV.3.b, one obtains statement (b) for ρ_H from statement (b) for ω_H.

(a): Since $\Theta(c^a_{\vartheta(j)}c^4_{\vartheta(j)}) = c^a_j c^4_j$, the Hamiltonian $H^{\rm spin} \in \mathfrak{A}$ of equation V.4 with coefficients V.5 gives rise to the Hamiltonian

$$\widehat{H} = -\sum_{\substack{(\mathfrak{I},A)\\(\mathfrak{I}',A')}} J^{AA'}_{\mathfrak{I}\,\mathfrak{I}'}\, i^{k+k'}\,\Theta\Big(c^{a_1}_{\vartheta(i_1)}c^4_{\vartheta(i_1)}\ldots c^{a_k}_{\vartheta(i_k)}c^4_{\vartheta(i_k)}\Big)\; c^{a'_1}_{i'_1}c^4_{i'_1}\ldots c^{a'_k}_{i'_{k'}}c^4_{i'_{k'}}\,. \tag{V.13}$$

in the Majorana algebra $\mathfrak{A}$. Equation (V.13) can thus be written

$$\widehat{H} = -\sum_{\widehat{\mathfrak{I}},\widehat{\mathfrak{I}}'} J^{\rm M}_{\widehat{\mathfrak{I}}\,\widehat{\mathfrak{I}}'}\Theta(C_{\widehat{\mathfrak{I}}}) \circ C_{\widehat{\mathfrak{I}}'},$$

where $J^{\rm M}$ is the matrix of Majorana coupling constants. It equals

$$J^{\rm M}_{\widehat{\mathfrak{I}}\,\widehat{\mathfrak{I}}'} = i^{k_{\mathfrak{I}}+k_{\mathfrak{I}'}}J^{AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'} \tag{V.14}$$

for the indices

$$\begin{aligned} \widehat{\mathfrak{I}} &= ((i_1,a_1),(i_1,4),\ldots,(i_k,a_k),(i_k,4))\,, \\ \widehat{\mathfrak{I}}' &= ((i'_1,a'_1),(i'_1,4),\ldots,(i'_k,a'_{k'}),(i'_{k'},4)) \end{aligned} \tag{V.15}$$

and zero elsewhere. With respect to an appropriate choice of basis, the matrix $i^{k_{\mathfrak{I}}+k_{\mathfrak{I}'}}J^{AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ is the only nonzero block in $J^{\rm M}_{\widehat{\mathfrak{I}}\,\widehat{\mathfrak{I}}'}$. Therefore, the latter is positive semidefinite if and only if the former is. The same holds for the matrices $J^{M0}_{\widehat{\mathfrak{I}}\,\widehat{\mathfrak{I}}'}$ and $i^{k_{\mathfrak{I}}+k_{\mathfrak{I}'}}J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ of couplings across the reflection plane.

The Majorana Hamiltonian $\widehat{H}$ is globally gauge invariant since each spin involves two Majoranas, and it is reflection invariant as $\widehat{J}$ is Hermitian. Since $J^{M0}_{\widehat{\mathfrak{I}}\,\widehat{\mathfrak{I}}'}$ is positive semidefinite, Theorem IV.3 yields reflection positivity of $\widehat{H}$. This implies reflection positivity of H, since

$$\begin{aligned} \mathrm{Tr}_{\,\rm spin}(\Theta(X)Xe^{-H}) &= \mathrm{Tr}_{\,M}(\Theta(\widehat{X})\widehat{X}e^{-\widehat{H}}P^5) \\ &= \mathrm{Tr}_{\,M}(\Theta(\widehat{X}P^5_+)(\widehat{X}P^5_+)e^{-\widehat{H}}) \geqslant 0\,. \end{aligned}$$

Here, we used $\mathrm{Tr}_{\rm spin}(X) = \mathrm{Tr}_M(\widehat{X}P^5)$, equation (V.10), and the fact that P^5_+ and $\Theta(P^5_+) = P^5_-$ commute with the other factors, with $P^5 = P^5_-P^5_+$.

(b): This is analogous to the proof of Theorem IV.2.b. Choose $X \in \mathfrak{A}_+^{\rm spin}$ such that $\mathrm{Tr}_{\rm spin}(\Theta(X)X) = 0$. Expand X as

$$X = \sum_{(\mathfrak{I}',A')} x_{\mathfrak{I}'}^{A'} \Sigma_{(\mathfrak{I}',A')}\,,$$

with the coefficient $b_\varnothing$ of $\Sigma_\varnothing = I$ equal to zero. Using equation (V.3), one finds

$$\Theta(X) = \sum_{(\mathfrak{I},A)} (-1)^{k_\mathfrak{I}} \overline{x}_\mathfrak{I}^A \Sigma_{\vartheta(\mathfrak{I},A)}\,.$$

Since $\rho_{\beta H}(\Theta(X)X) = \mathrm{Tr}_{\rm spin}(\Theta(X)Xe^{-\beta H})$ is nonnegative and zero for $\beta = 0$, one finds

$$0 \leqslant \frac{d}{d\beta}\mathrm{Tr}_{\rm spin}(\Theta(X)Xe^{-\beta H})\Big|_{\beta=0} = -\mathrm{Tr}_{\rm spin}(\Theta(X)XH)\,. \qquad \text{(V.16)}$$

Using the expansion (V.6) and the orthogonality relations (V.2) of $\Sigma_{(\mathfrak{I},A)}$ with respect to the trace pairing, one thus obtains

$$0 \leqslant \sum_{\substack{(\mathfrak{I},A)\\(\mathfrak{I}',A')}} (-1)^{k_\mathfrak{I}} \overline{x}_\mathfrak{I}^A J_{\vartheta(\mathfrak{I})\mathfrak{I}'}^{AA'} x_{\mathfrak{I}'}^{A'}\,.$$

Since $x_\varnothing = 0$, only the coupling constants $J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ across the reflection plane contribute. Substituting $y_\mathfrak{I}^A := i^{k_\mathfrak{I}} x_\mathfrak{I}^A$ yields

$$0 \leqslant \sum_{\substack{(\mathfrak{I},A)\\(\mathfrak{I}',A')}} \overline{y}_\mathfrak{I}^A \left(i^{k_\mathfrak{I}+k_{\mathfrak{I}'}} J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}\right) y_{\mathfrak{I}'}^{A'}\,,$$

so that $i^{k_\mathfrak{I}+k_{\mathfrak{I}'}} J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ is positive semidefinite, as required. □

VI. Automorphisms that Yield New Reflections

In Sections IV and V, we have given a characterization of reflection positivity with respect to a standard reflection Θ. In this section, we show how these results extend to other reflections $\Theta' = \alpha^{-1}\Theta\alpha$, where α is an automorphism. The special case where α is a gauge transformation, can be very useful in applications.

VI.1. **Relation to Other Reflections.** We formulate this in the more general context of a $\mathbb{Z}_2$-graded algebra $\mathfrak{A}$ which is the super tensor product of two isomorphic subalgebras $\mathfrak{A}_+$ and $\mathfrak{A}_-$. This means that $\mathfrak{A}$ is $\mathfrak{A}_+ \otimes \mathfrak{A}_-$ as a vector space, with multiplication defined by

$$(A \otimes B)(A' \otimes B') = (-1)^{|A||B|} AA' \otimes BB'$$

on homogeneous elements. The twisted product $A \circ B$ is then defined as in Definition I.2. It reduces to the ordinary product on algebras that are purely even, such as the spin algebra $\mathfrak{A}^{\mathrm{spin}}$.

A reflection $\Theta \colon \mathfrak{A} \to \mathfrak{A}$ is an antilinear automorphism such that $\Theta(\mathfrak{A}_\pm) = \mathfrak{A}_\mp$ and $\Theta^2 = I$. Two different reflections Θ and Θ' are related by the linear automorphism $\beta := \Theta\Theta'$, which maps $\mathfrak{A}_\pm$ to $\mathfrak{A}_\pm$, and satisfies $\Theta\beta = \beta^{-1}\Theta$. Conversely, if Θ is a reflection and β satisfies $\beta(\mathfrak{A}_\pm) = \mathfrak{A}_\pm$ and $\Theta\beta = \beta^{-1}\Theta$, then $\Theta' := \Theta\beta$ is also a reflection.

Recall that a linear functional $\omega \colon \mathfrak{A} \to \mathbb{C}$ is reflection positive on $\mathfrak{A}_+$ with respect to Θ', if $0 \leqslant \omega(\Theta'(A) \circ A)$ for all $A \in \mathfrak{A}_+$. If Θ' is related to Θ by a square $\beta = \alpha^2$, then reflection positivity with respect to Θ and Θ' are related as follows.

Proposition VI.1. *Let α be a linear automorphism of $\mathfrak{A}$ such that $\alpha(\mathfrak{A}_\pm) = \mathfrak{A}_\pm$ and $\Theta\alpha = \alpha^{-1}\Theta$. Let*

$$\Theta' := \alpha^{-1}\Theta\alpha \, .$$

Then the pullback $\alpha^{-1*}\omega(A) := \omega(\alpha^{-1}(A))$ is reflection positive with respect to Θ on $\mathfrak{A}_+$, if and only if ω is reflection positive with respect to Θ' on $\mathfrak{A}_+$.

Proof. Since α is a linear automorphism, $\alpha(A_- \circ A_+) = \alpha(A_-) \circ \alpha(A_+)$ for $A_\pm \in \mathfrak{A}_\pm$. For $A \in \mathfrak{A}_+$, one has

$$\begin{aligned} \alpha^{-1*}\omega(\Theta(A) \circ A) &= \omega(\alpha^{-1}\Theta(A) \circ \alpha^{-1}(A)) \\ &= \omega(\Theta'(\alpha^{-1}(A)) \circ \alpha^{-1}(A))) \, . \end{aligned}$$

Thus the first term is positive for all $A \in \mathfrak{A}_+$, if and only if the last term is positive. □

We apply this to the algebras of Majoranas and spins, with the Gibbs functional $\rho_H(A) = Z_H^{-1} \operatorname{Tr}(Ae^{-H})$.

Corollary VI.2. *The Hamiltonian $H' := \alpha(H)$ is invariant under the reflection Θ if and only if H is invariant under $\Theta' := \alpha^{-1}\Theta\alpha$. The Gibbs functional ρ_H is reflection positive with respect to Θ' on $\mathfrak{A}_+$, if and only if $\rho_{H'}$ is reflection positive with respect to Θ on $\mathfrak{A}_+$.*

Proof. The first statement follows as $\Theta(\alpha(H)) = \alpha(H)$ is equivalent to $\alpha^{-1}\Theta\alpha(H) = H$. For the second statement, note that the normalized trace is unique on the algebras of Majoranas and spins. Thus $\alpha^* \operatorname{Tr} = \operatorname{Tr}$ for every automorphism α, and one has

$$\begin{aligned} \alpha^{-1*}\rho_H(A) &= Z_H^{-1} \operatorname{Tr}(\alpha^{-1}(A)e^{-H}) = Z_H^{-1} \operatorname{Tr}(\alpha(\alpha^{-1}(A)e^{-H})) \\ &= Z_H^{-1} \operatorname{Tr}(Ae^{-\alpha(H)}) = \rho_{\alpha(H)}(A) \, . \end{aligned}$$

□

Note that in the above, we do *not* require Θ, Θ' or α to respect the involution $*$ on the algebra $\mathfrak{A}$. If $\mathfrak{A}$ is either the spin algebra or the algebra of Majoranas, then the canonical reflection Θ preserves the involution. In this case, $\Theta' = \alpha^{-1}\Theta\alpha$ will preserve the involution if and only if α^2 does so.

VI.2. **Gauge Automorphisms.** In the context of a (super) tensor product $\mathfrak{A}$ of $\mathbb{Z}_2$-graded $*$-algebras $\mathfrak{A}_j$

$$\mathfrak{A} = \bigotimes_{j\in\Lambda} \mathfrak{A}_j,$$

we define the *gauge automorphism* α_τ, parameterized by a collection $\{\tau_j\}_{j\in\Lambda}$ of automorphisms of $\mathfrak{A}_j$, as

$$\alpha_\tau := \otimes_{j\in\Lambda}\tau_j \,.$$

If the $\mathfrak{A}_j$ can be canonically identified which each other, and all τ_j are the same, then α_τ is called a *global* gauge transformation.

Suppose that $\mathfrak{A}$ has a reflection Θ such that $\Theta(\mathfrak{A}_j)$ is isomorphic to $\mathfrak{A}_{\vartheta(j)}$. Then the gauge automorphism α_τ is called *reflection invariant* if $\tau_j = \Theta\tau^{-1}_{\vartheta(j)}\Theta$ for all $j \in \Lambda$. Every reflection invariant gauge automorphism satisfies

$$\alpha_\tau(\mathfrak{A}_\pm) = \mathfrak{A}_\pm \quad \text{and} \quad \alpha_\tau\Theta = \Theta\alpha_\tau^{-1}\,.$$

VI.2.1. *Majorana Algebras with 1 generator.* In the case of the Majorana algebra generated by c_j with $j \in \Lambda$, $\mathfrak{A}_j$ is the two-dimensional algebra generated by I and c_j, and the only two automorphisms are $\tau_j(c_j) = \pm c_j$. There is a unique nontrivial global gauge automorphism $c_j \mapsto -c_j$.

VI.2.2. *Majorana Algebras with 4 generators.* In the case of the algebra generated by Majoranas c_j^α with $j \in \Lambda$ and $\alpha \in \{1, 2, 3, 4\}$, the algebra $\mathfrak{A}_i$ is the Clifford algebra $\mathrm{Cl}(4,\mathbb{C})$ generated by the c_i^α with i fixed. The automorphisms τ_j can be taken to be conjugation by an invertible element $g_j \in \mathrm{Cl}(4,\mathbb{C})^\times$, that is, $\tau_j(A) = g_jAg_j^{-1}$. The spin group $\mathrm{Spin}(4)$ is the group of even elements $g \in \mathrm{Cl}(4,\mathbb{C})^\times$ such that $gc^\alpha g^{-1} = R^\alpha_\beta c^\beta$ for some $R \in \mathrm{SO}(4,\mathbb{R})$.

VI.2.3. *Spin Algebras.* In the next section the most relevant case will be the spin algebra $\mathfrak{A}^{\mathrm{spin}}$, where $\mathfrak{A}_i$ is the purely even algebra $M^2(\mathbb{C})$. If τ_i is conjugation by a matrix $g_i \in \mathrm{SL}(2,\mathbb{C})$, we denote the gauge automorphism corresponding to the collection $\{g_j\}_{j\in\Lambda}$ by α_g. The requirement $g_{\vartheta(j)} = \Theta g_j^{-1}\Theta$ translates to $g_{\vartheta(j)} = g_j^*$. It is an automorphism of $*$-algebras if and only if $g_i \in \mathrm{SU}(2,\mathbb{C})$ for every $i \in \Lambda_+$.

VII. Examples of Spin Models

We apply the characterization of reflection positivity in Theorem V.2 to a number of spin systems: the Ising model, the quantum rotator, and the anti-ferromagnetic Heisenberg model. Nearest neighbor couplings are treated in §VII.1, and long range interactions in §VII.2.

Many of these examples are well-understood, and we include those mainly to show that they have a natural interpretation within our general framework. Some relevant references are [DLS76, FILS78, DLS78, FL78, Bis09].

In this section, the lattice Λ has a geometric interpretation. It is a finite, fixed point free subset of a manifold $\mathcal{M}$ with involution $\vartheta_{\mathcal{M}}$, as explained in §I.1. An important example is $\mathcal{M} = \mathbb{R}^d$ with $\vartheta\colon \mathbb{R}^d \to \mathbb{R}^d$ the orthogonal reflection in a hyperplane Π. Periodic boundary conditions can be handled by taking $\mathcal{M} = \mathbb{T}^d$ the d-dimensional torus.

VII.1. **Nearest Neighbor Couplings.**

The nearest neighbor *Heisenberg model* is given in terms of the Pauli matrices σ_j^a on a lattice $j \in \Lambda$ by the Hamiltonian

$$-H = \sum_{a=1}^{3} \sum_{\langle jj' \rangle} J_{jj'}^a \sigma_j^a \sigma_{j'}^a + \sum_{a=1}^{3} \sum_{j} h_j^a \sigma_j^a \,. \tag{VII.1}$$

Here the sum is over the nearest neigbour pairs $\langle jj' \rangle$, and $J_{jj'}^a = J_{j'j}^a$. As H is Hermitian, the partition sum $Z_H = \mathrm{Tr}(e^{-\beta H})$ is nonzero.

In order to define nearest neighbor models, we assume that the lattice $\Lambda \subseteq \mathcal{M}$ has the property that "bonds are perpendicular to the reflection hyperplane". This means that two lattice points $j \in \Lambda_+$ and $j' \in \Lambda_-$ can only be nearest neighbors if $j' = \vartheta(j)$. (For example, this is the case in Fig. 1 and Fig. 2.)

Let $J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ denote the matrix of couplings across the reflection plane, defined in (V.4), (V.5). It is given by

$$J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'} = J^a_{\vartheta(j)j'}$$

for the indices $(\mathfrak{I}, A) = \{(j,a)\}$ and $(\mathfrak{I}', A') = \{(j',a)\}$ of equation (V.1), and zero in all other components. Here $j, j' \in \Lambda_+$ and $a \in \{1,2,3\}$. Note that $J^a_{\vartheta(j)j'}$ is only nonzero if $j = j'$, as sites $j' \in \Lambda_+$ and $\vartheta(j) \in \Lambda_-$ on different sides of the reflection plane can only be neighbors if $j = j'$.

VII.1.1. *Anti-Ferromagnetic Heisenberg Models.*

In order to show reflection positivity for the anti-ferromagnetic Heisenberg model, we restrict the coupling constants in (VII.1) as follows:

The full matrix of coupling constants is ϑ-symmetric, $J^a_{jj'} = J^a_{\vartheta(j)\vartheta(j')}$. The external field is antisymmetric, $h^a_{\vartheta(j)} = -h^a_j$, and couplings across the reflection plane are anti-ferromagnetic, $J_{\vartheta(j)j} \leqslant 0$.

Proposition VII.1 (Anti-ferromagnetic Heisenberg Model). *For the above restrictions on the coupling constants in the Hamiltonian H of (VII.1), the Gibbs state $\rho_{\beta H}$ is reflection positive with respect to the standard reflection $\Theta(\sigma^a_j) = -\sigma^a_{\vartheta(j)}$.*

Proof. Under the standard reflection Θ, the first term on the right side of (VII.1) is invariant if $J^a_{jj'} = J^a_{\vartheta(j)\vartheta(j')}$, while the second term is invariant if the external field satisfies $h^a_{\vartheta(j)} = -h^a_j$. By Theorem V.2, the Gibbs state $\rho_{\beta H}$ is reflection positive for all $\beta \geqslant 0$, if and only if the matrix $i^{k_{\mathfrak{I}}+k_{\mathfrak{I}'}} J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ is positive semidefinite. As $k_{\mathfrak{I}} = k_{\mathfrak{I}'} = 1$, this matrix is diagonal with entries entries $-J^a_{\vartheta(j)j}$, labelled by the $j \in \Lambda_+$ for which $\vartheta(j) \in \Lambda_-$. This matrix is positive definite if and only if $J^a_{\vartheta(j)j} \leqslant 0$. □

This includes the usual anti-ferromagnetic Heisenberg model, with constant couplings $J^1_{ij} = J^2_{ij} = J^3_{ij} = J \leqslant 0$, and vanishing external field $h^a_{ij} = 0$. The *quantum rotator model* is the special case $J^3_{ij} = 0$, and the *Ising model* is the special case $J^2_{ij} = J^3_{ij} = 0$. By the above proposition, they are reflection positive in the anti-ferromagnetic case of negative coupling constants with vanishing external field h^a_j.

VII.1.2. *Ferromagnetic Quantum Rotator Model.* The next example illustrates the gauge transformation method introduced in §VI. In order to show reflection positivity for the ferromagnetic quantum rotator model, we restrict the coupling constants in (VII.1) as follows:

We require $J^3_{jj'} = 0$ and $0 \leqslant J^a_{j'j}$ for $a = 1, 2$. (In fact, the proof only uses that the bonds $j' = \vartheta(j)$ across the reflection plane are ferromagnetic.) We assume that the couplings are symmetric around the reflection plane, $J^a_{jj'} = J^a_{\vartheta(j)\vartheta(j')} \leqslant 0$ for $a = 1, 2$. Finally, we require that the first two components of the external field are reflection symmetric, $h^a_{\vartheta(j)} = h^a_j$ for $a = 1, 2$, and that the third component is antisymmetric, $h^3_{\vartheta(j)} = -h^3_j$.

Proposition VII.2 (Ferromagnetic Quantum Rotator). *With the above restrictions on the coupling constants in the Hamiltonian H of (VII.1), the Gibbs state $\rho_{\beta H}$ is reflection positive with respect to the anti-linear reflection Θ' that satisfies*

$$\Theta'(\sigma^1_j) = \sigma^1_{\vartheta(j)}, \quad \Theta'(\sigma^2_j) = \sigma^2_{\vartheta(j)}, \quad \textit{and} \quad \Theta'(\sigma^3_j) = -\sigma^3_{\vartheta(j)}. \tag{VII.2}$$

Proof. We use the gauge transformation α_g of §VI.2.3, with $g_j = e^{i\frac{\pi}{4}\sigma_j^3}$ for $j \in \Lambda_+$ and $g_j = e^{-i\frac{\pi}{4}\sigma_j^3}$ for $j \in \Lambda_-$. This yields the clockwise rotation over $\pi/2$ around the third axis,

$$\alpha_g(\sigma_j^1) = -\sigma_j^2,\ \alpha_g(\sigma_j^2) = \sigma_j^1,\ \alpha_g(\sigma_j^3) = \sigma_j^3 \quad \text{for} \quad j \in \Lambda_+\,, \tag{VII.3}$$

and the counterclockwise rotation

$$\alpha_g(\sigma_j^1) = \sigma_j^2,\ \alpha_g(\sigma_j^2) = -\sigma_j^1,\ \alpha_g(\sigma_j^3) = \sigma_j^3 \quad \text{for} \quad j \in \Lambda_-\,. \tag{VII.4}$$

After the gauge transformation, the Hamiltonian H of (VII.1) becomes $H' = \alpha_g(H)$, which decomposes as $H' = H'_+ + H'_0 + H'_-$. Here

$$-H'_+ = \sum_{\langle jj'\rangle} J^1_{jj'}\sigma_j^2\sigma_{j'}^2 + \sum_{\langle jj'\rangle} J^2_{jj'}\sigma_j^1\sigma_{j'}^1 + \sum_j h_j^2\sigma_j^1 - h_j^1\sigma_j^2 + h_j^3\sigma_j^3,$$

with the sum over nearest neighbors $j, j' \in \Lambda_+$. Similarly,

$$-H'_- = \sum_{\langle jj'\rangle} J^1_{jj'}\sigma_j^2\sigma_{j'}^2 + \sum_{\langle jj'\rangle} J^2_{jj'}\sigma_j^1\sigma_{j'}^1 + \sum_j -h_j^2\sigma_j^1 + h_j^1\sigma_j^2 + h_j^3\sigma_j^3,$$

with the sum over nearest neighbors $j, j' \in \Lambda_-$. Finally,

$$-H'_0 = \sum_j -J^1_{\vartheta(j)j}\sigma^2_{\vartheta(j)}\sigma_j^2 + \sum_j -J^2_{\vartheta(j)j}\sigma^1_{\vartheta(j)}\sigma_j^1\,,$$

where $j \in \Lambda_+$ has $j' \in \Lambda_-$ as a nearest neigbor.

The Hamiltonian H' is invariant under the standard reflection defined by $\Theta(\sigma_j^a) = -\sigma^a_{\vartheta(j)}$, as long as $J^a_{\vartheta(j)\vartheta(j')} = J^a_{jj'}$ and $h^1_{\vartheta(j)} = h^1_j$, $h^2_{\vartheta(j)} = h^2_j$, and $h^3_{\vartheta(j)} = -h^3_j$. The matrix of coupling constants across the reflection plane is positive semidefinite if $0 \leqslant J^1_{\vartheta(j)j}$ and $0 \leqslant J^2_{\vartheta(j)j}$. From Theorem V.2, we see that under these conditions, the Gibbs state $\rho_{\beta H'}$ for the Hamiltonian H' is reflection positive with respect to Θ.

Applying Corollary VI.2, we infer that the Gibbs state $\rho_{\beta H}$ for the *original* Hamiltonian $H = \alpha^{-1}(H')$ is reflection positive for the gauge transformed reflection automorphism $\Theta' = \alpha^{-1}\Theta\alpha = \Theta\alpha^2$, given in equation (VII.2). □

VII.2. **Long-Range Interactions of Spin Pairs.** The Heisenberg model with long-range interactions is defined by the Hamiltonian

$$-\,H = \sum_{a=1}^{3} \sum_{\{x,x'\in\Lambda\,:\,x\neq x'\}} J^a\,\sigma^a_{x'}\sigma^a_x f(x-x')\,. \tag{VII.5}$$

Here f can be any reflection invariant, reflection positive function on $\mathbb{R}^d$, or on its compactification $\mathbb{T}^m\times\mathbb{R}^{d-m}$ in $m \leqslant d$ directions. For such functions the matrix $f(\vartheta(x)-x')$ for $x, x' \in \Lambda_+$ is positive semidefinite.

Here there is extensive analysis, and some relevant papers are [OS73, OS74, LM75, GJ79, FL10].

An important example is $f(x) = \|x\|^{-s}$ on $\mathbb{R}^d$, which is reflection positive for $s \geqslant \max\{0, d-2\}$ by [NÓ14, Proposition 6.1]. Reflection positive functions on the compactification can be obtained from reflection positive functions on $\mathbb{R}^d$ under suitable conditions on the rapidity of their decay, see for example [JJM14, Proposition 15].

For long-range interactions, the matrix of coupling constants across the reflection plane will not be diagonal, as was the case for nearest neighbor models.

VII.2.1. *Anti-Ferromagnetic Heisenberg Model.* For $J^a \leqslant 0$ (the anti-ferromagnetic case), we can use the standard reflection $\Theta(\sigma_j^a) = -\sigma_j^a$.

Proposition VII.3 (Long-Range Heisenberg Model)**.** *The Gibbs functional $\rho_{\beta H}$ for the Hamiltonian (VII.5) is reflection positive with respect to Θ for all $\beta \geqslant 0$, if and only if $J^a \leqslant 0$ for $a = 1, 2, 3$.*

Proof. The Hamiltonian (VII.5) is hermitian and Θ-invariant, so by Theorem V.2, it is reflection positive for all $\beta \geqslant 0$ if and only if the matrix $i^{k_{\mathfrak{I}}+k_{\mathfrak{I}'}} J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ is positive semidefinite.

The matrix of coupling constants across the reflection plane has entries

$$J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'} = J^a f(\vartheta(x) - x')$$

for the indices $(\mathfrak{I}, A) = \{(x, a)\}$ and $(\mathfrak{I}', A') = \{(x', a)\}$ of equation (V.1), and all other entries are zero. Since $k_{\mathfrak{I}} = k_{\mathfrak{I}'} = 1$, one finds

$$i^{k_{\mathfrak{I}}+k_{\mathfrak{I}'}} J^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'} = -J^a f(\vartheta(x) - x')\,.$$

As f is reflection positive, this matrix is positive semidefinite if and only if $J^a \leqslant 0$ for $a = 1, 2, 3$. $\square$

VII.2.2. *Ferromagnetic Rotator Model.* The long-range rotator model is given by the Hamiltonian (VII.5) with $J^3 = 0$.

In the anti-ferromagnetic case $J^{1,2} \leqslant 0$, Proposition VII.3 shows that it is reflection positive with respect to the standard reflection Θ, satisfying $\Theta(\sigma_j^a) = -\sigma_{\vartheta(j)}^a$ for $a = 1, 2, 3$. As in the nearest neighbor case, the ferromagnetic model $0 \leqslant J^{1,2}$ is reflection positive for a *different* reflection Θ', satisfying (VII.2).

Proposition VII.4 (Long-Range Quantum Rotator). *The Gibbs state $\rho_{\beta H}$ for the Hamiltonian (VII.5) is reflection positive with respect to the anti-linear reflection Θ' for all $\beta \geqslant 0$, if and only if $0 \leqslant J^a$ for $a = 1, 2$.*

Proof. By Corollary VI.2, $\rho_{\beta H}$ is reflection positive for $\Theta' = \alpha^{-1}\Theta\alpha$, if and only if $\rho_{\beta H'}$ is reflection positive for Θ. Here $H' = \alpha(H)$, and we choose $\alpha = \alpha_g$ to be the gauge transformation of equations (VII.3) and (VII.4).

The gauge transformed Hamiltonian H' has the form $H' = H'_+ + H'_0 + H'_-$, where the term H'_0 containing the couplings across the reflection plane is

$$-H'_0 = \sum_{x,x'\in\Lambda_+} -\left(J^1 f(\vartheta(x)-x')\sigma^2_{\vartheta(x)}\sigma^2_{x'} + J^2 f(\vartheta(x)-x')\sigma^1_{\vartheta(x)}\sigma^1_{x'}\right)\,.$$

It follows that the matrix of couplings across the reflection plane for the gauge transformed Hamiltonian H' is

$$J'^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'} = -J^{\widehat{a}} f(\vartheta(x)-x')\,,$$

for $(\mathfrak{I}, A) = \{(x,a)\}$ and $(\mathfrak{I}, A) = \{(x',a)\}$. Here $\widehat{a} = 1$ if $a = 2$ and vice versa. Since $k_{\mathfrak{I}} = k_{\mathfrak{I}'} = 1$, the matrix $i^{k_{\mathfrak{I}}+k_{\mathfrak{I}'}} J'^{0\,AA'}_{\vartheta(\mathfrak{I})\mathfrak{I}'}$ is positive semidefinite in the ferromagnetic case $0 \leqslant J^a$.

In order to apply Theorem V.2 to H', we still need to check that H' is reflection invariant under the standard reflection Θ. By Corollary VI.2, this is equivalent to reflection invariance of the original Hamiltonian H under Θ'. This is readily seen to be the case by using the explicit equation (VII.2) for Θ'.

As α_g ia a $*$-automorphism, H' is hermitian, so $Z_{\beta H'} \geqslant 0$. One then infers from Theorem V.2, that $\rho_{\beta H'}$ is reflection positive with respect to Θ. As mentioned in the start of the proof, Corollary VI.2 then yields that $\rho_{\beta H}$ is reflection positive for Θ'. $\square$

Remark VII.5. An external field $\sum_{a=1}^{3}\sum_j h^a_j\sigma^a_j$ can be added to (VII.5) under the same conditions as in the nearest neighbor case. For the anti-ferromagnetic Heisenberg model, $h^a_{\vartheta(j)} = -h^a_j$ for $a = 1,2,3$. For the ferromagnetic quantum rotator, $h^a_{\vartheta(j)} = h^a_j$ for $a = 1,2$, and $h^a_{\vartheta(j)} = -h^a_j$ for $a = 3$.

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