An Introduction to Quantum Spin Systems[1]

Notes for MA5020 (John von Neumann Guest Lectures)

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Contents

1. Introduction

Non-relativistic quantum mechanics describes atoms, molecules, and both small and large systems composed of atoms and molecules. Its validity is well-established in a range of conditions that includes room temperature and atmospheric pressure as well as near-zero temperatures and low densities. The traditional way in which quantum spin systems arise is by a reduction of the Hilbert space of states for each atom or molecule to a finite-dimensional subspace. Such a reduction can often be justified on physical grounds. Other ways in which quantum spin models arises is as a truncation of a lattice quantum field theory for the purpose of numerical simulation. More abstractly, quantum spin systems describe collections of qubits in quantum information theory. Finally, quantum spin systems are also used as toy models in some theories of quantum gravity.

While there certainly are situations where a quantum spin system description would be inadequate, for example in conditions where relativistic effects are important, it is fair to say that almost all interesting features of quantum many-body physics are found in quantum spin models. These include the complex dynamics due to interactions between the components (be it particles or spins), the possibility of phase transitions, the important role played by symmetries and spontaneous symmetry breaking, the unique behavior typical of quantum phases of matter such as Bose-Einstein condensation and superfluidity, superconductivity, the integer and fractional quantum Hall effects, topological order, exotic quasi-particles called anyons etc. Quantum spin models provide the simplest framework in which all these phenomena can be studied in detail. It is also the setting that has proved to be most amenable to rigorous mathematical analysis. In fact, research on quantum spin systems has led to significant new development in functional analysis (e.g., the theory of operator algebras) and representation theory (e.g., quantum groups).

We have two goals in these lectures. The first is to provide a basic introduction to the mathematical framework for the rigorous study of quantum spin models and to introduce the most important models. The second goal is to discuss in sufficient detail some of the most important directions of research on quantum spin models today so that the course provides a foundation for graduate level research in quantum spin systems.

2. Quantum Spin Systems

2.1. **Spins and Qudits.** In these lectures, by *spin* we will be referring to any quantum system with a finite-dimensional, complex Hilbert space of states, i.e. $\mathbb{C}^d$. This could be the space of physical spin states of a particle, atom, or molecule. For example, electrons are spin $1/2$ particles, meaning that in addition to its translational degrees of freedom, an electron also has a spin state described by a vector in $\mathbb{C}^2$. In other examples this finite-dimensional Hilbert space may be a subspace of an infinite dimensional Hilbert space, spanned by the most relevant states for the problem at hand. The finite-dimensional approximation may provide a convenient, more tractable description of the systems of interest, perhaps corresponding to finitely many orbitals in a molecule, or may be introduced for the purpose of simulating the system on a computer. The basic unit of quantum information, the *qubit*, has a two-dimensional state space. The d-dimensional generalization of a qubit is called a *qudit*.

We will commonly denote by $\mathcal{H}$ the complex Hilbert space of states of a quantum system, by $\langle \cdot, \cdot \rangle$ the inner-product, a sequilinear form, which is linear in its second argument and anti-linear in the first, following the convention standard in the physics literature. The norm induced by this inner-product is denoted by $\| \cdot \|$.

Unless stated otherwise, we use the standard inner product on $\mathcal{H} = \mathbb{C}^d$, given by

$$\langle u, v \rangle = \sum_{i=1}^{d} \overline{u_i} v_i. \tag{2.1}$$

To emphasize the relation with physical spin, one often writes the dimension d as $d = 2S + 1$ for half-integer values of the spin $S = 0, 1/2, 1, 3/2 \ldots$. The smallest non-trivial dimension, $d = 2$, corresponds to *spin 1/2*, $S = 1/2$. Common notations for a choice of orthonormal basis in $\mathbb{C}^2$ are $\{|0\rangle, |1\rangle\}$, $\{|+\rangle, |-\rangle\}$, and $\{|+1/2\rangle, |-1/2\rangle\}$.

2.2. **Observables.** The *algebra of observables* of a quantum system with Hilbert space $\mathcal{H}$ is the set of all bounded linear operators on $\mathcal{H}$, denoted by $\mathcal{B}(\mathcal{H})$. In the physics literature, the term *observables* usually refers to the self-adjoint elements of $\mathcal{B}(\mathcal{H})$. Since the algebra structure of $\mathcal{B}(\mathcal{H})$ will be useful, we will refer to $\mathcal{B}(\mathcal{H})$ as the algebra of observables and single out the self-adjoint observables when necessary. The default notation for the algebra of observables will be $\mathcal{A}$.

For a qudit we have $\mathcal{H} = \mathbb{C}^d$ and, hence, $\mathcal{A} = \mathcal{B}(\mathcal{H}) = M_d(\mathbb{C})$, the set of $d \times d$ matrices with entries in $\mathbb{C}$, which we will also write as M_d. Self-adjoint observables $A \in \mathcal{A}$, *i.e.* , A such that $A^* = A$, have *real spectrum*. In this case, the spectral values, $\mathrm{spec}(A) \subset \mathbb{R}$, correspond to measurable values that can be the outcome of a physical experiment.

Let us consider the case of $d = 2$. In this case, the Hilbert space is $\mathcal{H} = \mathbb{C}^2$, and the set of observables is $\mathcal{A} = M_2$. It is convenient to have a basis for the set of observables. One such choice are the identity matrix and the three *Pauli matrices*:

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.2}$$

In general, the observables $\mathcal{A} = M_d$ can be equipped with an inner-product

$$\langle A, B \rangle_{\mathrm{HS}} = \mathrm{Tr}(A^* B) \quad \text{for all } A, B \in \mathcal{A}, \tag{2.3}$$

where Tr denotes the trace. This inner product is often called the *Hilbert-Schmidt* inner product. With respect to $\frac{1}{2}\langle \cdot, \cdot \rangle_{\mathrm{HS}}$, the spin matrices (2.2) are orthonormal. The associated norm is the Hilbert-Schmidt norm. Note, however, that standard norm on observables is the operator norm on $\mathcal{B}(\mathcal{H})$, defined by

$$\|A\| = \sup_{\psi \neq 0} \frac{\|A\psi\|}{\|\psi\|}. \tag{2.4}$$

2.3. **States.** A *state* of a quantum system with algebra of observables $\mathcal{A}$, which for now is given by $\mathcal{B}(\mathcal{H})$ for some Hilbert space $\mathcal{H}$, is a *normalized, positive linear functional* on $\mathcal{A}$. This means ω is a state if it is a linear map $\omega : \mathcal{A} \to \mathbb{C}$ that satisfies

$$\omega(A^* A) \geq 0, \text{ for all } A \in \mathcal{A}, \text{ and } \omega(\mathbb{1}) = 1. \tag{2.5}$$

For $A \in \mathcal{A}$, $\omega(A)$ is the *expected value* or *expectation* of the observable A in the state ω. The expectation of self-adjoint observables is real and, in general, we have $\omega(A^*) = \overline{\omega(A)}$. The variance of A, $\mathrm{Var}(A)$, is given by the familiar formula:

$$\mathrm{Var}(A) = \omega((A - \omega(A)\mathbb{1})^*(A - \omega(A)\mathbb{1})) = \omega(A^* A) - |\omega(A)|^2. \tag{2.6}$$

For any unit vector $\psi \in \mathcal{H}$, one can define a state ω_ψ on $\mathcal{B}(\mathcal{H})$ by

$$\omega_\psi(A) = \langle \psi, A\psi \rangle \quad \text{for all } A \in \mathcal{A}. \tag{2.7}$$

States of this form are called *vector states*. An alternative expression for ω_ψ is

$$\omega_\psi = \mathrm{Tr} P_\psi A, \tag{2.8}$$

where P_ψ denotes the orthogonal projection defined by

$$P_\psi(\phi) = \langle \psi, \phi \rangle \psi, \quad \phi \in \mathcal{H}. \tag{2.9}$$

It follows from the definition of state given above that the set of states on $\mathcal{A}$ is convex. The extreme points of this convex set are called the *pure states*. In the finite-dimensional case, *i.e.* $\mathcal{A} = M_d$, the pure states are precisely the vector states and all states are finite convex combinations

of vector states, *i.e.* , for any state ω, there are $t_1, \ldots, t_n \geq 0$ and unit vectors $\psi_1 \ldots, \psi_n \in \mathcal{H}$, such that

$$\omega = \sum_{i=1}^{n} t_i \omega_{\psi_i}. \tag{2.10}$$

It follows that there is a non-negative matrix $\rho \in M_d$ such that

$$\omega(A) = \mathrm{Tr}(\rho A), \quad \text{for all } A \in M_d, \tag{2.11}$$

with

$$\rho = \sum_{i=1}^{n} t_i P_{\psi_i}. \tag{2.12}$$

Matrices ρ of the form (2.12) are non-negative and, since the t_i are the coefficients in a convex combination, $\mathrm{Tr}\rho = \sum_{i=1}^{n} t_i = 1$. Non-negative matrices of unit trace are called *density matrices*.

As an example, we now describe the set of density matrices in the case $\mathcal{A} = M_2$. $\rho \in M_2$ is a density matrix if and only if

$$\rho = \begin{pmatrix} r & \mu \\ \overline{\mu} & 1-r \end{pmatrix} \tag{2.13}$$

for some $r \in [0,1]$ and $\mu \in \mathbb{C}$ satisfying

$$|\mu|^2 \leq r(1-r) \tag{2.14}$$

Another useful parametrization of the 2×2 density matrices is obtained by expanding then in the orthornormal basis with respect the the Hilbert-Schmidt inner product given by the Pauli matrices and the identity, i.e. (2.2):

$$\rho = \frac{1}{2}\left(\mathbb{1} + \vec{x} \cdot \vec{\sigma}\right) \tag{2.15}$$

where $\vec{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ with $|\vec{x}| \leq 1$ and we have denoted by

$$\vec{x} \cdot \vec{\sigma} = x_1 \sigma^1 + x_2 \sigma^2 + x_3 \sigma^3 \tag{2.16}$$

This provides a bijection between the set of all density matrices in M_2 and the unit ball in $\mathbb{R}^3$. The extreme points of the unit ball correspond to the pure states, and are in one-to-one correspondence with the unit vectors $\vec{x} \in \mathbb{R}^3 : \|\vec{x}\| = 1$. This set is often referred to as the *Bloch sphere*.

2.4. **Dirac notation.** The *Dirac bra- and ket notation* is very commonly used in quantum mechanics and quantum information theory. It is popular because it provides a convenient way to present the most frequently encountered operations in Hilbert space. Here, we only give a brief account of the Dirac notation in the case of finite-dimensional Hilbert spaces. Many aspects generalize without significant change to the case of infinite-dimensional spaces. We do not consider here the more liberal usage of the Dirac notation encountered in many physics texts, where it is extended beyond the Hilbert space context into distribution theory.

Let $\mathcal{H}$ be a finite-dimensional Hilbert space. With each $\phi \in \mathcal{H}$ we can associate two linear maps, which we denote by $|\phi\rangle$ and $\langle\phi|$.:

$$|\phi\rangle : \mathbb{C} \to \mathcal{H}, z \mapsto z\phi, \quad \langle\phi| : \mathcal{H} \to \mathbb{C} : \psi \mapsto \langle\phi, \psi\rangle. \tag{2.17}$$

In fact, since the linear maps define above depend linearly and anti-linearly on ϕ, we can consider $|\ \rangle$, pronounced *ket*, and $\langle\ |$, pronounced *bra*, as linear and antilinear maps themselves:

$$|\ \rangle : \mathcal{H} \to \mathcal{L}(\mathbb{C}, \mathcal{H}), \phi \mapsto |\phi\rangle, \quad \langle\ | : \mathcal{H} \to \mathcal{L}(\mathcal{H}, \mathbb{C}), \phi \mapsto \langle\phi|. \tag{2.18}$$

$\langle\ |$ is the antilinear map identifying $\mathcal{H}$ with its dual space $\mathcal{H}^*$, as guaranteed by the Riesz Representation Theorem. Since $\mathcal{H} \cong \mathbb{C}^d$, with $d = \dim(\mathcal{H})$, we can identify $|\phi\rangle$ with column vector of length

d, and $\langle\phi|$ with a row vector of length d, and consider these vectors as the matrix representation of the linear maps defined in (2.17).

For any pair $\phi_1, \phi_2 \in \mathcal{H}$, we can define a rank-one linear map $\mathcal{H} \to \mathcal{H}$ by

$$\psi \mapsto \langle\phi_2, \psi\rangle\phi_1. \tag{2.19}$$

It is easy to see that this rank-one map is the composition of a $|\phi_1\rangle$ and $\langle\phi_2|$, which justifies the following elegant notation for it:

$$|\phi_1\rangle\langle\phi_2|(\psi) = |\phi_1\rangle(\langle\phi_2, \psi\rangle) = \langle\phi_2, \psi\rangle\phi_1. \tag{2.20}$$

It is now convenient to use the notation ψ and $|\psi\rangle$ for vectors interchangeably, and to use an alternate notation for the inner product as well:

$$\langle\phi, \psi\rangle = \langle\phi \mid \psi\rangle = \langle\phi||\psi\rangle. \tag{2.21}$$

Labeled sets of vectors, such as, *e.g.* , an orthonormal basis $\{e_1, \ldots, e_d\}$, can be written in Dirac notation using just the labels if this does not lead to confusion: $\{|1\rangle, \ldots, |d\rangle\}$.

Using the Dirac notation, orthonormality and completeness of the basis we can expressed by the following two equations:

$$\langle i \mid j\rangle = \delta_{i,j}, \quad \sum_{i=1}^{d} |i\rangle\langle i| = \mathbb{1}. \tag{2.22}$$

2.5. **Finite Quantum Spin Systems.** The observables of the quantum systems we have considered so far are given by the elements of $\mathcal{B}(\mathcal{H})$, the bounded linear operators on a complex Hilbert space. For a finite quantum spin system, $\mathcal{H}$ is finite-dimensional and the algebra of observables is the algebra of $d\times d$ matrices with complex entries, M_d, where d is the dimension of the Hilbert space. More generally, one can consider quantum systems with an infinite-dimensional complex Hilbert space. The algebra of observables will then consist of elements of $\mathcal{B}(\mathcal{H})$, the bounded linear operators on $\mathcal{H}$. $\mathcal{B}(\mathcal{H})$ is complete with respect to the metric topology derived from the operator norm defined in (2.4). It is straightforward to check that the operator norm satisfies $\|AB\| \leq \|A\|\|B\|$, for all $A, B \in \mathcal{B}(\mathcal{H})$, which in particular implies that the product of observables is continuous in the norm topology. The completeness and the continuity of the product make $\mathcal{B}(\mathcal{H})$ into a Banach algebra.

The operation of taking the adjoint of an operator A, denoted by A^*, is an anti-linear involution, meaning $(A^*)^* = A$, $(A+B)^* = A^* + B^*$, and $(zA)^* = \overline{z}A^*$, for all $A, B \in \mathcal{B}(\mathcal{H})$ and $z \in \mathbb{C}$, and is an algebra anti-morphism: $(AB)^* = B^*A^*$. One readily checks that $\|A^*\|$ and $\|A^*A\| = \|A\|^2$.

M_d and, more generally, $\mathcal{B}(\mathcal{H})$ are examples of C^*-algebras, which we introduce in the next section.

2.5.1. *C^*-algebras.* A C^*-algebra is a Banach algebra equipped with an involution, denoted by $*$, satisfying some special properties.

Definition 2.1. Let $\mathcal{A}$ be an associative algebra over $\mathbb{C}$ that is equipped with a norm $\|\cdot\|$. If $\mathcal{A}$ is complete with respect to this norm and

$$\|AB\| \leq \|A\|\|B\| \quad \text{for all } A, B \in \mathcal{A}, \tag{2.23}$$

then $\mathcal{A}$ is called a Banach algebra. A Banach algebra $\mathcal{A}$ is called unital if it has an identity element, which we denote by $\mathbb{1} \in \mathcal{A}$.

In this book the term *algebra*, unless explicitly stated otherwise, will always refer to an associative algebra over the complex numbers with a unit, which will routinely be denoted by $\mathbb{1}$. We will also assume that the algebra we consider are non-trivial, *i.e.* ., are not equal to $\{0\}$.

Definition 2.2. A C^*-algebra $\mathcal{A}$ is a Banach algebra with an anti-linear involution, which we will denote by $*$, satisfying the following properties:
i) $(AB)^* = B^*A^*$ for all $A, B \in \mathcal{A}$
ii) $\|A^*\| = \|A\|$ for all $A \in \mathcal{A}$ (This implies that the $*$ operation w.r.t. the norm $\|\cdot\|$.)
iii) $\|A^*A\| = \|A\|^2$ for all $A \in \mathcal{A}$. (This is called the C^*-property.)

If the C^*-algebra $\mathcal{A}$ has a unit, denoted by $\mathbb{1}$, it is called unital. It follows from the properties stated the unit is unique, that $\mathbb{1}^* = \mathbb{1}$ and, if $\mathcal{A} \neq \{0\}$, that $\|\mathbb{1}\| = 1$.

If $\mathcal{A}$ and $\mathcal{B}$ are two C^*-algebras, a *$*$-morphism* (often simply called a morphism) $\pi : \mathcal{A} \to \mathcal{B}$ is an algebra morphism that preserves the involution, i.e., $\pi(A^*) = \pi(A)^*$ for all $A \in \mathcal{A}$. A morphism $\pi : \mathcal{A} \to \mathcal{B}$ is called *unit preserving* if $\pi(\mathbb{1}_{\mathcal{A}}) = \mathbb{1}_{\mathcal{B}}$.

A *representation* of a C^*-algebra $\mathcal{A}$ on a Hilbert space $\mathcal{H}$ is a unit preserving morphism $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$. A representation π is called *faithful*, if $\ker \pi = \{0\}$, *i.e.* , if it is a $*$-isomorphism between $\mathcal{A}$ and $\pi(\mathcal{A})$. A morphism $\pi : \mathcal{A} \to \mathcal{A}$ is called an *automorphism* if π is invertible.

A *state* ω on $\mathcal{A}$ is a linear mapping $\omega : \mathcal{A} \to \mathbb{C}$ that is non-negative and normalized, i.e. $\omega(A^*A) \geq 0$, for all $A \in \mathcal{A}$, and $\omega(\mathbb{1}) = 1$.

In the finite dimensional case, i.e. $\mathcal{A} = M_d$, we already discussed that states are in one-to-one correspondence with density matrices. If $\mathcal{H}$ is infinite-dimensional, density matrices ρ, defined as positive operators of trace-class such that $\mathrm{Tr}\rho = 1$, also define states on $\mathcal{B}(\mathcal{H})$, by the formula $\omega(A) = \mathrm{Tr}\rho A$, but there are states on $\mathcal{B}(\mathcal{H})$ that are not of this form.

Let $\mathcal{A}$ be a C^*-algebra. $A \in \mathcal{A}$ is called *self-adjoint* if $A^* = A$. The set of all self-adjoint elements in $\mathcal{A}$ will be denoted by $\mathcal{A}_{\mathrm{sa}}$. $A \in \mathcal{A}$ is said to be *positive*, denoted by $A \geq 0$, if there exists $B \in A$

such that $A = B^*B$. This notion of positivity allows one to define a partial order on $\mathcal{A}_{\rm sa}$, i.e. for any $A, B \in \mathcal{A}_{\rm sa}$, we write $A \geq B$ if and only if $A - B \geq 0$.

For the derivation of the following important properties see Appendix A, or consult a text on operator algebras such as [10], [71], or [37].

i) For any $A, B \in \mathcal{A}_{\rm sa}$,

$$A \geq B \quad \Rightarrow \quad C^*AC \geq C^*BC \quad \text{for all } C \in \mathcal{A}. \tag{2.24}$$

ii) For any $A \geq 0$, $A \leq \|A\|\mathbb{1}$, and as a consequence, for any state ω, we have that

$$\|\omega\| = \sup_{A \neq 0} \frac{|\omega(A)|}{\|A\|} = \omega(\mathbb{1}) = 1. \tag{2.25}$$

iii) Similarly, for a morphism π, we also have that

$$\|\pi\| = \|\pi(\mathbb{1})\| = 1 \quad \text{if } \pi \neq 0. \tag{2.26}$$

iv) Let $\mathcal{A}$ be a C^*-algebra and ω be a state on $\mathcal{A}$. The mapping from $\mathcal{A} \times \mathcal{A}$ to $\mathbb{C}$ given by

$$(A, B) \mapsto \omega(A^*B) \tag{2.27}$$

is a sesquilinear form. As a consequence, we have a Cauchy-Schwartz inequality:

$$|\omega(A^*B)|^2 \leq \omega(A^*A)\omega(B^*B) \quad \text{for all } A, B \in \mathcal{A}\,. \tag{2.28}$$

v) Let $\mathcal{A}$ be a C^*-algebra and ω be a state on $\mathcal{A}$. The bound

$$|\omega(A^*BA)| \leq \omega(A^*A)\|B\| \tag{2.29}$$

holds for all $A, B \in \mathcal{A}$. As a consequence, for all $A \in \mathcal{A}$ with $\omega(A^*A) \neq 0$,

$$\omega_A(B) := \frac{\omega(A^*BA)}{\omega(A^*A)} \quad \text{for all } B \in \mathcal{A} \tag{2.30}$$

defines a state ω_A on $\mathcal{A}$. This is the quantum analogue of starting with a measure, e.g. dx on $[0, 1]$, considering a non-negative function μ with $\int_0^1 \mu(x)dx < \infty$, and defining a new, normalized measure via

$$\frac{\mu(x)}{\int_0^1 \mu(x)dx}dx \tag{2.31}$$

2.5.2. *Composite systems.* Any two quantum systems described by Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ can be considered as one, composite system. The Hilbert space of the composite system is given by the tensor product of $\mathcal{H}_1$ and $\mathcal{H}_2$. The simplest way to describe the tensor product of two finite-dimensional Hilbert spaces, say with dimensions n and m and inner product $\langle\cdot,\cdot\rangle_1$ and $\langle\cdot,\cdot\rangle_2$, respectively, is as the span of an orthonormal basis of simple tensors defined as follows. Let $e_1, \ldots, e_n$ and $f_1, \ldots, f_m$ be orthonormal bases for $\mathcal{H}_1$ and $\mathcal{H}_2$, then $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ is defined as the linear span of nm orthonormal vectors denoted $e_i \otimes f_j$, $1 \leq i \leq n, 1 \leq j \leq m$. The tensor notation is extended by linearity to identify $\phi_1 \otimes \phi_2 \in \mathcal{H}_1 \otimes \mathcal{H}_2$, for any $\phi_1 \in \mathcal{H}_1, \phi_2 \in \mathcal{H}_2$. Such vectors are called *simple tensors*. From the orthonormality of the basis it then follows that the the inner product is uniquely determined by the following formula for simple tensors:

$$\langle \phi_1 \otimes \phi_2, \psi_1 \otimes \psi_2 \rangle = \langle \phi_1, \psi_1 \rangle_1 \langle \phi_2, \psi_2 \rangle_2 \tag{2.32}$$

There are several ways to define the tensor product for infinite-dimensional, Hilbert spaces H_1 and H_2, all of which lead to a Hilbert space $\mathcal{H}$ with the following properties: (i) there is a bilinear bijection of $\mathcal{H}_1 \times \mathcal{H}_2$ into a subset of $\mathcal{H}$ (the set of simple tensors), (ii) the inner product of simple tensors factorizes as in (2.32), and (iii) the linear span of the simple tensors is dense in $\mathcal{H}$, which is unique up to unitary equivalence. See, e.g., [8, 65], for the details of a construction of the tensor product of two arbitrary Hilbert spaces. It is straightforward to extend the notion of tensor product from two to any finite number of Hilbert spaces.

The combination of two (or more) spins, meaning, considering a physical context in which both exist, is described as a composite systems using the tensor product of the Hilbert spaces of the individual systems.

Let us start by considering two spins, with Hilbert spaces of dimension d_1 and d_2. The Hilbert space for the composite system is then:

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \cong \mathbb{C}^{d_1 d_2} \tag{2.33}$$

Such a system is often referred to as *bipartite*. The algebra of observables is again given by $\mathcal{B}(\mathcal{H})$, and it can also be obtained as a tensor product since

$$M_{d_1 d_2} \cong M_{d_1} \otimes M_{d_2}, \tag{2.34}$$

where $M_{d_1} \otimes M_{d_2}$ is the linear span of the tensor products of two matrices $A = (a_{i,j}) \in M_{d_1}$, and $B = (b_{k,l}) \in M_{d_2}$, defined by

$$A \otimes B = (c_{i,k;j,l}), \text{ with } c_{i,k;j,l} = a_{i,j} b_{k,l}. \tag{2.35}$$

Systems 1 and 2 are called subsystems of the composite system. One can identify their algebra of observables with subalgebras of $M_{d_1 d_2}$. E.g., $M_{d_1} \cong M_{d_1} \otimes \mathbb{1}_2 \subset M_{d_1} \otimes M_{d_2}$.

One way to appreciate the uniquely quantum (versus classical) behavior of states is to consider marginals of pure states. Pure states of a classical bipartite system with a finite state space $\Omega = \Omega_1 \times \Omega_2$, are given by Dirac measures concentrated in a point $(\xi_1, \xi_2) \in \Omega$. The marginals of classical pure states are then Dirac measures in the points $\xi_i \in \Omega_i$, which are also pure. In contrast, what distinguishes quantum from classical structure states (quantum probability versus classical probability) can be seen as exactly the property that *any* state of system 1 is the marginal of a pure state on for composite system containing system 1 as a tensor factor [15].

The marginals of a pure state for a bipartite quantum system given by a unit vector $\psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$, are pure iff the pure state is separable, *i.e.* , ψ is a simple tensor [66]. The marginals of the Bell states coincide with the maximally mixed state described by the density matrix $\frac{1}{2}\mathbb{1}_2$ (see the Example below).

Considering the marginals of a state of a bipartite system is simply considering its restrictions from $\mathcal{A}_1 \otimes \mathcal{A}_2$ to the subalgebras $\mathcal{A}_1 \otimes \mathbb{1}$ and $\mathbb{1} \otimes \mathcal{A}_2$. In the case of finite-dimensional state spaces, all states are uniquely represented by a density matrix. Hence there is a corresponding well-defined operation on density matrices describing the restriction process. For all density matrices $\rho \in M_{d_1} \otimes M_{d_2}$ there is a unique density matrix ρ_1 in M_{d_1}, such that

$$\mathrm{Tr}\rho(A \otimes \mathbb{1}) = \mathrm{Tr}\rho_1 A \tag{2.36}$$

The map $\rho \mapsto \rho_1$ is often denoted by Tr_2 and is called the *partial trace*.

Example: Take $d_1 = d_2 = 2$. Denote by $\{|0\rangle, |1\rangle\}$ an orthonormal basis of $\mathbb{C}^2$. Let $\psi \in \mathcal{H}_1 \otimes \mathcal{H}_2 = \mathbb{C}^2 \otimes \mathbb{C}^2$ be the normalized vector

$$\psi = \frac{1}{\sqrt{2}} \left(|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle \right) \tag{2.37}$$

Note that ψ is a maximally entangled state. For $A \in \mathcal{A}_1$, $A \otimes \mathbb{1} \in \mathcal{A}$. The restriction (or marginal) of the state defined by ψ is easily calculated:

$$\begin{aligned} \mathrm{Tr}|\psi\rangle\langle\psi|(A \otimes \mathbb{1}) &= \langle \psi, (A \otimes \mathbb{1})\psi \rangle \\ &= \frac{1}{2} \left(\langle 0|A|0\rangle + \langle 1|A|1\rangle \right) = \frac{1}{2}\mathrm{Tr}A. \end{aligned} \tag{2.38}$$

Hence

$$\mathrm{Tr}_2|\psi\rangle\langle\psi| = \frac{1}{2}\mathbb{1}. \tag{2.39}$$

Vector states given by simple tensors are product states. More generally, a state ω on an algebra of observables of the form $\mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2$, is called a *product state* if there exist states ω_1 on $\mathcal{A}_1$ and ω_2 on $\mathcal{A}_2$, such that for all $A_1 \in \mathcal{A}_1$ and $A_2 \in \mathcal{A}_2$, one has $\omega(A_1 \otimes A_2) = \omega_1(A_1)\omega_2(A_2)$.

Definition 2.3. A state on a tensor product algebra $\mathcal{A}_1 \otimes \mathcal{A}_2$ is called separable if it is a convex combination of product states. A state is called entangled if it is not separable.

If $d_1, d_2 \geq 2$ not all vectors $\psi \in \mathcal{H}$ can be written as $\psi = \psi_1 \otimes \psi_2$, and only those that are of this form define separable states. A vector state is either a product state or entangled. There is no analogue of entangled states for classical systems. Quantum information theory is of interest exactly due to the existence of entangled states.

One of the most commonly used measures of entanglement for a bipartite system is the *entanglement entropy*. For a pure state given by a unit vector $\psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$, the entanglement entropy, $S_E(\psi)$, is defined as the entropy of the restriction of the state to either one of its subsystems (the value is the same for both subsystems). Concretely:

$$S_E(\psi) = -\mathrm{Tr}\rho_1 \log \rho_1, \text{ with } \rho_1 = \mathrm{Tr}_{\mathcal{H}_2}|\psi\rangle\langle\psi|. \tag{2.40}$$

For a general state given by a density matrix ρ, the entanglement entropy is defined by the following minimization problem:

$$S_E(\rho) = \inf\{\sum t_i S_E(\psi_i) \mid \rho = \sum t_i |\psi_i\rangle\langle\psi_i|\} \tag{2.41}$$

which is an infinum over all decompositions of ρ as a convex combination of pure states. This measure of entanglement is also called *entanglement of formation*, because of an equivalent operational definition [52]. One can easily check that $S_E(\rho) = 0$ iff ρ is separable. The maximum value of S_E is $\min(\log d_1, \log d_2)$, and it is easy to construct states that attain this maximal value. Such states are called *maximally entangled*. In the case $d_1 = d_2 = 2$, the maximally entangled states are the so-called Bell states of the form $(e_1 \otimes f_1 + e_2 \otimes f_2)/\sqrt{2}$, for two arbitrary orthonormal bases $\{e_1, e_2\}$ and $\{f_1, f_2\}$ of $\mathbb{C}^2$.

2.5.3. *Dynamics.* One to the most important observables of any quantum spin system is the *Hamiltonian*, which has the physical interpretation of the total energy of the system. For a system consisting of N spins, the Hilbert space is

$$\mathcal{H}_N = \bigotimes_{j=1}^{N} \mathcal{H}_j \tag{2.42}$$

and the algebra of observables is

$$\mathcal{A}_N = \bigotimes_{j=1}^{N} \mathcal{A}_j \tag{2.43}$$

where $\mathcal{A}_j = \mathcal{B}(\mathcal{H}_j)$. The Hamiltonian is a selfadoint element $H^* = H \in \mathcal{A}_N$. Its importance stems from its role as generator of the *dynamics* of the system. For any pure state of the system at time $t = 0$, given by $\psi_0 \in \mathcal{H}_N$, the state at any time $t \in \mathbb{R}$ is given by the solution of the Schrödinger equation:

$$i\frac{d}{dt}\psi(t) = H\psi(t) \quad \text{with} \quad \psi(0) = \psi_0. \tag{2.44}$$

As is well-known, the solution of this vector-valued linear equation is given by

$$\psi(t) = U_t\psi_0, \text{ with } U_t = e^{-itH}. \tag{2.45}$$

Since H is self-adjoint, U_t is unitary for all $t \in \mathbb{R}$ and it is easy to see that $U_t^* = U_{-t}$, and that $U_t U_s = U_{t+s}$, $t, s \in \mathbb{R}$, *i.e.* , $\{U_t \mid t \in \mathbb{R}\}$ is a one-parameter group of unitaries.

Denote by $\rho_0 = |\psi_0\rangle\langle\psi_0|$. Then the density matrix corresponding to the solution of (2.44), i.e. (2.45), is

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| = U_t\rho_0 U_t^*. \tag{2.46}$$

This is the solution of the operator-valued equation

$$i\frac{d}{dt}\rho(t) = [H, \rho(t)] \quad \text{with} \quad \rho(0) = \rho_0 \tag{2.47}$$

This is sometimes called the *Schrödinger-Liouville equation*. It has a unique solution ρ_t which, for an arbitrary initial density matrix ρ_0, is a density matrix for all t.

The dynamics of a finite spin system can equivalently be described in the so-called *Heisenberg picture*, by evolving the observables rather than the states. This change of perspective is particularly useful in the context of infinite systems because, while there is no a priori infinite volume Hilbert space, there is a well-defined observable algebra for the infinite system (see following lectures). The equivalence of the Schrödinger and Heisenberg descriptions of the dynamics is established by the following relations:

$$\omega_{\rho(t)}(A) = \mathrm{Tr}\rho(t)A = \mathrm{Tr}U_t\rho_0 U_t^* A = \mathrm{Tr}\rho_0 U_t^* A U_t = \omega_{\rho_0}(U_t^* A U_t), \tag{2.48}$$

for any observable $A \in \mathcal{A}$. This justifies the following definition of time-evolved observables:

$$A(t) = U_t^* A U_t \quad \text{for any } A \in \mathcal{A} \quad \text{and } t \in \mathbb{R}. \tag{2.49}$$

These time-dependent observables satisfy the *Heisenberg equation*:

$$\frac{d}{dt}A(t) = i[H, A(t)] \quad \text{with } A(0) = A, \tag{2.50}$$

and (2.48) becomes, for any $A \in \mathcal{A}$,

$$\mathrm{Tr}\rho(t)A = \mathrm{Tr}\rho_0 A(t). \tag{2.51}$$

Example: The Quantum Heisenberg Model, introduced by Heisenberg almost a century ago [35].

To each $x \in \mathbb{Z}$ associate the single-site Hilbert space $\mathcal{H}_x = \mathbb{C}^2$. For any finite interval $\Lambda = [a, b] \subset \mathbb{Z}$, consider the Hilbert space

$$\mathcal{H}_\Lambda = \bigotimes_{x=a}^{b} \mathbb{C}^2 = \mathbb{C}^{2^{b-a+1}} \tag{2.52}$$

and the corresponding observable algebra

$$\mathcal{A}_\Lambda = \bigotimes_{x=a}^{b} M_2 = M_{2^{b-a+1}} \tag{2.53}$$

To each $i = 1, 2, 3$, and any $x \in \Lambda$ associate a self-adjoint observable $\sigma_x^i \in \mathcal{A}_\Lambda$ by setting

$$\sigma_x^i = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \sigma^i \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \tag{2.54}$$

where the only non-trivial operator, σ^i above, occurs in the xth factor of $\mathcal{A}_\Lambda$. The quantum Heisenberg Hamiltonian on volume Λ is then the self-adjoint observable

$$\begin{aligned} H_\Lambda &= -J\sum_{j=a}^{b-1} \vec{\sigma}_x \cdot \vec{\sigma}_{x+1} \\ &= -J\sum_{x=a}^{b-1} \left(\sigma_x^1\sigma_{x+1}^1 + \sigma_x^2\sigma_{x+1}^2 + \sigma_x^3\sigma_{x+1}^3\right) \end{aligned} \tag{2.55}$$

with $J \in \mathbb{R}$ a parameter.

If $J > 0$, this is called the (quantum) *ferromagnetic* Heisenberg chain.

If $J < 0$, this is called the (quantum) *anti-ferromagnetic* Heisenberg chain.

In the Exercises you are asked to prove some basic properties of the Heisenberg chain with periodic boundary conditions.

3. Appendix: C^*-algebras

It this appendix, we review some of the basic properties of abstract C^*-algebras. These properties are familiar when the C^*-algebra is a subalgebra of $\mathcal{B}(\mathcal{H})$, for some Hilbert space $\mathcal{H}$. Since the algebra of observables of an infinite quantum spin system, introduced in **??**, is *a priori* not represented on a Hilbert space, it is important to understand the basic properties of abstract C^*-algebras. This appendix is based on Sections 2.1-2.3 - of [10], to which we refer the reader for complete details and further information.

3.1. **C^*-algebras.** A complex vector space $\mathcal{A}$ is an *associative algebra* if it is equipped with a bilinear product, i.e. to each pair $A, B \in \mathcal{A}$ there corresponds a unique element $AB \in \mathcal{A}$, in such a way that:

i) $A(BC) = (AB)C$ for all $A, B, C \in \mathcal{A}$,

ii) $A(B + C) = AB + AC$ for all $A, B, C \in \mathcal{A}$,

iii) $\alpha\beta(AB) = (\alpha A)(\beta B)$ for all $\alpha, \beta \in \mathbb{C}$ and all $A, B \in \mathcal{A}$.

If an algebra $\mathcal{A}$ contains an identity element, i.e., $\mathbb{1} \in \mathcal{A}$ such that $\mathbb{1}A = A = A\mathbb{1}$, for all $A \in \mathcal{A}$, $\mathcal{A}$ is called *unital*. A subspace $\mathcal{B} \subset \mathcal{A}$ that is also an algebra with respect to the operations of $\mathcal{A}$ is called a subalgebra of $\mathcal{A}$.

An associative algebra $\mathcal{A}$ is a $*$-algebra if it has a map $A \mapsto A^*$ with the properties:

i) $(A^*)^* = A$ for all $A \in \mathcal{A}$ (* is an *involution*),

ii) $(AB)^* = B^*A^*$ for all $A, B \in \mathcal{A}$ (* is an *antimorphism*),

iii) $(\alpha A + \beta B)^* = \overline{\alpha}A^* + \overline{\beta}B^*$ for all $\alpha, \beta \in \mathbb{C}$ and all $A, B \in \mathcal{A}$ (* is *antilinear*).

Here, and below, we will denote by $\overline{z}$ and $|z|$ the complex conjugate and modulus of $z \in \mathbb{C}$, respectively. A subset $\mathcal{B}$ of a $*$-algebra A is called *self-adjoint* if $A \in \mathcal{B}$ implies $A^* \in \mathcal{B}$.

An algebra $\mathcal{A}$ is called a *normed algebra* if there is a mapping $\|\cdot\| : \mathcal{A} \to \mathbb{R}$ with the properties:

i) $\|A\| \geq 0$ for all $A \in \mathcal{A}$ and $\|A\| = 0$ if and only if $A = 0$,

ii) $\|\alpha A\| = |\alpha|\|A\|$ for all $\alpha \in \mathbb{C}$ and all $A \in \mathcal{A}$,

iii) $\|A + B\| \leq \|A\| + \|B\|$ for all $A, B \in \mathcal{A}$,

iv) $\|AB\| \leq \|A\|\|B\|$ for all $A, B \in \mathcal{A}$.

For any $A \in \mathcal{A}$, the quantity $\|A\|$ is called the norm of A. The norm on a normed algebra $\mathcal{A}$ defines a metric topology on $\mathcal{A}$, called the *uniform topology* or *norm topology*, and if $\mathcal{A}$ is complete with respect to this topology, then $\mathcal{A}$ is called a *Banach algebra*. A $*$-algebra $\mathcal{A}$ is a normed $*$-algebra $\mathcal{A}$ if one has $\|A^*\| = \|A\|$ for all $A \in \mathcal{A}$. A normed $*$-algebra is a *Banach $*$-algebra* if it is complete with respect to its norm topology.

The main object of interest in the section can now be defined.

Definition 3.1. A C^*-algebra is a Banach $*$-algebra $\mathcal{A}$ with the property that

$$\|A^*A\| = \|A\|^2 \quad \text{for all } A \in \mathcal{A}. \tag{3.1}$$

The condition (3.1) is called the *C^*-property*. It is easy to see that (3.1) implies the $*$ property of the norm: $\|A^*\| = \|A\|$ for all $A \in \mathcal{A}$. Here are some important examples.

Example: Let $\mathcal{H}$ be a complex Hilbert space and denote by $\mathcal{A} = \mathcal{B}(\mathcal{H})$ the set of bounded linear operators over $\mathcal{H}$. With the $*$ operation given by the adjoint operation and the norm corresponding to the operator norm, $\mathcal{A}$ is a C^*-algebra. □

Example: Let X be a topological space and let $C(X)$ denote the space of bounded and continuous complex-valued functions on X. $C(X)$ is a an commutative algebra for the pointwise multiplication of functions. Equipped with the supremum norm and the $*$-operation given by complex conjugation, $C(X)$ becomes a C^*-algebra. □

Example: Let $\mathcal{H}$ be a complex Hilbert space and denote by $\mathcal{C} \subset \mathcal{B}(\mathcal{H})$ the set of compact operators over $\mathcal{H}$. One easily checks that any uniformly closed subalgebra of $\mathcal{B}(\mathcal{H})$ that is also a self-adjoint subset, is a C^*-sub-algebra of $\mathcal{B}(\mathcal{H})$. This is the case with the algebra of compact operators $\mathcal{C}$. Note that $\mathbb{1} \notin \mathcal{C}$. □

The following theorem shows that, as in the last example, any C^* algebra can be regarded as a closed subalgebra of $\mathcal{B}(\mathcal{H})$ for some Hilbert space $\mathcal{H}$.

Theorem 3.2. *Any C^*-algebra $\mathcal{A}$ is isomorphic to a norm-closed self-adjoint algebra of bounded linear operators on a Hilbert space $\mathcal{H}$.*

For a proof of this theorem see, e.g., [10, Theorem 2.1.10].

The availability of an identity in a C^*-algebra describing the observables of a physical system is important. Let $\mathcal{A}$ be a C^*-algebra. If $\mathcal{A}$ has an indentity, it is necessarily unique; if both $\mathbb{1}$ and $\mathbb{1}'$ are identities, then $\mathbb{1} = \mathbb{1}\mathbb{1}' = \mathbb{1}'$. It is easy to verify that $\mathbb{1}^*$ is an identity, and hence we must have $\mathbb{1}^* = \mathbb{1}$. Moreover,

$$\|\mathbb{1}\| = \|\mathbb{1}^*\mathbb{1}\| = \|\mathbb{1}\|^2 \quad \text{and} \quad \|A\| = \|\mathbb{1}A\| \leq \|\mathbb{1}\|\|A\|. \tag{3.2}$$

Thus either $\|\mathbb{1}\| = 1$ or $\mathcal{A} = \{0\}$, which is a trivial case we shall ignore; we will always assume that $\|\mathbb{1}\| = 1$. A C^*-algebra $\mathcal{A}$ with an identity is called a *unital* C^*-algebra.

It is not the case that all C^*-algebras possess an identity. As mentioned above, the C^*-algebra of the compact operators on a Hilbert space $\mathcal{H}$ has an identity if and only if $\mathcal{H}$ is finite-dimensional. In general, it is possible to *adjoin an identity* to any C^*-algebra. We briefly describe this procedure.

Let $\mathcal{A}$ be a C^*-algebra with no identity. Consider the collection of pairs

$$\tilde{\mathcal{A}} = \{(\alpha, A) : \alpha \in \mathbb{C} \text{ and } A \in \mathcal{A}\}\,. \tag{3.3}$$

Equip $\tilde{\mathcal{A}}$ with the vector space properties

$$(\alpha, A) + (\beta, B) = (\alpha + \beta, A + B) \quad \text{and} \quad \alpha(\beta, B) = (\alpha\beta, \alpha B) \tag{3.4}$$

In addition, declare a product and involution by setting

$$(\alpha, A)(\beta, B) = (\alpha\beta, \alpha B + \beta A + AB) \quad \text{and} \quad (\alpha, A)^* = (\overline{\alpha}, A^*) \tag{3.5}$$

One can check, see also Proposition 2.1.5 in [10], that the quantity

$$\|(\alpha, A)\| = \sup\{\|\alpha B + AB\| : B \in \mathcal{A}, \|B\| = 1\} \tag{3.6}$$

defines a norm on $\tilde{\mathcal{A}}$ and with respect to this norm, $\tilde{\mathcal{A}}$ is a C^*-algebra. The algebra $\mathcal{A}$ can be identified with the C^*-subalgebra of $\tilde{\mathcal{A}}$ formed by the pairs $(0, A)$. $\tilde{A}$ is often called the C^*-algebra obtained by adjoining an identity to $\mathcal{A}$. The notation $\tilde{\mathcal{A}} =: \mathbb{C}\mathbb{1} + \mathcal{A}$ and similarly $(\alpha, A) =: \alpha\mathbb{1} + A$ is common.

With this construction in mind, we will only work with unital C^*-algebras in these notes.

3.2. **Spectral theory in a C^*-algebra.** The goal of this section is to provide quick introduction to the basic facts of spectral theory in a C^*-algebra. For more details and more general statements, we refer the interested reader to, e.g., [10, Section 2.2.1]. Unless otherwise state, we will assume $\mathcal{A}$ is a unital C^*-algebra..

An element $A \in \mathcal{A}$ is said to be *invertible* if there exists an element $A^{-1} \in \mathcal{A}$, called the *inverse* of A, which satisfies

$$AA^{-1} = A^{-1}A = \mathbb{1}\,. \tag{3.7}$$

One readily checks that if A is invertible, then the inverse is unique. A number of other properties also immediately follow:

i) If A is invertible, then so is A^{-1} and $(A^{-1})^{-1} = A$.

ii) If A is invertible, then so is A^* and $(A^*)^{-1} = (A^{-1})^*$.

iii) If A and B are invertible, then so is AB and $(AB)^{-1} = B^{-1}A^{-1}$.

Definition 3.3. The resolvent set of an element $A \in \mathcal{A}$, denoted by $\mathrm{res}_{\mathcal{A}}(A)$, is the set of all $\lambda \in \mathbb{C}$ for which $\lambda\mathbb{1} - A$ is invertible. The spectrum of any $A \in \mathcal{A}$, denoted by $\mathrm{spec}_{\mathcal{A}}(A)$, is then defined to be the complement of $\mathrm{res}_{\mathcal{A}}(A)$ in $\mathbb{C}$. Given $A \in \mathcal{A}$ and $\lambda \in \mathrm{res}_{\mathcal{A}}(A)$, the inverse $(\lambda\mathbb{1} - A)^{-1}$ is called the resolvent of A at λ.

For a non-unital C^*-algebras $\mathcal{A}$, one can still define the notion of spectrum by setting $\mathrm{spec}_{\mathcal{A}}(A) := \mathrm{spec}_{\tilde{\mathcal{A}}}(A)$, where $\tilde{\mathcal{A}}$ is the unique algebra obtained from $\mathcal{A}$ by adjoining an identity.

For all $A \in \mathcal{A}$ and any $\lambda \in \mathbb{C}$ with $\|A\| < |\lambda|$, it is easy to see that

$$\frac{1}{\lambda}\sum_{n=0}^{\infty}\left(\frac{A}{\lambda}\right)^n \tag{3.8}$$

defines a norm-convergent sum. It is then readily checked that this element is the inverse of $\lambda\mathbb{1} - A$. Hence, $\lambda \in \mathrm{res}_{\mathcal{A}}(A)$ and thus $\mathrm{spec}_{\mathcal{A}}(A)$ is a bounded subset of $\mathbb{C}$; namely

$$\mathrm{spec}(A) \subset \{\lambda \in \mathbb{C} : |\lambda| \leq \|A\|\}\,. \tag{3.9}$$

Straightforward manipulations with Neumann series, defined similarly to (3.8), allow one to show that for any $A \in \mathcal{A}$, $\mathrm{res}_{\mathcal{A}}(A)$ is open, and thus $\mathrm{spec}_{\mathcal{A}}(A)$ is closed. One readily verifies that the mapping $\lambda \mapsto (\lambda\mathbb{1} - A)^{-1}$ is continuous on $\mathrm{res}_{\mathcal{A}}(A)$. It is also important to observe that for every $A \in \mathcal{A}$, $\mathrm{spec}_{\mathcal{A}}(A)$ is non-empty. This fact is a consequence of the next result.

First, an important definition. For any $A \in \mathcal{A}$ define the *spectral radius* of A by

$$\rho(A) = \sup\{|\lambda| : \lambda \in \mathrm{spec}_{\mathcal{A}}(A)\}\,. \tag{3.10}$$

Proposition 3.4. *For any $A \in \mathcal{A}$, one has that*

$$\rho(A) = \lim_{n\to\infty}\|A^n\|^{1/n} = \inf_n \|A^n\|^{1/n} \leq \|A\|\,. \tag{3.11}$$

In particular, the above limit exists and if the righthand side of (3.11) vanishes, then $0 \in \mathrm{spec}(A)$. Therefore, the spectrum of any $A \in \mathcal{A}$ is a non-empty compact set.

A proof of this result can be found, e.g., in [10, Proposition 2.2.2].

One can characterize the spectrum of certain special classes of elements $A \in \mathcal{A}$. An element $A \in \mathcal{A}$ is said to be *normal* if $A^*A = AA^*$, and $A \in \mathcal{A}$ is called *self-adjoint* if $A^* = A$. The set of all self-adjoint elements of $\mathcal{A}$ will be denoted by $\mathcal{A}_{\mathrm{sa}}$. It is often useful to observe that each $A \in \mathcal{A}$ can be written as a linear combination of self-adjoint elements:

$$A = A_1 + iA_2 \quad \text{with } A_1 = \frac{A + A^*}{2} \text{ and } A_2 = \frac{A - A^*}{2i} \tag{3.12}$$

and A_1 and A_2 are commonly referred to as the real and imaginary parts of A respectively.

An element $A \in \mathcal{A}$ is called an *isometry* if $A^*A = \mathbb{1}$, and $A \in \mathcal{A}$ is said to be *unitary* if $A^*A = \mathbb{1} = AA^*$.

The following statement collects some facts proven, e.g., [10, Theorem 2.2.5].

Theorem 3.5. *Let $\mathcal{A}$ be a unital C^*-algebra.*

i) If $A \in \mathcal{A}$ is normal, then $\rho(A) = \|A\|$.

ii) If $A \in \mathcal{A}$ is unitary, then

$$\mathrm{spec}_{\mathcal{A}}(A) \subset \{\lambda \in \mathbb{C} : |\lambda| = 1\}\,.$$

iii) If $A \in \mathcal{A}$ is self-adjoint, then

$$\mathrm{spec}_{\mathcal{A}}(A) \subset [-\|A\|, \|A\|]\,.$$

iv) For any $A \in \mathcal{A}$ and any polynomial P,

$$\mathrm{spec}_{\mathcal{A}}\left(P(A)\right) = P\left(\mathrm{spec}_{\mathcal{A}}(A)\right)\,.$$

Two important consequences follow now from the results previously stated.

First, if $\mathcal{A}$ is a $*$-algebra and there exists a norm on $\mathcal{A}$ with the C^* property and with respect to which $\mathcal{A}$ is closed, then this norm is unique. Hence the norm on a C^*-algebra is unique.

Next, let $\mathcal{B}$ be a C^*-sub-algebra of some C^*-algebra $\mathcal{A}$. Then, for any $A \in \mathcal{B}$,

$$\mathrm{spec}_{\mathcal{A}}(A) = \mathrm{spec}_{\mathcal{B}}(A)$$

Thus, there is no ambiguity in the definition of the spectrum of an element A in a C^*-algebra, and so we may simply write $\mathrm{spec}(A)_{\mathcal{A}} = \mathrm{spec}(A)$.

3.3. **Positive elements.** In this section, we review some of their basic properties of positive elements a unital C^*-algebra $\mathcal{A}$. As we shall see, the cone of positive elements introduces a partial order on $\mathcal{A}$.

Definition 3.6. An element $A \in \mathcal{A}$ is said to be *positive* if A is self-adjoint and $\mathrm{spec}(A) \subset [0, \infty)$. We will denote by $\mathcal{A}_+$ the set of all positive elements $A \in \mathcal{A}$.

As a consequence of Theorem 3.5 iii), we actually know that if $A \in \mathcal{A}$ is positive, then

$$\mathrm{spec}(A) \subset [0, \|A\|] \,.$$

In fact, since it is easy to verify that

$$\mathrm{spec}(\lambda \mathbb{1} - A) = \lambda - \mathrm{spec}(A) \quad \text{for all } \lambda \in \mathbb{C} \text{ and } A \in \mathcal{A} \,,$$

we immediately conclude that

$$A \in \mathcal{A}_+ \quad \Rightarrow \quad \|A\| \mathbb{1} - A \in \mathcal{A}_+ \,. \tag{3.13}$$

Similar arguments allow one to prove that if $A \in \mathcal{A}_{\mathrm{sa}}$, then A is positive if and only if

$$\left\| \mathbb{1} - \frac{A}{\|A\|} \right\| \leq 1 \,. \tag{3.14}$$

Positive elements allow for the definition of a square root, which is an important building block for developing functional calculus in C^*-algebras. A first result in this direction is the following.

Theorem 3.7. *[10, Theorem 2.2.10] $A \in \mathcal{A}_{\mathrm{sa}}$ is positive if and only if $A = B^2$ for some $B \in \mathcal{A}_{\mathrm{sa}}$. In fact, for each $A \in \mathcal{A}_+$, there is a unique $B \in \mathcal{A}_+$ for which $A = B^2$.*

Given the above result, we can now make the following definitions. For any $A \in \mathcal{A}_+$, the *square-root of A*, which we denote by $A^{1/2}$, is defined by $A^{1/2} = B$, where $B \in \mathcal{A}_+$ is the unique element described in Theorem 3.7 above. Moreover, for any $A \in \mathcal{A}_{\mathrm{sa}}$, it is clear that $\mathrm{spec}(A^2) \subset [0, \|A\|^2]$, combine e.g. Theorem 3.5 iii) and iv). Thus $A^2 \in \mathcal{A}_+$, and so we may therefore define the *modulus of A*, which we denote at $|A|$, by setting $|A| = (A^2)^{1/2}$.

The following fact is a useful observation about the set of positive operators.

Proposition 3.8. *The set $\mathcal{A}_+ \subset \mathcal{A}$ of positive elements is a uniformly closed convex cone satisfying $\mathcal{A}_+ \cap (-\mathcal{A}_+) = \{0\}$. Moreover, if $A \in \mathcal{A}_{\mathrm{sa}}$, then with $A_\pm = (|A| \pm A)/2$ one sees that*
i) $A_\pm \in \mathcal{A}_+$,
ii) $A = A_+ - A_-$,
iii) $A_+ A_- = 0$.
The elements $A_\pm$ are the unique elements with these properties.

A proof of Proposition 3.8 can be found e.g. in [10, Proposition 2.2.11]. The decomposition for $A \in \mathcal{A}_{\mathrm{sa}}$, i.e. $A = A_+ - A_-$ in ii) above, is called the *orthogonal decomposition of A*.

The following fact is crucial.

Theorem 3.9. *$A \in \mathcal{A}_+$ if and only if $A = B^* B$ for some $B \in \mathcal{A}$.*

A proof of this result can be found in [10, Theorem 2.2.12].

Given Theorem 3.9, one can now extend the notion of modulus to all $A \in \mathcal{A}$. In fact, for any $A \in \mathcal{A}$, it is clear that $A^* A \in \mathcal{A}_+$. In this case, we define $|A| = (A^* A)^{1/2}$ to be the modulus of A. Moreover, if $A \in \mathcal{A}$ is invertible, then an analogue of the polar decomposition holds:

$$A = U|A| \quad \text{with} \quad U = A|A|^{-1} \tag{3.15}$$

and one can check that the U given above is unitary. One final result on decompositions is occasionally of use.

Lemma 3.10. *Every $A \in \mathcal{A}$ can be written as*

$$A = \sum_{j=1}^{4} a_j U_j \text{ where each } a_j \in \mathbb{C} \text{ satisfies } |a_j| \leq \frac{\|A\|}{2}\,, \tag{3.16}$$

and each U_j is unitary.

The proof of the above follows from (3.12) and the observation that for any $A \in \mathcal{A}_{\rm sa}$ with $\|A\| \leq 1$, one can readily check that

$$A = \frac{U_+ + U_-}{2} \quad \text{with unitaries} \quad U_\pm = A \pm i\sqrt{\mathbb{1} - A^2}\,. \tag{3.17}$$

Using the fact that $\mathcal{A}_+$ is a convex cone, one can introduce an order relation on the self-adjoint elements of $\mathcal{A}$. If $A, B \in \mathcal{A}_{\rm sa}$, we write that $A \geq B$, or $B \leq A$, if $A - B \in \mathcal{A}_+$.

The following proposition identifies some important features of this partial order.

Proposition 3.11. *Let $\mathcal{A}$ be a unital C^*-algebra.*
i) If $A \geq 0$ and $A \leq 0$, then $A = 0$.
ii) If $A \geq B$ and $B \geq C$, then $A \geq C$.
iii) If $A \geq 0$, then $\|A\|\mathbb{1} \geq A$.
iv) If $A \geq B \geq 0$, then $C^*AC \geq C^*BC \geq 0$ for all $C \in \mathcal{A}$.

3.4. **Representations.** It is often useful to consider mappings between C^*-algebras that preserve the structure. These are $*$-morphism. A particularly important sub-class of these are the representations. We introduce these notions in this subsection.

Definition 3.12. Let $\mathcal{A}$ and $\mathcal{B}$ be unital C^*-algebras. A mapping $\pi : \mathcal{A} \to \mathcal{B}$ is called a $*$-morphism between $\mathcal{A}$ and $\mathcal{B}$ if it satisfies:
i) $\pi(\alpha A + \beta B) = \alpha\pi(A) + \beta\pi(B)$ for all $\alpha, \beta \in \mathbb{C}$ and $A, B \in \mathcal{A}$,
ii) $\pi(AB) = \pi(A)\pi(B)$ for all $A, B \in \mathcal{A}$,
iii) $\pi(A^*) = \pi(A)^*$ for all $A \in \mathcal{A}$.

Remarks:
1) The phrase *morphism* may refer to mappings satisfying only properties i) and ii) above. Property iii) makes π a $*$-morphism. We only consider $*$-morphisms below.
2) A $*$-morphism $\pi : \mathcal{A} \to \mathcal{B}$ is said to be *unit preserving* if $\pi(\mathbb{1}_{\mathcal{A}}) = \mathbb{1}_{\mathcal{B}}$.
3) Any $*$-morphism π from $\mathcal{A}$ to $\mathcal{B}$ necessarily preserves positivity in the sense that: $\pi : \mathcal{A}_+ \to \mathcal{B}_+$. Indeed, for any $A \in \mathcal{A}_+$, $A = B^*B$ and hence,

$$\pi(A) = \pi(B^*B) = \pi(B^*)\pi(B) = \pi(B)^*\pi(B) \in \mathcal{B}_+\,.$$

The following proposition demonstrates that $*$-morphism are bounded, hence continuous.

Proposition 3.13. *Let $\mathcal{A}$ and $\mathcal{B}$ be unital C^*-algebras. Any $*$-morphism $\pi : \mathcal{A} \to \mathcal{B}$ is bounded, in fact*

$$\|\pi(A)\| \leq \|A\| \quad \text{for all } A \in \mathcal{A}. \tag{3.18}$$

In addition, the range of π, namely $\pi(\mathcal{A}) := \{\pi(A) : A \in \mathcal{A}\}$, is a C^*-subalgebra of $\mathcal{B}$.

Proof. We begin with the following observation. Let $P = \pi(\mathbb{1}_{\mathcal{A}})$. It is easy to check that $P \in \mathcal{B}_{\rm sa}$ and moreover, $P^2 = P$, i.e. P is a projection. As a consequence, $\mathcal{B}' = P\mathcal{B}P$ is a C^*-subalgebra of $\mathcal{B}$. On this C^*-sub-algebra, P acts as the identity, and it is also the case that $\pi(\mathcal{A}) \subset \mathcal{B}'$.

Now, it is sufficient to check (3.18) for $A \in \mathcal{A}_{\rm sa}$. In fact, suppose this bound holds for all $A \in \mathcal{A}_{\rm sa}$. Then, for any $A \in \mathcal{A}$,

$$\|\pi(A)\|^2 = \|\pi(A)^*\pi(A)\| = \|\pi(A^*A)\| \leq \|A^*A\| = \|A\|^2 \tag{3.19}$$

where we have used the C^*-property in both $\mathcal{A}$ and $\mathcal{B}'$.

Now, suppose $A \in \mathcal{A}_{\text{sa}}$. It is clear then that $\pi(A) \in \mathcal{B}'_{\text{sa}}$, i.e. $\pi(A)^* = \pi(A^*) = \pi(A)$. Using Theorem 3.5 i), the norm of $\pi(A)$ can be calculated using the spectral radius, i.e.,

$$\|\pi(A)\| = \rho(\pi(A)) = \sup\{|\lambda| : \lambda \in \text{spec}_{\mathcal{B}'}(\pi(A))\}\,. \tag{3.20}$$

One readily checks that

$$\text{spec}_{\mathcal{B}'}(\pi(A)) \subset \text{spec}_{\mathcal{A}}(A)\,, \tag{3.21}$$

and therefore,

$$\|\pi(A)\| \leq \sup\{|\lambda| : \lambda \in \text{spec}_{\mathcal{A}}(A)\} = \|A\| \tag{3.22}$$

since $A \in \mathcal{A}_{\text{sa}}$. An argument for the remainder of this proof can be found in [10, Proposition 2.3.1]. □

Let $\mathcal{A}$ and $\mathcal{B}$ be unital C^*-algebras. A $*$-morphism π from $\mathcal{A}$ to $\mathcal{B}$ is said to be a $*$-*isomorphism* if it is one-to-one and onto. Clearly π is a $*$-isomorphism if and only if $\ker(\pi) = \{0\}$, where

$$\ker(\pi) := \{A \in A : \pi(A) = 0\}\,.$$

Definition 3.14. Let $\mathcal{A}$ be a C^*-algebra. A representation of $\mathcal{A}$ is a pair $(\mathcal{H}, \pi)$ where $\mathcal{H}$ is a complex Hilbert space and π is a $*$-morphism from $\mathcal{A}$ to $\mathcal{B}(\mathcal{H})$. The representation $(\mathcal{H}, \pi)$ is said to be faithful if and only if π is a $*$-isomorphism from $\mathcal{A}$ to $\pi(\mathcal{A})$, i.e., if and only if $\ker(\pi) = \{0\}$.

If $\mathcal{A}$ is a C^*-algebra and $(\mathcal{H}, \pi)$ is a representation, then $\mathcal{H}$ is called the *representation space*; the operators $\pi(A) \in \mathcal{B}(\mathcal{H})$ are called the *representatives of* $\mathcal{A}$, and π is often referred to as a *representation of* $\mathcal{A}$ *on* $\mathcal{H}$.

Proposition 3.15. *Let $(\mathcal{H}, \pi)$ be a representation of a C^*-algebra $\mathcal{A}$. The representation is faithful if and only if it satisfies each of the following equivalent conditions:*
i) $\ker(\pi) = \{0\}$,
ii) $\|\pi(A)\| = \|A\|$ *for all* $A \in \mathcal{A}$,
iii) for all $A \in \mathcal{A}_+$, $A \neq 0$, *we have* $\pi(A) \geq 0$ *and* $\pi(A) \neq 0$.

A proof of this result can be found in [10, Proposition 2.3.3].

Definition 3.16. Let $\mathcal{A}$ be a C^*-algebra. A $*$-isomorphism τ from $\mathcal{A}$ to $\mathcal{A}$ is called an automorphism on $\mathcal{A}$.

An immediate consequence of Proposition 3.15 and Definition 3.16 is the following.

Corollary 3.17. *Let $\mathcal{A}$ be a C^*-algebra and τ be an automorphism on $\mathcal{A}$. τ is norm-preserving, i.e.*

$$\|\tau(A)\| = \|A\| \quad \textit{for all } A \in \mathcal{A}. \tag{3.23}$$

3.5. **States.** Another notion of crucial importance for the theory of C^*-algebras is that of states. States are essential, of course, also in applications to physical systems. Again, let $\mathcal{A}$ be a unital C^*-algebra.

The *dual* of $\mathcal{A}$, which we denote by $\mathcal{A}^*$, is the collection of all continuous linear functionals over $\mathcal{A}$. For any $f \in \mathcal{A}^*$, we define the *norm* of f to be

$$\|f\| := \sup\{|f(A)| : A \in \mathcal{A} \text{ and } \|A\| = 1\}. \tag{3.24}$$

Definition 3.18. A linear functional ω over $\mathcal{A}$ is said to be positive if

$$\omega(A^*A) \geq 0 \quad \text{for all } A \in \mathcal{A}.$$

A positive linear functional ω over a C^*-algebra $\mathcal{A}$ is said to be a state if $\|\omega\| = 1$.

Recall that $A \in \mathcal{A}_+$ if and only if $A = B^*B$ for some $B \in \mathcal{A}$. Moreover, for $A, B \in \mathcal{A}_{\rm sa}$, $A \geq B$ if and only if $A - B \in \mathcal{A}_+$. It follows that $\omega(A) \in \mathbb{R}$ if $A \in \mathcal{A}_{\rm sa}$, and $A \geq B$ implies $\omega(A) \geq \omega(B)$.

States and representations are intimately connected. To see this, let $\mathcal{A}$ be a unital C^*-algebra, and let $(\mathcal{H}, \pi)$ be a representation of $\mathcal{A}$. For any non-zero $\Omega \in \mathcal{H}$, define

$$\omega_\Omega(A) = \langle \Omega, \pi(A)\Omega \rangle \quad \text{for all } A \in \mathcal{A}\,. \tag{3.25}$$

It is clear that any such ω_Ω is linear on $\mathcal{A}$. In addition,

$$\omega_\Omega(A^*A) = \langle \Omega, \pi(A^*A)\Omega \rangle = \|\pi(A)\Omega\|^2 \geq 0 \tag{3.26}$$

and so ω_Ω is positive as well. If $\|\Omega\| = 1$ and π is non-degenerate, then one can check that $\|\omega_\Omega\| = 1$. In this case, then ω_Ω is a state on $\mathcal{A}$. States of this type are called *vector states* of the representation $(\mathcal{H}, \pi)$. In fact, one can prove that every state over a C^*-algebra is a vector state in a suitable representation **??**.

The following lemma underlies the most basic properties of states .

Lemma 3.19 (Cauchy-Schwarz)**.** *Let ω be a positive linear functional over $\mathcal{A}$. It follows that*
i) $\omega(A^*B) = \overline{\omega(B^*A)}$ for all $A, B \in \mathcal{A}$,
ii) $|\omega(A^*B)|^2 \leq \omega(A^*A)\omega(B^*B)$ for all $A, B \in \mathcal{A}$.

Proof. Let $A, B \in \mathcal{A}$ and $\lambda \in \mathbb{C}$. By positivity of ω

$$\omega\left((\lambda A + B)^*(\lambda A + B)\right) \geq 0\,. \tag{3.27}$$

Using linearity, one finds that this is equivalent to

$$|\lambda|^2\omega(A^*A) + \overline{\lambda}\omega(A^*B) + \lambda\omega(B^*A) + \omega(B^*B) \geq 0 \tag{3.28}$$

The necessary and sufficient conditions for the positivity of this quadratic form on λ are exactly the conditions given above. □

There are a number of immediate and important consequences.

Corollary 3.20. *Let ω be a positive linear functional over $\mathcal{A}$. It follows that*
i) $\omega(A^*) = \overline{\omega(A)}$ for all $A \in \mathcal{A}$.
ii) $\omega(\mathbb{1}) = \|\omega\| = \sup\{\omega(A^*A) : \|A\| = 1\}$.
iii) $|\omega(A)|^2 \leq \omega(A^*A)\|\omega\|$ for all $A \in \mathcal{A}$.
iv) $|\omega(A^*BA)| \leq \omega(A^*A)\|B\|$ for all $A, B \in \mathcal{A}$.

Proof. The proof of i) follows from Lemma 3.19 i) by taking $B = \mathbb{1}$. To see that the first equality in ii) is true, observe that

$$0 \leq \omega(\mathbb{1}^*\mathbb{1}) = \omega(\mathbb{1}) = \frac{\omega(\mathbb{1})}{\|\mathbb{1}\|} \leq \|\omega\| \tag{3.29}$$

where we have used uniqueness of the identity, i.e. that $\mathbb{1}^* = \mathbb{1}$, and non-triviality of $\mathcal{A}$, i.e. that $\|\mathbb{1}\| = 1$. It is also clear that, for any $A \in \mathcal{A}$

$$|\omega(A)|^2 = |\omega(\mathbb{1}^*A)|^2 \leq \omega(\mathbb{1})\omega(A^*A) \tag{3.30}$$

where we have applied Lemma 3.19 ii). If we further assume that $A \in \mathcal{A}$ satisfies $\|A\| = 1$, then (3.30) implies

$$\|\omega\|^2 \leq \omega(\mathbb{1})\|\omega\| \tag{3.31}$$

where we have used that $\|A^*A\| = \|A\|^2 = 1$. If $\|\omega\| = 0$, then (3.29) shows that $\omega(\mathbb{1}) = 0$ as well. Otherwise, $\omega(\mathbb{1}) = \|\omega\|$ now follows by combining the inequalities proven in (3.29) and (3.31). The claim in iii) now follows from (3.30). In fact, the second equality in ii) also follows from (3.30). Finally, iv) follows from the application of ii) to the positive functional $B \mapsto \omega(A^*BA)$. □

Note that iv) implies that, for any $A \in \mathcal{A}$ with $\omega(A^*A) \neq 0$,

$$\omega_A(B) := \frac{\omega(A^*BA)}{\omega(A^*A)} \quad \text{for all } B \in \mathcal{A} \tag{3.32}$$

defines a state ω_A on $\mathcal{A}$. This is the quantum analogue of starting with a measure, e.g. dx on $[0,1]$, considering a non-negative function μ with $\int_0^1 \mu(x)dx < \infty$, and defining a new, normalized measure via

$$\frac{\mu(x)}{\int_0^1 \mu(x)dx}dx \tag{3.33}$$

4. General Framework for Finite and Infinite Quantum Spin Systems

The general framework introduced in this chapter will allow us to consider infinite quantum spin systems as C^*-dynamical systems. In particular we will construct the dynamics for infinite quantum spin systems as a strongly continuous one-parameter group of automorphism of the algebra of quasi-local observables. We start by studying the dynamics of finite quantum spin systems.

4.1. **The Dynamics of Finite Systems.** Let Λ be a finite set. For each $x \in \Lambda$ we have a quantum system described by a finite-dimensional Hilbert space of dimension $d_x \geq 2$. These are the 'spins' that form the spin system. The Hilbert space for the finite spin system is then

$$\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathbb{C}^{d_x}. \tag{4.1}$$

The algebra of observables of the systems is

$$\mathcal{A}_\Lambda = \bigotimes_{x\in\Lambda} M_{d_x}. \tag{4.2}$$

Due to the tensor product structure, for any $\Lambda_1 \subset \Lambda$, the collection of observables $\mathcal{A}_{\Lambda_1}$ may be regarded as a subset of the observables in $\mathcal{A}_\Lambda$ by identifying $A \in \mathcal{A}_{\Lambda_1}$ with $A \otimes \mathbb{1}_{\Lambda\setminus\Lambda_1} \in \mathcal{A}_{\Lambda_1} \otimes \mathcal{A}_{\Lambda\setminus\Lambda_1} = \mathcal{A}_\Lambda$. With this in mind, we will consider $\mathcal{A}_{\Lambda_1}$ as a subalgebra of $\mathcal{A}_\Lambda$.

An interaction Φ is a mapping $\Phi : \mathcal{P}(\Lambda) \to \mathcal{A}_\Lambda$ (where $\mathcal{P}(\Lambda)$ denotes the set of all subsets of Λ) with the property that: For each $X \in \mathcal{P}(\Lambda)$, $\Phi(X) \in \mathcal{A}_X$ and $\Phi(X)^* = \Phi(X)$. For any $Z \subset \Lambda$, the Hamiltonian corresponding to Φ in the volume Z is given by

$$H_Z = \sum_{X\in\mathcal{P}(Z)} \Phi(X) \tag{4.3}$$

Example An interaction, Φ_H, for the Heisenberg spin chain on an interval $[a, b] \subset \mathbb{Z}$ is given by

$$\Phi_H(X) = \begin{cases} -J\vec{\sigma}_j\vec{\sigma}_{j+1} & \text{if } X = \{j, j+1\} \\ 0 & \text{otherwise} \end{cases} \tag{4.4}$$

and therefore we have

$$H_{[a,b]} = \sum_{X\in\mathcal{P}([a,b])} \Phi_H(X) = -J\sum_{j=a}^{b-1} \vec{\sigma}_j\vec{\sigma}_{j+1} \tag{4.5}$$

as in (2.55) above.

The Heisenberg dynamics, which we will denote by τ_t^Λ, generated by the Hamiltonian H_Λ (corresponding to the interaction Φ) is an automorphism of the algebra $\mathcal{A}_\Lambda$ defined as follows:

$$\tau_t^\Lambda(A) = U_\Lambda^*(t)AU_\Lambda(t), \quad \text{for all } A \in \mathcal{A}_\Lambda, \tag{4.6}$$

where $U_\Lambda(t)$ is the unitary operator

$$U_\Lambda(t) = e^{-itH_\Lambda} \in \mathcal{A}_\Lambda. \tag{4.7}$$

The automorphisms τ_t^Λ provide the solutions to the Heisenberg equation for the time-evolution of observables:

$$\frac{d}{dt}\tau_t^\Lambda(A) = i[H_\Lambda, \tau_t^\Lambda(A)]. \tag{4.8}$$

Often, we consider finite volume subsystems of some infinite system of spins labeled by a countable set Γ. A common situation is a spin systems defined on the lattice $\mathbb{Z}^\nu$.

A typical model will be defined by specifying a global interaction Φ which is a mapping

$$\Phi : \mathcal{P}_0(\mathbb{Z}^\nu) \to \bigcup_{n\geq 1} \mathcal{A}_{\Lambda_n} \tag{4.9}$$

with $\mathcal{P}_0(\mathbb{Z}^\nu)$ being the set of *finite* subsets of $\mathbb{Z}^\nu$ and the union of the observable algebras is defined inductively using that $\mathcal{A}_{\Lambda_n} \subset \mathcal{A}_{\Lambda_{n+1}}$. (Under the additional assumption that the sequence is *exhaustive*, i.e., $\cup_n \Lambda_n = \mathbb{Z}^\nu$, this union is independent of the chosen sequence.) The same conditions on the interaction, i.e., $\Phi(X)^* = \Phi(X) \in \mathcal{A}_X$ apply. We often investigate properties of finite-volume Hamiltonians corresponding to this fixed interaction:

$$H_n = H_{\Lambda_n} = \sum_{X \in \mathcal{P}(\Lambda_n)} \Phi(X) \tag{4.10}$$

For the dynamics, it is clear that if $\Lambda_1 \subset \Lambda$, then

$$\tau_t^{\Lambda_1}(A) \in \mathcal{A}_{\Lambda_1} \quad \text{for any } A \in \mathcal{A}_{\Lambda_1} \text{ and all } t \in \mathbb{R}. \tag{4.11}$$

However, it is generally the case that

$$\tau_t^{\Lambda}(A) \notin \mathcal{A}_{\Lambda_1} \quad \text{for any } A \in \mathcal{A}_{\Lambda_1} \text{ and } t \neq 0. \tag{4.12}$$

Let's examine this further in the context of a one-dimensional systems with nearest neighbor interactions, such as the one-dimensional Heisenberg model. Let H_N denote the Hamiltonian for such a system on $[-N, N] \subset \mathbb{Z}$:

$$H_N = \sum_{j=-N}^{N-1} h_{j,j+1} \quad \text{with} \quad h_{j,j+1} = -J\vec{\sigma}_j \cdot \vec{\sigma}_{j+1} \in \mathcal{A}_{\{j,j+1\}} \tag{4.13}$$

The corresponding Heisenberg dynamics, i.e. $\tau_t^N(\cdot)$, can be defined by the series for the exponential of its generator $i[H_N, \cdot]$:

$$\tau_t^N(A) = e^{it[H_N,\cdot]}(A) = A + it[H_N, A] + \frac{(it)^2}{2!}[H_N, [H_N, A]] + \cdots, \quad \text{for any } A \in \mathcal{A}_{[-N,N]}. \tag{4.14}$$

To gain some insight in the structure of the dynamics, consider $A \in \mathcal{A}_{\{0\}}$ i.e. an observable that acts non-trivially only at the origin. Then, using the local form of the Hamiltonian, i.e. (4.13), and the fact that observables with spatially disjoint support commute, we find that the first order term is

$$[H_N, A] = ([h_{-1,0}, A] + [h_{0,1}, A]) \in \mathcal{A}_{\{-1,0,1\}}. \tag{4.15}$$

A similar calculation shows that

$$[H_N, [H_N, A]] \in \mathcal{A}_{\{-2,-1,0,1,2\}} \tag{4.16}$$

and in for general $n \geq 0$,

$$([H_N, \cdot])^n(A) \in \mathcal{A}_{[-\min(n,N), \min(n,N)]}. \tag{4.17}$$

As a consequence, if we take $B \in \mathcal{A}_{\{x\}}$ for some $x \in [-N, N]$, one readily sees that

$$[\tau_t^N(A), B] = \mathcal{O}(|t|^{|x|}), \tag{4.18}$$

suggesting that, for $A \in \mathcal{A}_{\{0\}}$, the commutator of $\tau_t^N(A)$ with $B \in \mathcal{A}_{\{x\}}$, is small for t small and x large. One observes, however, that direct analysis of the series expansion does not look appealing due to the fast growth in n of the number of terms that contribute at order n. In any case, we are interested in an explicit estimate for the norm of commutators of this type. The following Lemma shows how such estimates could be used.

Lemma 4.1. *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two complex Hilbert spaces. Suppose that, for $\epsilon > 0$, $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ satisfies*

$$\|[A, \mathbb{1} \otimes B]\| \leq \epsilon \|B\|, \tag{4.19}$$

for all $B \in \mathcal{B}(\mathcal{H}_2)$. Then there exists $A' \in \mathcal{B}(\mathcal{H}_1)$, $\|A'\| \leq \|A\|$, such that

$$\|A' \otimes \mathbb{1} - A\| \leq \epsilon \tag{4.20}$$

So, if $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ has a small commutator with all $B \in \mathcal{B}(\mathcal{H}_2)$, then A is well-approximated by observable in $\mathcal{B}(\mathcal{H}_1)$, i.e., one with support in the complement of the support of the B's.

If $\dim(\mathcal{H}_2) < \infty$, the local operator in the statement of the lemma can be taken to be

$$A' = \frac{1}{\dim(\mathcal{H}_2)} \mathrm{Tr}_2 A, \tag{4.21}$$

where Tr_2 denotes the partial trace over $\mathcal{H}_2$.

Proof of Lemma 4.1 in the finite-dimensional case: If $\dim \mathcal{H}_2 < \infty$, a simple application of Schur's Lemma shows that, for $B \in \mathcal{B}(\mathcal{H}_2)$,

$$\frac{1}{\dim(\mathcal{H}_2)} \mathrm{Tr} B = \int_{U(\mathcal{H}_2)} U^* B U \, dU, \tag{4.22}$$

where $U(\mathcal{H}_2)$ is the unitary group and dU is the normalized Haar-measure on $U(\mathcal{H}_2)$. From this expression, we see that A' as defined in (4.21) can be expressed by

$$A' \otimes \mathbb{1} = \int_{U(\mathcal{H}_2)} (\mathbb{1} \otimes U^*) A (\mathbb{1} \otimes U) \, dU \tag{4.23}$$

Then,

$$A' \otimes \mathbb{1} - A = \int_{U(\mathcal{H}_2)} \{ (\mathbb{1} \otimes U^*) A (\mathbb{1} \otimes U) - (\mathbb{1} \otimes U^*)(\mathbb{1} \otimes U) A \} \, dU, \tag{4.24}$$

and so

$$\| A' \otimes \mathbb{1} - A \| \leq \int_{U(\mathcal{H}_2)} \| (\mathbb{1} \otimes U^*)[A, (\mathbb{1} \otimes U)] \| \, dU \leq \epsilon \tag{4.25}$$

since $\|U\| \leq 1$. This completes the proof for the case of finite-dimensional $\mathcal{H}_2$. For a proof in the case of arbitrary Hilbert spaces and further discussion see [50]. □

In our analysis of commutator bounds we will use solutions of Schrödinger equations with time-dependent Hamiltonians, or so-called non-autonomous quantum systems. This is of course an interesting subject in its own right. Here, we limit ourselves to the simplest situation: that of a norm-continuous function $t \mapsto H(t) \in \mathcal{B}(\mathcal{H})$. We are interested in the initial value problem

$$\begin{aligned} \frac{d}{dt}\psi(t) &= -iH(t)\psi(t) \\ \psi(0) &= \psi_0 \in \mathcal{H}. \end{aligned} \tag{4.26}$$

Existence and uniqueness of the solutions follows from standard results for differential equantions. The following construction shows that the solution can be expressed in terms of a family of unitary operators on $\mathcal{H}$, which, for reasons that will become clear later, we will denote by $U(t,0)$. $U(t,0)$ is given by the following absolutely convergent series, called the Dyson series or sometimes 'time-ordered exponential':

$$U(t,0) = \mathbb{1} + \sum_{n=1}^{\infty} (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \, H(t_1) H(t_2) \cdots H(t_n). \tag{4.27}$$

It is straightforward to verify that

$$\frac{d}{dt} U(t,0) = -iH(t)U(t,0), \quad U(0,0) = \mathbb{1}, \tag{4.28}$$

which immediately implies that $\psi(t) = U(t,0)\psi(0)$ solved (4.26), for all $\psi_0 \in \mathcal{H}$. By taking adjoints of both sides of (4.28) we obtain a similar equation for $U(t,0)^*$:

$$\frac{d}{dt} U(t,0)^* = iU(t,0)^* H(t), \quad U(0,0)^* = \mathbb{1}, \tag{4.29}$$

Using (4.28) and (4.29) we find that the derivative of $U(t,0)^*U(t,0)$ vanishes for all $t \in \mathbb{R}$, and we conclude that $U(t,0)$ is unitary as claimed. Therefore, for $s,t \in \mathbb{R}$, we can define a unitary $U(t,s) = U(t,0)U(s,0)^*$. It is easy to verify that $U(t,s)$ satisfies $U(t,s)^* = U(t,s)^{-1} = U(s,t)$ and the cocycle property: $U(t,s)U(s,r) = U(t,r)$, for $r,s,t \in \mathbb{R}$.

The Heisenberg dynamics of observables can then be given in terms of a co-cycle of automorphisms $\tau_{t,s}$ defined by

$$\tau_{t,s}(A) = U(t,s)^* A U(t,s), A \in \mathcal{B}(\mathcal{H}). \tag{4.30}$$

The automorphisms satisfy the equation

$$\frac{d}{dt}\tau_{t,0}(A) = i\tau_{t,0}([H(t),A]) = i[\tau_{t,0}(H(t)), \tau_{t,0}(A)]). \tag{4.31}$$

4.2. **Infinite Systems.** We already indicated that one is often interested in families of finite systems defined on finite subsets Λ of an infinite set Γ, with an interaction Φ defined on $\mathcal{P}_0(\Gamma)$, the finite subsets of Γ. This will be the starting point for the definition of infinite quantum spin systems.

Let (Γ, d) be a countable metric space. We will impose certain regularity conditions on (Γ, d). An example to keep in mind is $\mathbb{Z}^\nu$ with the usual graph (i.e., the ℓ^1) distance. To each $x \in \Gamma$, we associate a finite-dimensional, single-site Hilbert space of states $\mathcal{H}_x = \mathbb{C}^{d_x}$. As before, the algebra of observables at the site x will be denoted by $\mathcal{A}_x = \mathcal{B}(\mathcal{H}_x) = M_{d_x}$. For any finite volume $\Lambda \subset \Gamma$, we then have

$$\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{H}_x \quad \text{and} \quad \mathcal{A}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{A}_x \tag{4.32}$$

As we have seen, if $\Lambda_0 \subset \Lambda$ are two finite subsets of Γ, then $\mathcal{A}_{\Lambda_0} \subset \mathcal{A}_\Lambda$. It therefore makes sense to consider the union over all finite subsets of Γ:

$$\mathcal{A}_\Gamma^{\mathrm{loc}} = \bigcup_{\Lambda\subset\Gamma} \mathcal{A}_\Lambda. \tag{4.33}$$

The C^*-algebra of all quasi-local observables is the norm completion of $\mathcal{A}_\Gamma^{\mathrm{loc}}$:

$$\mathcal{A}_\Gamma = \overline{\mathcal{A}_\Gamma^{\mathrm{loc}}}^{\|\cdot\|}. \tag{4.34}$$

An *interaction* Φ is a map from the finite subsets of Γ to $\mathcal{A}_\Gamma^{\mathrm{loc}}$, $\Phi : \mathcal{P}_0(\Gamma) \to \mathcal{A}_\Gamma^{\mathrm{loc}}$, that satisfies

$$\Phi(X)^* = \Phi(X) \in \mathcal{A}_X \quad \text{for each } X \in \mathcal{P}_0(\Gamma). \tag{4.35}$$

The Heisenberg dynamics associated to this interaction is then defined for any finite $\Lambda \subset \Gamma$ in terms of the self-adjoint finite-volume Hamiltonian

$$H_\Lambda = \sum_{X\subset\Lambda} \Phi(X), \tag{4.36}$$

For each $\Lambda \in \mathcal{P}_0(\Gamma)$, the finite-volume dynamics is given by

$$\tau_t^\Lambda(A) = e^{itH_\Lambda} A e^{-itH_\Lambda} \quad \text{for any } A \in \mathcal{A}_\Lambda \text{ and } t \in \mathbb{R}. \tag{4.37}$$

So far, we have a family, labeled by $\Lambda \in \mathcal{P}_0(\Gamma)$, of one-parameter groups of $*$-automorphisms on $\mathcal{A}_\Lambda$. We are interested in a framework where it makes sense to consider infinite systems describing bulk matter. Note that one can regard the τ_t^Λ as automorphisms defined on $\mathcal{A}_{\Lambda'}$, with $\Lambda \subset \Lambda'$, $\mathcal{A}_\Gamma^{\mathrm{loc}}$, or $\mathcal{A}_\Gamma$, for which $\mathcal{A}_\Lambda$ is an invariant subspace. Therefore, it makes sense to consider the convergence of τ_t^Λ as automorphisms on $\mathcal{A}_\Gamma$ as $\Lambda \nearrow \Gamma$.

A convenient way to express sufficient conditions for the existence of the infinite-volume limit of the dynamics (and other quantities), is by means of a function $F : [0,\infty) \to (0,\infty)$, which we will refer to as an *F-function* if it satisfies the following properties:

i. *Non-increasiing:* for $0 \le r \le s$, we have $F(r) \ge F(s)$;

ii. *Uniform integrability:*

$$\|F\| = \sup_{x\in\Gamma} \sum_{y\in\Gamma} F(d(x,y)) < \infty \tag{4.38}$$

iii. *Convolution condition:* There exists $C_F < \infty$ such that for any $x, y \in \Gamma$

$$\sum_{z\in\Gamma} F(d(x,z))F(d(z,y)) \leq C_F F(d(x,y)) \tag{4.39}$$

For example, if $\Gamma = \mathbb{Z}^\nu$, then for any $\epsilon > 0$, one can take

$$F(r) = (1+r)^{-(\nu+\epsilon)} \tag{4.40}$$

which is clearly, uniformly integrable. Moreover, it is easy to check that the convolution property holds with

$$C_F = 2^{\nu+\epsilon}\|F\| \tag{4.41}$$

works in (4.39).

It is also convenient to observe that if F is an F-function on (Γ, d) - as described above, then for any $a \geq 0$,

$$F_a(r) = e^{-ar}F(r) \tag{4.42}$$

also satisfies the required properties required i-iii) above (i.e. F_a is also an F-function on (Γ, d)) with $\|F_a\| \leq \|F\|$ and $C_{F_a} \leq C_F$.

In terms of any F-function on (Γ, d), we can define a Banach space of interactions Φ with the norm

$$\|\Phi\|_F = \sup_{x,y\in\Gamma} \frac{1}{F(d(x,y))} \sum_{\substack{X\subset\Gamma:\\ x,y\in X}} \|\Phi(X)\|. \tag{4.43}$$

Then, $\mathcal{B}_F(\Gamma) = \{\Phi \mid \Phi \text{ is an interaction s.t. } \|\Phi\|_F < \infty\}$. This norm $\|\cdot\|_F$, often referred to as an F-norm, expresses the decay of the interaction strength at long distances: for each pair of points $x, y \in \Gamma$, the sum over all interaction terms which involve this pair must decay faster than F, in the sense that for any $x, y \in \Gamma$, we have

$$\sum_{\substack{X\subset\Gamma:\\ x,y\in X}} \|\Phi(X)\| \leq \|\Phi\|_F F(d(x,y)). \tag{4.44}$$

A commonly used bound for the total interaction energy per spin is

$$|||\Phi|||_0 = \sup_{x\in\Gamma} \sum_{\substack{X\in\mathcal{P}_0(\Gamma)\\ x\in X}} \frac{1}{|X|}\|\Phi(X)\|. \tag{4.45}$$

and is an easy exercise to show $|||\Phi|||_0 \leq \|F\|\|\Phi\|_F$. We then also have the frequently used bound

$$\sup_{x\in\Gamma} \sum_{\substack{X\in\mathcal{P}_0(\Gamma)\\ x\in X}} \|\Phi(X)\| \leq \|F\|\|\Phi\|_F. \tag{4.46}$$

5. Lieb-Robinson Bounds

We will now state and prove a version of the quasi-locality estimates known as Lieb-Robinson bounds. Lieb-Robinson bounds can be expressed a number of different forms, and the precise manner typically depends on the application one has in mind. Often one is considering a dynamics generated by nearest neighbor interactions. In this case, it seems intuitively clear that the spread of the interactions through the system should depend on the surface area of the support of a local observable, not its volume.

Let $\Lambda \in \mathcal{P}_0(\Gamma)$. For any $X \subset \Lambda$, we will denote the surface of X in Λ by

$$S_\Lambda(X) = \{Z \subset \Lambda : Z \cap X \neq \emptyset \text{ and } Z \cap (\Lambda \setminus X) \neq \emptyset\} \tag{5.1}$$

and set $S(X) = S_\Gamma(X)$ for brevity. The Φ-boundary of a set $X \in \mathcal{P}_0(\Gamma)$ is then defined to be

$$\partial_\Phi X = \{x \in X : \exists Z \in S(X) \text{ with } x \in Z \text{ and } \Phi(Z) \neq 0\}. \tag{5.2}$$

It is clear that for general Φ, $\partial_\Phi X = X$, but if Φ is finite range and X is sufficiently large, we have that $\partial_\Phi X$ is a proper subset of X.

A Lieb-Robinson bound may be stated as follows.

Theorem 5.1 (Lieb-Robinson Bound [**?**, 34, 44, 51])**.** *Let $\Phi \in \mathcal{B}_F(\Gamma)$, $X, Y, \Lambda \in \mathcal{P}_0(\Gamma)$, such that $X, \cap Y = \emptyset$. Then, for all $A \in \mathcal{A}_X$ and $B \in \mathcal{A}_Y$, we have the estimate*

$$\left\| [\tau_t^\Lambda(A), B] \right\| \leq \frac{2\,\|A\|\,\|B\|}{C_F} \left(e^{2\,\|\Phi\|_F\, C_F\,|t|} - 1 \right) D(X, Y), \tag{5.3}$$

holds for all $t \in \mathbb{R}$. Here the quantity $D(X, Y)$ is given by

$$D(X, Y) = \min \left\{ \sum_{x \in X} \sum_{y \in \partial_\Phi Y} F\left(d(x, y)\right), \sum_{x \in \partial_\Phi X} \sum_{y \in Y} F\left(d(x, y)\right) \right\}. \tag{5.4}$$

Before we prove this bound, a number of comments are useful in interpreting this theorem.

First, one always has the trivial bound $\|[\tau_t^\Lambda(A), B]\| \leq 2\|A\|\|B\|$. This trivial estimate is usually better when $|t|$ is large and also holds when $X \cap Y \neq \emptyset$.

Next, if Φ is exponentially decaying, i.e. there is $a > 0$ for which $\Phi \in \mathcal{B}_{F_a}(\Gamma)$ with $F_a(r) = e^{-ar} F(r)$, then

$$\begin{aligned} D(X, Y) &\leq \min \left\{ \sum_{x \in X} \sum_{y \in \partial_\Phi Y} F\left(d(x, y)\right), \sum_{x \in \partial_\Phi X} \sum_{y \in Y} F\left(d(x, y)\right) \right\} e^{-a d(X, Y)} \\ &\leq \min\left\{ |\partial_\Phi X|, |\partial_\Phi Y| \right\} \|F\| e^{-a d(X, Y)} \end{aligned} \tag{5.5}$$

In this case, the bound (5.3) implies

$$\left\| [\tau_t^\Lambda(A), B] \right\| \leq \frac{2\,\|A\|\,\|B\|\,\|F\|}{C_a} \min\left\{ |\partial_\Phi X|, |\partial_\Phi Y| \right\} e^{-a \left[d(X, Y) - \frac{2\|\Phi\|_a C_a}{a} |t| \right]}, \tag{5.6}$$

If Φ is finite range on $\mathbb{Z}^\nu$, then $\Phi \in \mathcal{B}_{F_a}(\mathbb{Z}^\nu)$ for all $a > 0$. For $\Phi \in \mathcal{B}_{F_a}$, with $a > 0$, (5.6) can be interpreted as a bound on the velocity of propagation given by

$$v_{\Phi, a} = \frac{2\|\Phi\|_a C_a}{a}. \tag{5.7}$$

It is also important to observe that for fixed local observables A and B, the bounds above, (5.3) and similarly (5.6) if applicable, are independent of the volume $\Lambda \in \mathcal{P}_0(\Gamma)$. This will be key in our proof of the existence of the infinite-volume dynamics.

Finally, we note that the bound above only depends on the minimal cardinality of Φ-boundaries. Hence, one may still obtain useful estimates even in cases where one of the corresponding observables has support growing with the volume Λ.

In the proof of Theorem 5.1 we will use the lemma below, which provide a simple estimate for the growth of solutions of a class of differential equations in a Banach space. In this lemma the derivative is to be interpreted as a limit in the Banach space norm and the integrals in the proof may be interpreted as Riemann or Bochner integrals.

Let X be a Banach space and let I be a finite or infinite interval $\subset \mathbb{R}$. Suppose $A : I \to \mathcal{B}(X)$ be a continuous function with values in the bounded linear operators on X considered with the operator norm, and denote by $x(t)$ the solution of the differential equation

$$\partial_t x(t) \;=\; A(t)\, x(t) \tag{5.8}$$

with initial condition $x(t_0) = x_0 \in X$. We say that the family of operators $A(t)$ is *norm-preserving* if for every $x_0 \in X$, the mapping $\gamma_t : X \to X$ which associates $x_0 \to x(t)$, i.e., $\gamma_t(x_0) = x(t)$, satisfies

$$\| \gamma_t(x_0) \| \;=\; \| x_0 \| \quad \text{for all } t \in I. \tag{5.9}$$

Some obvious examples are the case where X is a Hilbert space and $A(t)$ is anti-hermitian for each t, or when X is a $*$-algebra of operators on a Hilbert space with a spectral norm and, for each t, $A(t)$ is a derivation commuting with the $*$-operation.

Lemma 5.2. *Let $A(t)$, for $t \in I \subset \mathbb{R}$, be a family of norm preserving operators on a Banach space X. For any continuous function $b : I \to X$, the solution of*

$$\partial_t y(t) \;=\; A(t) y(t) \;+\; b(t), \tag{5.10}$$

with boundary condition $y(t_0) = y_0$, satisfies the bound

$$\| y(t) \;-\; \gamma_t(y_0) \| \;\leq\; \int_{\min(t_0,t)}^{\max(t_0,t)} \| b(s) \|\, ds. \tag{5.11}$$

Proof. For any $t \in \mathbb{R}$, let $x(t)$ be the solution of

$$\partial_t x(t) \;=\; A(t)\, x(t) \tag{5.12}$$

with boundary condition $x(0) = x_0$, and let γ_t be the linear mapping which takes x_0 to $x(t)$. By variation of constants, the solution of the inhomogeneous equation (5.10) may be expressed as

$$y(t) \;=\; \gamma_t \left(y_0 \;+\; \int_0^t (\gamma_s)^{-1} \left(b(s) \right) ds \right). \tag{5.13}$$

The estimate (5.11) follows from (5.13) as $A(t)$ is norm preserving. □

Proof of Theorem 5.1: We prove (5.3) in two steps. First, we use Lemma 5.2 to establish a basic inequality, see (5.20) below. Next, using properties of the F-function, iteration of (5.20) yields (5.3) as claimed. Without loss of generality we may assume that $X, Y \subset \Lambda$.

First note that, the roles of A and B, and hence the roles their respective supports, X and Y, can be interchanged. This is due to the automorphism property of the dynamics, which gives

$$\|[\tau^\Lambda_{-t}(B), A]\| = \|\tau^\Lambda_t \left([\tau^\Lambda_{-t}(B), A] \right) \| = \|[\tau^\Lambda_t(A), B]\| \tag{5.14}$$

and the argument below can be applied to the left hand side of (5.14).

Therefore, without loss of generality, we can assume that

$$D(X, Y) = \sum_{x \in \partial_\Phi X} \sum_{y \in Y} F\left(d(x, y) \right) \tag{5.15}$$

To prove (5.20), consider the function

$$f(t) = \left[\tau^\Lambda_t \left(\tau^X_{-t}(A) \right), B \right], \tag{5.16}$$

where A and B are as in the statement of the theorem. Note that the inner dynamics, $\tau^X_{-t}(A)$, corresponds to evolution by the local Hamiltonian H_X, as defined e.g. in (4.3), with X being the

support of the observable A. It is straightforward to verify

$$\begin{aligned} f'(t) &= i\left[\tau_t^\Lambda\left(\left[H_\Lambda - H_X, \tau_{-t}^X(A)\right]\right), B\right] \\ &= i\sum_{Z\in S_\Lambda(X)}\left[\left[\tau_t^\Lambda\left(\Phi(Z)\right), \tau_t^\Lambda\left(\tau_{-t}^X(A)\right)\right], B\right] \\ &= i\sum_{Z\in S_\Lambda(X)}\left[\tau_t^\Lambda\left(\Phi(Z)\right), f(t)\right] - i\sum_{Z\in S_\Lambda(X)}\left[\tau_t^\Lambda(\tau_{-t}^X(A)), \left[\tau_t^\Lambda\left(\Phi(Z)\right), B\right]\right]. \end{aligned} \tag{5.17}$$

where for the last equality we used the Jacobi identity. The first term in (5.17) above is norm preserving, and therefore, Lemma 5.2 implies that

$$\|[\tau_t^\Lambda(\tau_{-t}^X(A)), B]\| \le \|[A,B]\| + 2\|A\| \sum_{Z\in S_\Lambda(X)} \int_{\min\{0,t\}}^{\max\{0,t\}} \left\|[\tau_s^\Lambda(\Phi(Z)), B]\right\| ds. \tag{5.18}$$

To ease notation, we will assume that $t \ge 0$ for the remainder of the argument. Changing the sign of t is equivalent to changing the sign of Φ and therefore leaves the estimate unchanged. For any $Z \in \mathcal{P}_0(\Gamma)$, introduce the quantity

$$C_B^\Lambda(Z;t) = \sup_{\substack{A\in\mathcal{A}_Z:\\ A\neq 0}} \frac{\|[\tau_t^\Lambda(A), B]\|}{\|A\|}. \tag{5.19}$$

Since $\mathrm{supp}(\tau_{-t}^X(A)) \subset X$ and $\|\tau_{-t}^X(A)\| = \|A\|$ (both for all $t \in \mathbb{R}$), the inequality (5.18) clearly implies

$$C_B^\Lambda(X;t) \le C_B^\Lambda(X;0) + 2\sum_{Z\in S_\Lambda(X)} \|\Phi(Z)\| \int_0^t C_B^\Lambda(Z;s) ds. \tag{5.20}$$

Note: it is clear from (5.20) that single-site interaction terms, i.e. those of the form $\Phi(\{z\})$ for some $z \in \Gamma$, do not contribute to this locality estimate.

The claim in (5.3) now follows from (5.20) by iteration. In fact, it is clear from the definition, see (5.19), that for any finite $Z \subset \Lambda$,

$$C_B^\Lambda(Z;0) \le 2\|B\|\,\delta_Y(Z) \tag{5.21}$$

where δ_Y is defined by

$$\delta_Y(Z) = \begin{cases} 1 & \text{if } Z\cap Y \neq \emptyset, \\ 0 & \text{otherwise.} \end{cases} \tag{5.22}$$

To prove (5.3), let $N \ge 1$. Iteration of (5.20) using (5.21) yields

$$C_B^\Lambda(X;t) \le 2\|B\|\left(\delta_Y(X) + \sum_{n=1}^N a_n \frac{(2t)^n}{n!}\right) + R_{N+1}(t) \tag{5.23}$$

where

$$a_n = \sum_{Z_1\in S_\Lambda(X)} \sum_{Z_2\in S_\Lambda(Z_1)} \cdots \sum_{Z_n\in S_\Lambda(Z_{n-1})} \left(\prod_{j=1}^n \|\Phi(Z_j)\|\right) \delta_Y(Z_n) \tag{5.24}$$

and

$$\begin{aligned} R_{N+1}(t) &= 2^{N+1} \sum_{Z_1\in S_\Lambda(X)} \sum_{Z_2\in S_\Lambda(Z_1)} \cdots \sum_{Z_{N+1}\in S_\Lambda(Z_N)} \int_0^t \int_0^{s_1} \cdots \int_0^{s_N} \times \\ &\quad \times \left(\prod_{j=1}^{N+1} \|\Phi(Z_j)\|\right) C_B^\Lambda(Z_{N+1}; s_{N+1}) ds_{N+1} ds_N \cdots ds_1 \end{aligned} \tag{5.25}$$

The remainder term $R_{N+1}(t)$ is estimated as follows. First, we bound $C_B^\Lambda(Z_{N+1}; s_{N+1})$ with $2\|B\|$ using its definition (5.19). Next, we note that the sums above are over chains of sets $(Z_1, Z_2, \cdots, Z_{N+1})$ which satisfy $Z_1 \cap \partial_\Phi X \neq \emptyset$ and $Z_j \cap Z_{j-1} \neq \emptyset$ for $2 \leq j \leq N+1$. Therefore, there are points $w_1, w_2, \cdots, w_{N+1} \in \Lambda$ with $w_1 \in Z_1 \cap \partial_\Phi X$ and $w_j \in Z_j \cap Z_{j-1}$ for all $2 \leq j \leq N+1$. A simple upper bound on these sums is then obtained by estimating

$$\sum_{Z_1 \in S_\Lambda(X)} \sum_{Z_2 \in S_\Lambda(Z_1)} \cdots \sum_{Z_{N+1} \in S_\Lambda(Z_N)} * \quad \leq \sum_{w_1 \in \partial_\Phi X} \sum_{w_2, \ldots, w_{N+2} \in \Lambda} \sum_{\substack{Z_1, \ldots, Z_{N+1} \subset \Lambda: \\ w_k, w_{k+1} \in Z_k, k=1, \ldots, N+1}} * \tag{5.26}$$

where we have used that the last set Z_{N+1} must contain more than one point since $Z_{N+1} \in S_\Lambda(Z_N)$. By (4.44)

$$\sum_{\substack{Z_k \subset \Lambda: \\ w_k, w_{k+1} \in Z_k}} \|\Phi(Z_k)\| \leq \|\Phi\|_F F(d(w_k, w_{k+1})) \tag{5.27}$$

and the convolution property, we find that

$$\begin{aligned} R_{N+1}(t) &\leq 2\|B\| \cdot \frac{(2t)^{N+1}}{(N+1)!} \sum_{Z_1 \in S_\Lambda(X)} \sum_{Z_2 \in S_\Lambda(Z_1)} \cdots \sum_{Z_{N+1} \in S_\Lambda(Z_N)} \left(\prod_{j=1}^{N+1} \|\Phi(Z_j)\| \right) \\ &\leq 2\|B\| \cdot \frac{(2t\|\Phi\|_F)^{N+1}}{(N+1)!} \sum_{w_1 \in \partial_\Phi X} \sum_{w_2, \ldots, w_{N+2} \in \Lambda} \prod_{k=1}^{N+1} F(d(w_k, w_{k+1})) \\ &\leq \frac{2\|B\|}{C_F} \cdot \frac{(2t\|\Phi\|_F C_F)^{N+1}}{(N+1)!} \sum_{w_1 \in \partial_\Phi X} \sum_{w_{N+2} \in \Lambda} F(d(w_1, w_{N+2})) \end{aligned} \tag{5.28}$$

Since F is uniformly summable and X is finite, this bound clearly shows that $R_{N+1}(t)$ goes to 0 as $N \to \infty$. We have proven that

$$C_B^\Lambda(X; t) \leq 2\|B\| \sum_{n=1}^{\infty} a_n \cdot \frac{(2t)^n}{n!} \tag{5.29}$$

The coefficients a_n are bounded similarly. In fact, using the additional constraint that the final set Z_n must intersect Y, we find that

$$a_n \leq \frac{(C\|\Phi\|_F)^n}{C_F} \sum_{y \in Y} \sum_{x \in \partial_\Phi X} F(d(x, y)) \tag{5.30}$$

and therefore,

$$C_B(X; t) \leq \frac{2\,\|B\|}{C_F} \left(e^{2C_F \|\Phi\|_F t} - 1 \right) \sum_{y \in Y} \sum_{x \in \partial_\Phi X} F(d(x, y)), \tag{5.31}$$

□

In combination with Lemma 4.1, the Lieb-Robinson bounds of Theorem 5.1 show that the time evolution of a local observable with support in $X \in \mathcal{P}_0(\Gamma)$, yields an observable which, up to a small correction, is localized in a larger but still finite region. More precisely, for $X \in \mathcal{P}_0(\Gamma)$, and with $\|\Phi\|_a < \infty$, for some $a > 0$ and $v_{\Phi,a}$ is the quantity defined in (5.7), define

$$X(v_{\Phi,a}|t| + r) = \{x \in \Gamma \mid d(x, X) \leq v_{\Phi,a}|t| + r\}.$$

Then, for $A \in \mathcal{A}_X$, define

$$(\tau_t^\Lambda(A))_{X(v_{\Phi,a}|t|+r)} = \mathrm{Tr}_{\mathcal{H}_{\Lambda \setminus X(v_{\Phi,a}|t|+r)}} \tau_t^\Lambda(A).$$

Then $(\tau_t^\Lambda(A))_{X(v_{\Phi,a}|t|+r)} \in \mathcal{A}_{X(v_{\Phi,a}|t|+r)} \subset \mathcal{A}_\Lambda$ and

$$\|\tau_t^\Lambda(A) - (\tau_t^\Lambda(A))_{X(v_{\Phi,a}|t|+r)}\| \leq \frac{2\,\|A\|\,|X|}{C_a}\,\|F\|\,e^{-ar}.$$

This observation, and the fact that the bound above is uniform in Λ, is a clear indication that the dynamics of local observables under the interaction with the infinite system on Γ, should be well-defined. We prove that this is indeed the case in the next section.

5.1. **Existence of the Dynamics.** Lieb-Robinson bounds can be used to establish the existence of a limiting dynamics for interactions $\Phi \in \mathcal{B}_F(\Gamma)$. To see this we will consider limits of the finite volume dynamics along increasing, exhaustive sequences $\{\Lambda_n\}$, i.e., for all $n \geq 1$, $\Lambda_n \in \mathcal{P}_0(\Gamma)$, $\Lambda_n \subset \Lambda_{n+1}$, and for any $z \in \Gamma$, there exists an $n \geq 1$ for which $z \in \Lambda_n$.

Theorem 5.3. *Let $\Phi \in \mathcal{B}_F(\Gamma)$. Along any increasing, exhaustive sequence $\{\Lambda_n\}$ of finite subsets of Γ, the norm limit*

$$\tau_t(A) = \lim_{n\to\infty} \tau_t^{\Lambda_n}(A) \tag{5.32}$$

exists for all $t \in \mathbb{R}$ and $A \in \mathcal{A}_\Gamma^{\mathrm{loc}}$. The convergence in (5.32) is uniform for t in compact sets, and moreover, it is independent of the choice of exhaustive sequence $\{\Lambda_n\}$. The collection $\{\tau_t\}_{t\in\mathbb{R}}$, which we denote by the infinite volume dynamics corresponding to Φ, defines a strongly continuous, one parameter group of $*$-automorphisms on $\mathcal{A}_\Gamma$.

Proof. Let $A \in \mathcal{A}_\Gamma^{\mathrm{loc}}$ and denote by $X = \mathrm{supp}(A) \in \mathcal{P}_0(\Gamma)$. Take $m \geq 1$ large enough so that $X \subset \Lambda_m$. For any $n \geq m$, we have that,

$$\tau_t^{\Lambda_n}(A) - \tau_t^{\Lambda_m}(A) \;=\; \int_0^t \frac{d}{ds}\left(\tau_s^{\Lambda_n}\left(\tau_{t-s}^{\Lambda_m}(A)\right)\right)\,ds, \tag{5.33}$$

and since

$$\frac{d}{ds}\left(\tau_s^{\Lambda_n}\left(\tau_{t-s}^{\Lambda_m}(A)\right)\right) = i\tau_s^{\Lambda_n}\left(\left[H_{\Lambda_n} - H_{\Lambda_m}, \tau_{t-s}^{\Lambda_m}(A)\right]\right), \tag{5.34}$$

it is clear that for $t > 0$

$$\|\tau_t^{\Lambda_n}(A) - \tau_t^{\Lambda_m}(A)\| \;\leq\; \sum_{Z\in S_{\Lambda_n}(\Lambda_m)} \int_0^t \|[\tau_s^{\Lambda_m}(A), \Phi(Z)]\|\,ds. \tag{5.35}$$

(Again, analogous results hold for $t \leq 0$.) The estimate continues by dividing the above sum on Z:

$$\begin{aligned}
\|\tau_t^{\Lambda_n}(A) - \tau_t^{\Lambda_m}(A)\| \;&\leq\; 2\|A\|t \sum_{\substack{Z\in S_{\Lambda_n}(\Lambda_m):\\ Z\cap X\neq\emptyset}} \|\Phi(Z)]\| + \sum_{\substack{Z\in S_{\Lambda_n}(\Lambda_m):\\ Z\cap X=\emptyset}} \int_0^t \|[\tau_s^{\Lambda_m}(A), \Phi(Z)]\|\,ds \\
&\leq\; 2\|A\|t \sum_{x\in X} \sum_{z\in\Lambda_n\setminus\Lambda_m} \sum_{\substack{Z\subset\Lambda_n:\\ x,z\in Z}} \|\Phi(Z)\| \\
&\quad + \frac{2\|A\|}{C}\int_0^t (e^{2\|\Phi\|_F C_F s} - 1)\,ds \sum_{\substack{Z\in S_{\Lambda_n}(\Lambda_m):\\ Z\cap X=\emptyset}} \|\Phi(Z)\| \sum_{x\in X, z\in Z} F(d(x,z))
\end{aligned} \tag{5.36}$$

where we have used Theorem 5.1 on the second sum above. Observe that

$$\begin{aligned}\sum_{\substack{Z\in S_{\Lambda_n}(\Lambda_m):\\ Z\cap X=\emptyset}} \|\Phi(Z)\| \sum_{x\in X, z\in Z} F(d(x,z)) &\leq \sum_{x\in X}\sum_{z'\in\Lambda_n\setminus\Lambda_m}\sum_{z\in\Lambda_n} F(d(x,z)) \sum_{\substack{Z\subset\Lambda_n:\\ z,z'\in Z}} \|\Phi(Z)\| \\ &\leq \|\Phi\|_F \sum_{x\in X}\sum_{z'\in\Lambda_n\setminus\Lambda_m}\sum_{z\in\Lambda_n} F(d(x,z))F(d(z,z')) \\ &\leq C\|\Phi\|_F \sum_{x\in X}\sum_{z'\in\Lambda_n\setminus\Lambda_m} F(d(x,z')) \qquad (5.37)\end{aligned}$$

Altogether then, we have shown that

$$\|\tau_t^{\Lambda_n}(A) - \tau_t^{\Lambda_m}(A)\| \leq 2\|A\|\|\Phi\|_F \left(\int_0^t e^{2\|\Phi\|_F C_F s} ds\right) \sum_{x\in X}\sum_{z\in\Lambda_n\setminus\Lambda_m} F(d(x,z)) \qquad (5.38)$$

This proves that the sequence of finite volume evolutions is Cauchy and hence convergent; at least on $\mathcal{A}_\Gamma^{\mathrm{loc}}$. The remaining claims follow by elementary arguments. In particular, see the Exercise 15 of Sections 1-3. □

By general arguments of semi-group theory (see, e.g., [11][Proposition 6.2.3]), the strongly continuous, one-parameter group of $*$-automorphisms $\{\tau_t\}_{t\in\mathbb{R}}$ is generated by a closed operator δ in the following sense. For all $A \in \mathcal{A}_\Gamma^{\mathrm{loc}}$, using an estimate in terms of $\|\Phi\|_F$, one can show the existence of the limit in $\mathcal{A}_\Gamma$:

$$\delta(A) = \lim_{\Lambda\to\Gamma} [H_\Lambda, A]. \qquad (5.39)$$

and δ is the closure of this operator, meaning the domain of the generally unbounded operator δ, $\mathrm{dom}(\delta)$, contains $\mathcal{A}_\Gamma^{\mathrm{loc}}$ as a core. For $A \in \mathrm{dom}(\delta)$, we have

$$\frac{d}{dt}\tau_t(A) = i\delta(\tau_t(A)) = i\tau_t(\delta(A)), \qquad (5.40)$$

and it is customary to write $\tau_t = e^{it\delta}$.

6. Ground States and Equilibrium States

For a quantum spin system associated with a finite set Λ, the Hamiltonian $H_\Lambda = H_\Lambda^* \in \mathcal{A}_\Lambda$ is a self-adjoint operator acting on a finite-dimensional complex Hilbert space $\mathcal{H}_\Lambda$. Its spectrum is a finite set of real eigenvalues and a *ground state* is defined to be any state ω_0 that minimizes the energy, *i.e.* , such that

$$\omega_0(H_\Lambda) = \min\{\omega(H_\Lambda) \mid \omega \text{ a state on } \mathcal{A}_\Lambda\}. \tag{6.1}$$

It is a simple exercise to show that ground states of finite quantum spin systems are exactly those states that have density matrices with a range that is a subspace of the eigenspace corresponding to the smallest eigenvalue of H_Λ. The ground state of the system is unique if and only if this eigenvalue is simple.

For a finite quantum spin system with Hamiltonian H_Λ, thermal equilibrium at inverse temperature $\beta \in [0, \infty)$ is the unique state, the *Gibbs state*, given by the density matrix ρ_β defined as follows:

$$\rho_\beta = \frac{1}{Z_\beta} e^{-\beta H_\Lambda}, \quad Z_\beta = \mathrm{Tr} e^{-\beta H_\Lambda}. \tag{6.2}$$

In the sections below we derive some basic properties and equivalent characterizations of ground states and equilibrium states, which will be useful to formulate these concepts in the infinite system setting.

6.1. **Ground States.**

Let $E_0(\Lambda)$ denote the smallest eigenvalue of the Hamiltonian H_Λ on a finite-dimensional Hilbert space $\mathcal{H}_\Lambda$. In this context $E_0(\Lambda)$ is the *ground-state energy*, and any state ω on $\mathcal{A}_\Lambda$ such that $\omega(H_\Lambda) = E_0(\Lambda)$ is a *ground state*. In the following proposition it is shown that the set of all ground states for the system with Hamiltonian H_Λ is the set of all states satisfying $\omega(A^*[H_\Lambda, A]) \geq 0$, for all $A \in \mathcal{A}_\Lambda$, and that this property is inherited by limits of sequences of ground states of finite-volume systems defined on a sequence $\Lambda_n \in \mathcal{P}_0(\Gamma)$, defined by an interaction $\Phi \in \mathcal{B}_F(\Gamma)$, for any F-function F.

It is clear that to any sequence of finite volumes $\{\Lambda_n\}$ with $\Lambda_n \to \Gamma$, there correspond one or more sequences of ground-states ω_{Λ_n}. Using the Banach-Alaoglu theorem, it is easy to see that each of these sequences has an accumulation point (and a convergent subsequence).

Note that there is no simple definition of a limit of the Hilbert spaces $\mathcal{H}_{\Lambda_n}$, nor of the Hamiltonians H_{Λ_n}, but it makes perfect sense to consider the limiting states on $\mathcal{A}_\Gamma^{\mathrm{loc}}$, and, by unique continuous extension, also on $\mathcal{A}_\Gamma$. This provides a good option for defining *ground states* for the infinite volume Γ.

Proposition 6.1.
(i) Let ω be a state of a system with Hamiltonian H on a finite-dimensional Hilbert space $\mathcal{H}$, i.e. , suppose that the range of the density matrix ρ of ω is a subspace of the eigenspace of H corresponding to its smallest eigenvalue E_0. Then we have

$$\omega(A^*[H, A]) \geq 0, \text{ for all } A \in \mathcal{B}(\mathcal{H}). \tag{6.3}$$

Conversely, every state on $\mathcal{B}(\mathcal{H})$ satisfying (6.3) is a ground state of the system.
(ii) Let $\{\Lambda_n\}$ be an exhaustive sequence of finite volumes in Γ. For each $n \geq 1$, let ω_n be a ground state of H_{Λ_n}. If

$$\omega_n(A) \to \omega(A) \quad \text{for all } A \in \mathcal{A}_\Gamma^{\mathrm{loc}} \tag{6.4}$$

and

$$\delta_{\Lambda_n}(A) := [H_{\Lambda_n}, A] \to \delta(A) \quad \text{for all } A \in \mathcal{A}_\Gamma^{\mathrm{loc}} \tag{6.5}$$

in the strong sense (i.e. in norm), then ω is a state on $\mathcal{A}_\Gamma^{\mathrm{loc}}$ satisfying

$$\omega(A^*\delta(A)) \geq 0, \text{ for all } A \in \mathcal{A}_\Gamma^{\mathrm{loc}}. \tag{6.6}$$

Proof. (i). Observe that

$$\begin{aligned} \omega(A^*[H,A]) &= \mathrm{Tr}\rho A^*[H,A] \\ &= \mathrm{Tr}\rho A^*HA - \mathrm{Tr}H\rho A^*A = \mathrm{Tr}\rho A^*(H-E_0\mathbb{1})A \geq 0 \end{aligned} \tag{6.7}$$

where we have used $H\rho = E_0\rho$ and $H_\Lambda \geq E_0\mathbb{1}$.

To prove the converse, assume that there exists $0 \neq \psi \in \mathrm{ran}\rho$ such that $H\psi \neq E_0\psi$ and consider $A = |\psi_0\rangle\langle\psi|$ where $\psi_0 \neq 0$ and $H\psi_0 = E_0\psi_0$. An easy calculation shows that $\omega(A^*[H,A]) < 0$. Therefore, ω does not satisfy (6.3).

(ii). To study the limit $n \to \infty$, we write

$$\begin{aligned} &\omega(A^*\delta(A)) - \omega_{\Lambda_n}(A^*\delta_{\Lambda_n}(A)) \\ &= \omega\left(A^*\left(\delta(A) - \delta_{\Lambda_n}(A)\right)\right) + (\omega - \omega_{\Lambda_n})\left(A^*\left(\delta_{\Lambda_n}(A) - \delta(A)\right)\right) + (\omega - \omega_{\Lambda_n})(A^*\delta(A)). \end{aligned} \tag{6.8}$$

The limit of the first terms vanishes because of (6.5) and the fact that states are bounded linear functionals of unit norm. For the last term, for each $\epsilon > 0$, pick $B \in \mathcal{A}_\Gamma^{\mathrm{loc}}$ such that $\|A^*\delta(A) - B\| \leq \epsilon$ and use this to see that

$$\limsup_n |(\omega - \omega_{\Lambda_n})(A^*\delta(A))| \leq 2\epsilon. \tag{6.9}$$

Since ϵ is arbitrary, we can conclude that also the third term of (6.8) vanishes in the limit $n \to \infty$, and the claimed result follows. □

Note that there are in general many sequences H_{Λ_n} such that (6.5) holds with the same generator δ. The limits of ground states of each such sequence of finite-volume Hamiltonians will all satisfy (6.3) and it will make sense to consider them all as ground states of the C^*-dynamical system $(\mathcal{A}_\Gamma, \{\tau_t = e^{it\delta} \mid t \in \mathbb{R}\})$. Therefore, we adopt the following definition.

Definition 6.2. Let $\mathcal{A}$ be a C^*-algebra and $\{\tau_t = e^{it\delta} \mid t \in \mathbb{R}\}$ be a strongly continuous one-parameter group of automorphisms of $\mathcal{A}$. Then, a state ω on $\mathcal{A}$ is a ground-state for τ_t if

$$\omega(A^*\delta(A)) \geq 0 \quad \text{for all } A \in \mathrm{dom}(\delta). \tag{6.10}$$

Note that it suffices to require (6.10) for A in a core for δ. In the context of quantum spin systems defined by an interaction $\Phi \in \mathcal{B}_F(\Gamma)$, a convenient core for δ is given by the local observables $\mathcal{A}_\Gamma^{\mathrm{loc}}$.

The next proposition shows that ground states are time-invariant, *i.e.* , $\omega \circ \tau_t = \omega$, for all $t \in \mathbb{R}$.

Proposition 6.3. *Let $\mathcal{A}$ be a C^*-algebra and $\{\tau_t = e^{it\delta} \mid t \in \mathbb{R}\}$ be a strongly continuous one-parameter group of automorphisms of $\mathcal{A}$. Then, the following three conditions are equivalent:*

i. $\omega \circ \tau_t = \omega$, *for all* $t \in \mathbb{R}$;
ii. $\omega(\delta(A)) = 0$, *for all* $A \in \mathrm{dom}(\delta)$;
iii. $\omega(A^*\delta(A)) \in \mathbb{R}$, *for all* $A \in \mathrm{dom}(\delta)$.

We leave the proof of this proposition as an exercise for the reader. (Hint: $\omega(\delta(A^*A)) = 2i\mathrm{Im}[\omega(A^*\delta(A))]$.)

6.2. **Thermal Equilibrium, the Free Energy, and the Variational Principle for Gibbs States.** For a finite spin systems, the thermal equilibrium state at inverse temperature $\beta \in [0,\infty)$, can be defined as the minimizer of the *free energy* functional. This provides a definition of equilibrium states analogous to the definition of ground states as those states that minimize the energy. As we shall see, ground states correspond to zero temperature, *i.e.* , $\beta = +\infty$.

In order to define the free energy functional, we start with von Neumann's definition of the *entropy*, $S(\rho)$, of a state defined by a density matrix ρ:

$$S(\rho) = -\mathrm{Tr}\rho\log\rho. \tag{6.11}$$

Here $\rho \log \rho$ is defined through the functional calculus with the continuous function $x \log x : [0,1] \to \mathbb{R}$. When $\mathcal{H}$ is finite-dimensional the entropy is finite for all ρ and satisfies the bound

$$0 \leq S(\rho) \leq \log \dim \mathcal{H}, \tag{6.12}$$

the proof of which we leave as an exercise.

Let $H = H^* \in \mathcal{B}(\mathcal{H})$ be the Hamiltonian of a finite quantum spin system. The *Gibbs state* at inverse temperature $\beta \in (0, \infty)$ for the system with Hamiltonian H is defined by the density matrix

$$\rho_\beta = \frac{1}{Z(\beta)} e^{-\beta H}, \text{ with } Z(\beta) = \mathrm{Tr} e^{-\beta H}. \tag{6.13}$$

The normalization factor $Z(\beta)$ is called the *partition function*. We will denote the Gibbs state by ω_β. The parameter β corresponds to the temperature T in the sense that $\beta = (k_B T)^{-1}$, where k_B is Boltzmann's constant. Thus $T = 0$ corresponds to $\beta \to \infty$, and in turn to the ground state.

For $\beta \in (0, \infty)$, the free-energy functional F_β is given by

$$F_\beta(\rho) = \mathrm{Tr} \rho H - \beta^{-1} S(\rho). \tag{6.14}$$

Proposition 6.4. *ρ_β is the unique density matrix that minimizes F_β, i.e. , for all density matrices ρ we have*

$$F_\beta(\rho_\beta) \leq F_\beta(\rho), \text{ and } F_\beta(\rho) = F_\beta(\rho_\beta) \Rightarrow \rho = \rho_\beta. \tag{6.15}$$

Using this proposition, the minimum value of F_β is easily seen to be given by $f(\beta) = -\beta^{-1} \log Z(\beta)$ and is called the *free energy* of the system at inverse temperature β.

The proof of this proposition follows from a simple application of the following lemma.

Lemma 6.5 (Klein [58], Ohya-Petz [53])**.** *Let A and B be two non-negative definite matrices satisfying $0 \leq A, B \leq \mathbb{1}$ and such that $\ker B \subset \ker A$. Then*

$$\mathrm{Tr} A(\log A - \log B) \geq \mathrm{Tr}(A - B) + \frac{1}{2} \mathrm{Tr}(A - B)^2 \tag{6.16}$$

Proof. The function $f(x) = -x \log x$, $x > 0$, continuously extended such that $f(0) = 0$, is easily seen to be concave. In fact $f \in C^2((0, \infty))$ with

$$f''(x) = -\frac{1}{x} \tag{6.17}$$

By the Taylor Remainder Theorem and the expression for f'', it follows that for all x and y such that $0 \leq x < y \leq 1$, there exists a ξ such that $x \leq \xi \leq y$ and

$$f(y) - f(x) - (y - x) f'(y) = -\frac{1}{2}(x - y)^2 f''(\xi) \geq \frac{1}{2}(x - y)^2 \tag{6.18}$$

As A and B are non-negative definite, they are diagonalizable. Denote their eigenvalues by a_i and b_i, and the corresponding orthonormal eigenvectors by φ_i and ψ_i, respectively. From the assumptions it follows that $0 \leq a_i, b_i \leq 1$. Using the spectral decompositions of A and B, i.e.,

$$A = \sum_i a_i |\varphi_i\rangle\langle\varphi_i| \tag{6.19}$$

$$B = \sum_i b_i |\psi_i\rangle\langle\psi_i| \tag{6.20}$$

$$\sum_i |\varphi_i\rangle\langle\varphi_i| = \sum_i |\psi_i\rangle\langle\psi_i| = \mathbb{1} \tag{6.21}$$

we see that

$$\begin{aligned}
&\mathrm{Tr}A(\log A - \log B) - \mathrm{Tr}(A-B) - \frac{1}{2}\mathrm{Tr}(A-B)^2 \\
&= \sum_{ij} \mathrm{Tr}|\psi_i\rangle\langle\psi_i||\varphi_j\rangle\langle\varphi_j| \left[-f(A) + f(B) + (A-B)f'(B) - \frac{1}{2}(A^2+B^2-2AB)\right] \\
&= \sum_{ij} \mathrm{Tr}|\psi_i\rangle\langle\psi_i||\varphi_j\rangle\langle\varphi_j| \left[-f(a_j) + f(b_i) + (a_j-b_i)f'(b_i) - \frac{1}{2}(a_j-b_i)^2\right] \\
&\geq 0
\end{aligned}$$

where the last inequality follows from applying (6.18) term by term. □

Now to prove Proposition 6.4, we can apply Lemma 6.5 with $A = \rho$, where ρ is an arbitrary density matrix, and $B = \rho_\beta$. Note than $\ker B = \{0\}$. This gives

$$\beta(f_\beta - F(\beta)) = \mathrm{Tr}\rho\log\rho - \mathrm{Tr}\rho\log\left(\frac{e^{-\beta H}}{Z(\beta)}\right) \tag{6.22}$$

$$\geq \frac{1}{2}\mathrm{Tr}(\rho-\rho_\beta)^2 \geq 0 \tag{6.23}$$

If the RHS vanishes, we have $\rho = \rho_\beta$. Hence the minimum of F_β is uniquely attained for $\rho = \rho_\beta$.

6.3. **The Kubo-Martin-Schwinger condition.** Again, we consider a finite-dimensional Hilbert space $\mathcal{H}$, and a Hamiltonian $H = H^* \in \mathcal{A} = \mathcal{B}(\mathcal{H})$. Denote the Heisenberg dynamics by τ_t. Since H is bounded it is straightforward to define the analytic continuation of $\tau_t(A)$ for all $t \in \mathbb{C}$. A state ω on $\mathcal{A}$ is called a β-KMS state if, for all $A, B \in \mathcal{A}$, it satisfies

$$\omega(A\tau_{i\beta}(B)) = \omega(BA). \tag{6.24}$$

Proposition 6.6. *ω is a β-KMS state if and only if $\omega = \omega_\beta$, i.e. , the KMS state coincides with the Gibbs state.*

Proof. First, the KMS property of the Gibbs state follows from a simple computation using the dynamics and the cyclicity of the trace:

$$\mathrm{Tr}e^{-\beta H}Ae^{itH}Be^{-itH}|_{t=i\beta} = \mathrm{Tr}e^{-\beta H}Ae^{-\beta H}Be^{\beta H} = \mathrm{Tr}e^{-\beta H}BA. \tag{6.25}$$

For the other direction, we use an orthonormal basis of eigenvectors of H, $|1\rangle, \ldots, |n\rangle$, with eigenvalues $\lambda_1, \ldots, \lambda_n$. The β-KMS property of state with density matrix ρ with $A = |i\rangle\langle j|$ and $B = |k\rangle\langle l|$ then reads

$$\mathrm{Tr}\rho|i\rangle\langle j|e^{\beta(\lambda_l-\lambda_k)}|k\rangle\langle l| = \mathrm{Tr}\rho|k\rangle\langle l||i\rangle\langle j|, \tag{6.26}$$

which translates into

$$\delta_{k,j}\langle l \mid \rho \mid i\rangle e^{\beta(\lambda_l-\lambda_k)} = \delta_{i,l}\langle j \mid \rho \mid k\rangle. \tag{6.27}$$

since ρ is a density matrix, at least on of its diagonal matrix elements is non-zero, say $\langle i \mid \rho \mid i\rangle > 0$. With $l = i$ and $k \neq j$, the above relation implies that ρ is in fact diagonal in the eigenbasis of H. Finally, with $l = i$ and $k = j$, we obtain that there is a constant c such that

$$\langle i \mid \rho \mid i\rangle e^{\beta\lambda_i} = c. \tag{6.28}$$

It follows that ρ is the Gibbs state. □

Note that the arguments in the proof of this proposition rely on the finite-dimensionality of the Hilbert space.

6.4. **The Energy-Entropy Balance inequalities.** A third criterion for thermal equilibrium is expressed by a family of inequalities called the Energy-Entropy- Balance (EEB) inequalities. Again, for now we only consider finite systems and define $\delta(\cdot) = [H, \cdot]$. Then, we say that ω satisfies EEB at inverse temperature β if, for all $X \in \mathcal{A}$

$$\omega\left(X^*[H,X]\right) \geq \beta^{-1}\omega(X^*X)\log\left(\frac{\omega(X^*X)}{\omega(XX^*)}\right) \quad \text{for all } X \in \mathcal{A}. \tag{6.29}$$

Our next goal is to prove that, for a finite system, the EEB inequalities uniquely characterize the Gibbs state. First we prepare some auxiliary material that is also useful more generally.

The formulation of the EEB inequalities uses the function $f : [0,+\infty) \times [0,+\infty) \to (-\infty,+\infty]$ defined by

$$f(x,y) = \begin{cases} x\log\frac{x}{y} & \text{if } x,y > 0 \\ 0 & \text{if } x = 0, y \geq 0 \\ +\infty & \text{if } x > 0, y = 0 \end{cases} \tag{6.30}$$

In the following, whenever we write something of the form $x\log(x/y)$, we mean f as defined above. We will use the following elementary properties of f.

Proposition 6.7. *The function f defined in (6.30) has the following properties:*
(i) f is lower semicontinuous.
(ii) f is jointly convex in (x,y).
(iii) f is homogeneous of degree one. i.e., for all $\lambda \geq 0$,

$$f(\lambda x, \lambda y) = \lambda f(x,y)$$

(iv) For all finite sequences of non-negative numbers t_i, x_i, y_i, $i = 1,\ldots,n$, one has

$$f(\sum_i t_i x_i, \sum_i t_i y_i) \leq \sum_i t_i f(x_i, y_i).$$

We leave the proof of this proposition as an exercise for the reader.

Theorem 6.8 ([25,26])**.** *Let ω be a state on $\mathcal{A}$. The following are equivalent conditions:*
(i) ω is the Gibbs state corresponding to H and inverse temperature β.
(ii) For all $X \in \mathcal{A}$ one has

$$\beta\omega(X^*[H,X]) \geq \omega(X^*X)\log\frac{\omega(X^*X)}{\omega(XX^*)} = f(\omega(X^*X),\omega(XX^*)) \tag{6.31}$$

It is worth noting that the equilibrium condition expressed by the EEB is equivalent to the KMS condition in the general context of C^*-dynamical systems (see [11][Theorem 5.3.15]).

In the context of finite quantum spin systems, the theorem says that the Gibbs state satisfies the inequalities (6.31) for all $X \in \mathcal{A}$, and that it is the only state that does so. We will derive this property from the variational principle following a common procedure: we will define suitable curves in the space of all states that pass through the Gibbs state, or emanate from it, and compute and estimate the derivative of the free energy functional along these curves. The EEB inequalities will follow from expressing that the state ω minimizes the free energy functional. The converse direction will be proved by explicit computation. In order to define curves in the space of all states we use a class of semigroups on $\mathcal{A}$ described in the next section. Their definition and essential properties are as follows.

Let $X \in \mathcal{B}(\mathcal{H})$. Define $L_X : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, by

$$L_X(A) = X^*AX - \frac{1}{2}(X^*XA + AX^*X)$$

Clearly, as $\|L_X(A)\| \leq 2\|X\|^2\|A\|$, L_X is a bounded linear transformation on the Banach space $\mathcal{B}(H)$. Therefore, we can define

$$\gamma_t(A) = e^{tL_X}(A)$$

$(\gamma_t)_{t\geq 0}$ is a semigroup with the following properties: $\gamma_t(\mathbb{1}) = \mathbb{1}$, and $\gamma_t(A)$ is positive for all $t \geq 0$ and $A \geq 0$. For a prove of this and other important properties see, e.g., the lecture notes by Michael Wolf [70]. A map γ_t with this property is called a positive map and L_X generates a semigroup of such maps. From these properties it immediately follows that, for all t, there is a unique density matrix ρ_t such that

$$\mathrm{Tr}\rho_t A = \mathrm{Tr}\rho\gamma_t(A)$$

ρ_t is obtained from ρ by application of another semigroup of positive maps, γ_t^*, which are the adjoints of γ_t with respect to the Hilbert-Schmidt inner product on $\mathcal{B}(\mathcal{H})$. Its generator is given by

$$L_X^*(\rho) = X\rho X^* - \frac{1}{2}(X^*X\rho + \rho X^*X).$$

In the finite-dimensional context, γ_t is a well-defined bounded linear transformation on $\mathcal{A}$ for all $t \in \mathbb{R}$. The norm of it, however, diverges as $t \to -\infty$. So although we have curves ρ_t, in the space of density matrices defined for all $t \in \mathbb{R}$, we will only use $t \geq 0$. In infinite-dimensional situations γ_t is in general not defined for $t < 0$.

Proof of Theorem 6.8. The proof of the EEB inequalities consists in deriving the following two relations:

$$\lim_{t\downarrow 0} \frac{\mathrm{Tr}\rho_t H - \mathrm{Tr}\rho_\beta H}{t} = \omega_\beta(X^*[H, X]) \tag{6.32}$$

$$\lim_{t\downarrow 0} \frac{S(\rho_t) - S(\rho_\beta)}{t} \geq \omega_\beta(X^*X) \log \frac{\omega_\beta(X^*X)}{\omega_\beta(XX^*)} \tag{6.33}$$

Here, $\rho_\beta = \rho_0$, and $\omega_\beta(A) = \mathrm{Tr}\rho_\beta A$. The EEB inequalities then follow from the Variational Principle. Since

$$F_\beta(\rho_t) - F_\beta(\rho_\beta) \geq 0$$

and therefore, for all $t > 0$, we must have

$$\frac{\mathrm{Tr}\rho_t H - \mathrm{Tr}\rho_\beta H}{t} \geq \frac{1}{\beta}\frac{S(\rho_t) - S(\rho_\beta)}{t}$$

Below we take the limit $t \downarrow 0$, compute the LHS and prove a lower bound for the RHS. The resulting inequalities will turn out to be the EEB inequalities.

The derivative of the energy is easy to compute:

$$\frac{d}{dt}\omega(\gamma_t(H))\big|_{t=0} = \omega(L_X(H)) = \mathrm{Tr}\rho_\beta X^*HX - \frac{1}{2}\mathrm{Tr}\rho_\beta(X^*XH + HX^*X)$$

We are interested in the derivative in $\rho = \rho_\beta$. As $[\rho_\beta, H] = 0$, the last two terms are equal and can be combined. The result is (6.32).

For the entropy term we will need to differentiate operator valued functions of the type $\log A_t$. This is non-trivial. Usually the log function is defined by its series expansion around $\mathbb{1}$. To compute the derivative we will use the identity

$$\log x = \int_0^\infty \left[\frac{1}{1+t} - \frac{1}{x+t}\right] dt$$

for $x > 0$. So, for invertible $A_t \geq 0$, we consider

$$\begin{aligned}\frac{d}{dt}\log A_t &= \frac{d}{dt}\int_0^\infty \left[\frac{1}{1+s} - \frac{1}{A_t+s}\right] ds \\ &= \int_0^\infty (A_t+s)^{-1}\left(\frac{d}{dt}A_t\right)(A_t+s)^{-1} ds\end{aligned}$$

Here, we used the operator identity $A^{-1}(B-A)B^{-1} = A^{-1} - B^{-1}$ to compute

$$\frac{d}{dt}(A_t)^{-1} = -A_t^{-1}\left(\frac{d}{dt}A_t\right)A_t^{-1}$$

When we apply this to $-S(\rho_t)$ we get

$$\begin{aligned}\mathrm{Tr}\rho\frac{d}{dt}\log\rho_t\big|_{t=0} &= \mathrm{Tr}\rho\int_0^\infty \frac{1}{\rho+t}L_X^*(\rho)\frac{1}{\rho+t}dt \\ &= \mathrm{Tr}\rho\rho^{-1}L_X^*(\rho) \\ &= \mathrm{Tr}L_X^*(\rho)\end{aligned}$$

Now we can compute the derivative of the entropy term:

$$\begin{aligned}\frac{d}{dt}S(\rho_t)\big|_{t=0} &= -\mathrm{Tr}\frac{d}{dt}\rho_t\big|_{t=0} - \mathrm{Tr}\rho_t\frac{d}{dt}\log(\rho_t)\big|_{t=0} \\ &= -\mathrm{Tr}L_X^*(\rho)\log\rho - \mathrm{Tr}L_X^*(\rho) \\ &= -\mathrm{Tr}L_X^*(\rho)\log\rho\end{aligned}$$

where we used that $\mathrm{Tr}L_X^*(\rho) = \mathrm{Tr}\rho L_X(\mathbb{1}) = 0$.

Now we have to estimate (6.34). We will prove that

$$\begin{aligned}-\mathrm{Tr}\rho L_X(\log\rho) &= -\mathrm{Tr}\rho X^*(\log\rho)X + \frac{1}{2}\mathrm{Tr}\rho X^*X\log\rho + \frac{1}{2}\mathrm{Tr}\rho(\log\rho)X^*X \\ &\geq f(\mathrm{Tr}\rho X^*X, \mathrm{Tr}\rho XX^*)\end{aligned}$$

where f is the function defined in (6.30). To this end we use the spectral decomposition of ρ:

$$\rho = \sum_i \rho_i |\phi_i\rangle\langle\phi_i|\phi_i$$

Using this we can write the LHS of the inequality as follows:

$$-\sum_{ij}\rho_i\,\langle\phi_i, X^*\phi_j\rangle\log\rho_j\,\langle\phi_j, X\phi_i\rangle + \sum_{ij}\rho_i\log\rho_i\,\langle\phi_i, X^*\phi_j\rangle\,\langle\phi_j, X\phi_i\rangle$$

If we let a_{ij} denote the matrix elements $\langle\phi_j, X\phi_i\rangle$, this can be written as

$$\sum_{ij} f(\rho_i,\rho_j)|a_{ij}|^2$$

Property (iv) of Proposition 6.7 then yields

$$\begin{aligned}-\mathrm{Tr}\rho L_X(\log\rho) &\geq f(\sum_{ij}\rho_i|a_{ij}|^2, \sum_{ij}\rho_j|a_{ij}|^2) \\ &= f(\mathrm{Tr}\rho X^*X, \mathrm{Tr}\rho XX^*)\end{aligned}$$

This concludes the proof of (i) $\Rightarrow$ (ii) in Theorem 6.8.

The opposite direction proceeds by solving the EEB inequalities. Suppose the Hamiltonian has eigenvalues λ_i and an orthonormal basis of eigenvectors ϕ_i. We will use the basis E_{ij} for the matrices:

$$E_{ij} = |\phi_i\rangle\langle\phi_i|\phi_j, \quad E_{ij}^* = E_{ji}, \quad E_{ij}E_{kl} = \delta_{jk}E_{il} \quad .$$

The spectral decomposition of the Hamiltonian can then be written as

$$H = \sum_i \lambda_i E_{ii}.$$

First, we note that if ω satisfies (6.31), then the corresponding density matrix commutes with the Hamiltonian. This follows from the fact that the inequalities imply that, for all X,

$$\mathrm{Tr}\rho X^* H X - \mathrm{Tr}\rho X^* X H \in \mathbb{R}$$

and, as

$$\mathrm{Im}\ \mathrm{Tr}\rho X^* H X - \mathrm{Tr}\rho X^* X H = \mathrm{Tr} X^* X [\rho, H]$$

for arbitrary $X \in \mathcal{A}$, this implies $[\rho, H] = 0$. Hence, ρ has a spectral decomposition of the form

$$\rho = \sum_i \rho_i E_{ii}$$

Now, take $X = E_{ij}$ in the EEB inequalities. Then $[H, X] = (\lambda_i - \lambda_j) E_{ij}$, and the EEB inequality becomes:

$$\beta(\lambda_i - \lambda_j)\mathrm{Tr}\rho E_{jj} \geq f(\mathrm{Tr}\rho E_{jj}, \mathrm{Tr}\rho E_{ii})$$

By calculating the expectations this is

$$\beta(\lambda_i - \lambda_j)\rho_j \geq f(\rho_j, \rho_i) = \rho_j \log \frac{\rho_j}{\rho_i}. \tag{6.34}$$

We will first show that (6.34) implies that $\rho_i > 0$, for all i. Suppose that for some i, $\rho_i = 0$, and that $\rho_j > 0$ for some j, which must be the case since ρ is a density matrix. Then, the RHS of (6.34) equals $+\infty$, while the LHS is finite. We conclude that $\rho_i > 0$ for all i. Therefore we can divide both sides of (6.34) by ρ_j to obtain:

$$\beta(\lambda_i - \lambda_j) \geq \log \frac{\rho_j}{\rho_i}$$

By interchanging the roles of i and j in this inequality we see that the following equalities must hold for all i and j:

$$\beta(\lambda_i - \lambda_j) = \log \frac{\rho_j}{\rho_i}$$

or, equivalently

$$\rho_i = \text{constant} \times e^{-\beta\lambda_i},$$

where the constant is fixed by the normalization of ρ. This completes the proof that ρ_β is the only density matrix satisfying the EEB inequalities for a fixed H and $\beta \geq 0$. □

7. Infinite Systems and the GNS representation

There is a close connection between representations and states of a C^*-algebra. The key to this connection is the so-called GNS construction, attributed to Israel Gelfand and Mark Naimark and, independently, Irving Segal, whose initials provided the name. The GNS constructions associates with each state ω on a C^*-algebra a canonical representation, which is unique up to unitary equivalence. We will discuss the GNS representation in its general setting first, and then apply it to the context of quantum spin systems. In particular,in the case of ground states of infinite quantum spin systems we obtain a representation in which the dynamics is generated by a densely defined self-adjoint operator (the GNS Hamiltonian) which is bounded below and of which the ground state is given by an eigenvector of the smallest eigenvalue.

7.1. **The GNS Construction.** Let $\mathcal{A}$ be a unital C^*-algebra. A *representation* of $\mathcal{A}$ on a Hilbert space $\mathcal{H}$ is a linear mapping $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ for which:
i) $\pi(\mathbb{1}) = \mathbb{1}$
ii) $\pi(A^*) = \pi(A)^*$
iii) $\pi(AB) = \pi(A)\pi(B)$.

All C^*-algebras appearing in this book are assumed to have an identity, generically denoted by $\mathbb{1}$, and all representations of a C^*-algebra on a Hilbert space will be assumed to map the identity into the identity operator on the Hilbert space.

A vector $\Omega \in \mathcal{H}$ is called *cyclic* for a representation π if

$$\mathcal{D}_\Omega = \{\pi(A)\Omega : A \in \mathcal{A}\} \subset \mathcal{H} \tag{7.1}$$

is a dense subspace of $\mathcal{H}$. A representation π is said to be *cyclic* if there is a cyclic vector for it.

Theorem 7.1 (GNS construction)**.** *Let ω be a state on a C^*-algebra $\mathcal{A}$. Then there exists a Hilbert space $\mathcal{H}_\omega$, a representation π_ω of $\mathcal{A}$ on $\mathcal{H}_\omega$, and a vector $\Omega_\omega \in \mathcal{H}_\omega$, which is cyclic for π_ω and such that*

$$\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle \quad \text{for all } A \in \mathcal{A}. \tag{7.2}$$

Moreover, the triple $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ is uniquely determined by ω up to unitary equivalence. In other words, if there are two such cyclic representations $(\mathcal{H}_1, \pi_1, \Omega_1)$ and $(\mathcal{H}_2, \pi_2, \Omega_2)$ for the same state ω, then there exists a unitary mapping $U : \mathcal{H}_1 \to \mathcal{H}_2$ for which

$$\Omega_2 = U\Omega_1 \quad \text{and} \quad \pi_2(A) = U\pi_1(A)U^* \quad \text{for all } A \in \mathcal{A}. \tag{7.3}$$

The unitary U with these properties is itself unique.

Proof. First, we construct the Hilbert space. This is done in two steps. Note that

$$\langle A, B \rangle = \omega(A^*B) \tag{7.4}$$

defines a sesquilinear form on $\mathcal{A}$. Thus, $(\mathcal{A}, \langle \cdot, \cdot \rangle)$ is a pre-Hilbert space.

In general, this sesquilinear form may be degenerate; in which case it does not define an inner product. To remedy this, set

$$I = \{A \in \mathcal{A} : \omega(A^*A) = 0\}. \tag{7.5}$$

These correspond to the vectors with *zero norm*. One readily checks that I is a left ideal of $\mathcal{A}$. This means that I is a linear subspace of $\mathcal{A}$ for which given any $A \in \mathcal{A}$ and any $B \in I$, the product $AB \in I$. In words, I is invariant under left multiplication by elements in $\mathcal{A}$. To see this, we use $A^*A \leq \|A\|^2\mathbb{1}$. Since, for $B \in I$, $\omega(B^*B) = 0$, we then have

$$0 \leq \omega((AB)^*(AB)) = \omega(B^*A^*AB) \leq \omega(B^*B)\|A\|^2 = 0 \tag{7.6}$$

and thus $AB \in I$.

Let $\mathcal{H}_0$ be the quotient $\mathcal{A}/I$, which is the set of equivalence classes in $\mathcal{A}$ defined by I:

$$\psi_A = \{\tilde{A} \in \mathcal{A} : \tilde{A} = A + A' \text{ for some } A' \in I\} = A + I \tag{7.7}$$

As a quotient of a complex vector space by a subspace, $\mathcal{H}_0$ is a complex vector space, and we define a sesquilinear form in it by

$$\langle \psi_A, \psi_B \rangle = \langle A, B \rangle = \omega(A^* B) \tag{7.8}$$

for all equivalence classes ψ_A and ψ_B. It is clear that this form is well-defined: If $\tilde{A} = A + A'$ and $\tilde{B} = B + B'$ for some $A', B' \in I$, then

$$\omega((\tilde{A})^* \tilde{B}) = \omega(A^* B) + \omega(A^* B') + \omega((A')^* B) + \omega((A')^* B') = \omega(A^* B) \tag{7.9}$$

since the last three terms in the middle expression above vanish by Cauchy-Schwarz.

By construction, we now have a non-degenerate inner product space $\mathcal{H}_0$. We define $\mathcal{H}_\omega$ to be the Hilbert space obtained by completion of $\mathcal{H}_0$.

The next task is to define the representation π_ω of $\mathcal{A}$ on $\mathcal{B}(\mathcal{H}_\omega)$. Observe that, again by construction, $\{\psi_A : A \in \mathcal{A}\}$ is dense in $\mathcal{H}_\omega$. In this case, for any $A \in \mathcal{A}$, $\pi_\omega(A) \in \mathcal{B}(\mathcal{H}_\omega)$ will be uniquely defined if we define it on this dense subspace and show that

$$\|\pi_\omega(A)\| \leq \|A\|. \tag{7.10}$$

For any $A \in \mathcal{A}$, define a mapping $\pi_\omega(A)$ on $\mathcal{H}_0$ by setting

$$\pi_\omega(A)\psi_B = \psi_{AB} \tag{7.11}$$

This is well-defined because I is a left-ideal:

$$\pi_\omega(A)\psi_{B+B'} = \psi_{AB+AB'} = \psi_{AB} \quad \text{since } AB' \in I. \tag{7.12}$$

Since

$$\alpha\psi_C + \beta\psi_D = \psi_{\alpha C + \beta D}\,, \tag{7.13}$$

linearity of $\pi_\omega(A)$ is also easy to check. Moreover,

$$\|\pi_\omega(A)\psi_B\|^2 = \langle \psi_{AB}, \psi_{AB} \rangle = \omega(B^* A^* A B) \leq \|A\|^2 \omega(B^* B) = \|A\|^2 \|\psi_B\|^2 \tag{7.14}$$

which proves that $\|\pi_\omega(A)\| \leq \|A\|$ on $\mathcal{H}_0$. We will continue to denote by $\pi_\omega(A)$ the unique bounded extension of this mapping to all of $\mathcal{H}_\omega$. One easily checks that π_ω is a representation:

$$\begin{aligned}
&\pi_\omega(\mathbb{1})\psi_B = \psi_B \\
&\langle \pi_\omega(A^*)\psi_B, \psi_C \rangle = \omega((A^* B)^* C) = \omega(B^* A C) = \langle \psi_B, \pi_\omega(A)\psi_C \rangle \\
&\pi_\omega(A_1 A_2)\psi_B = \psi_{A_1 A_2 B} = \pi_\omega(A_1)\psi_{A_2 B} = \pi_\omega(A_1)\pi_\omega(A_2)\psi_B.
\end{aligned}$$

Finally, $\psi_{\mathbb{1}}$ is a cyclic vector with the desired properties. It is cyclic because

$$\{\pi_\omega(A)\Omega_\omega : A \in \mathcal{A}\} = \{\psi_A : A \in \mathcal{A}\} \tag{7.15}$$

is dense by construction of the Hilbert space. The desired relation with the state ω follows from the definition of the inner product on $\mathcal{H}_\omega$:

$$\langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle = \langle \psi_{\mathbb{1}}, \psi_A \rangle = \omega(A). \tag{7.16}$$

This completes the construction of a GNS triple $(\mathcal{H}_\omega, \pi_\omega, \Omega)$.

To prove the uniqueness statement, suppose there are two GNS triples, $(\mathcal{H}_1, \pi_1, \Omega_1)$ and $(\mathcal{H}_2, \pi_2, \Omega_2)$, with

$$\langle \Omega_1, \pi_1(A)\Omega_1 \rangle = \omega(A) = \langle \Omega_2, \pi_2(A)\Omega_2 \rangle \quad \text{for all } A \in \mathcal{A} \tag{7.17}$$

In this case, define a mapping $U : \mathcal{H}_1 \to \mathcal{H}_2$ by setting

$$U\pi_1(A)\Omega_1 = \pi_2(A)\Omega_2 \quad \text{for all } A \in \mathcal{A}. \tag{7.18}$$

Since Ω_1 is cyclic, and due to (7.17), this defines an isometry U on a dense set of vectors in $\mathcal{H}_1$; we will continue to denote by U the unique linear extension of this mapping to all of $\mathcal{H}_1$. Observe that

$$\begin{aligned} \langle U\pi_1(A)\Omega_1, U\pi_1(B)\Omega_1\rangle &= \langle \pi_2(A)\Omega_2, \pi_2(B)\Omega_2\rangle \\ &= \langle \Omega_2, \pi_2(A^*B)\omega_2\rangle \\ &= \omega(A^*B) = \langle \pi_1(A)\Omega_1, \pi_1(B)\Omega_1\rangle. \end{aligned} \tag{7.19}$$

This shows that U is an isometry. Since ran$U$ is dense, it follows that U is unitary, i.e. $U^*U = UU^* = \mathbb{1}$. It is straightforward to check the remaining properties of U. □

The uniqueness property of the GNS triple for a given state ω, which we henceforth denote by $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$, has an important consequence.

Corollary 7.2. *Let $\mathcal{A}$ be a C^*-algebra, ω a state on $\mathcal{A}$ and α an automorphism of $\mathcal{A}$ that leaves ω invariant, i.e. , such that $\omega \circ \alpha = \omega$. Then, α is implementable in the GNS representation of ω. Explicitly, there exists a unique unitary $U \in \mathcal{B}(\mathcal{H}_\omega)$ such that for all $A \in \mathcal{A}$ we have*

$$\pi_\omega(\alpha(A)) = U\pi_\omega(A)U^*, \quad U\Omega = \Omega. \tag{7.20}$$

Proof. If $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ is a GNS triple for ω, one can immediately check that $(\mathcal{H}_\omega, \pi_\omega \circ \alpha, \Omega_\omega)$ is a GNS triple for $\omega \circ \alpha$. By Theorem 7.1, the existence and uniqueness of a unitary operator U on $\mathcal{H}_\omega$ with the desired properties is then guaranteed:

$$U\Omega_\omega = \Omega_\omega, \quad \pi_\omega(\alpha(A)) = U\pi_\omega(A)U^*. \tag{7.21}$$

□

As a first application of this corollary, we explore its consequences for ground states, which are invariant under the automorphisms τ_t describing the time evolution (see Proposition 6.3).

Let ω be a ground state. From Corollary 7.2 we then have, for each $t \in \mathbb{R}$, a unique unitary U_t on $\mathcal{H}_\omega$ implementing τ_t (for consistency with the standard conventions in the quantum mechanics literature, we interchange the roles of U_t and U_t^*. Concretely, we have

$$U_t\Omega_\omega = \Omega_\omega \quad \text{and} \quad U_t^*\pi_\omega(A)U_t = \pi_\omega(\tau_t(A)) \quad \text{for all } A \in \mathcal{A}_\Gamma. \tag{7.22}$$

Using the uniqueness, one sees that the group property of the τ_t carries over to the U_t. and the continuity for the norm on $\mathcal{A}$ of $t \mapsto \tau_t(A)$ implies that $t \mapsto U_t\psi$ is continuous for all $\psi \in \mathcal{H}_\omega$. This is the strong continuity property of the one-parameter group of unitaries. To verify this, consider, for all $A \in \mathcal{A}$,

$$\begin{aligned} \|U_t^*\pi_\omega(A)\Omega_\omega - \pi_\omega(A)\Omega_\omega\| &= \|U_t^*\pi_\omega(A)U_tU_t^*\Omega_\omega - \pi_\omega(A)\Omega_\omega\| \\ &= \|\pi_\omega(\tau_t(A))\Omega_\omega - \pi_\omega(A)\Omega_\omega\| \\ &= \|\pi_\omega(\tau_t(A) - A)\Omega_\omega\|. \end{aligned} \tag{7.23}$$

The last quantity vanishes as $t \to 0$ by the strong continuity of τ_t.

Using Stone's Theorem 7.3, we now conclude that there is a densely defined self-adjoint operator H_ω acting on (a dense subset of) $\mathcal{H}_\omega$ for which

$$U_t = e^{-itH_\omega}. \tag{7.24}$$

We are now back to quantum mechanics on a Hilbert space, i.e., the Schrödinger picture in which one studies self- adjoint operators on a Hilbert space.

Note that using

$$U_t\Omega_\omega = \Omega_\omega, \tag{7.25}$$

and the ground state property of ω, we have that

$$\begin{aligned} 0 \leq \omega(A^*\delta(A)) &= \frac{1}{i}\frac{d}{dt}\omega(A^*\tau_t(A))|_{t=0} \\ &= \frac{1}{i}\frac{d}{dt}\langle\Omega_\omega, \pi_\omega(A^*\tau_t(A))\Omega_\omega\rangle|_{t=0} \\ &= \frac{1}{i}\frac{d}{dt}\langle\pi_\omega(A)\Omega_\omega, U_t^*\pi_\omega(A)U_t\Omega_\omega\rangle|_{t=0} \\ &= \langle\pi_\omega(A)\Omega_\omega, H_\omega\pi_\omega(A)\Omega_\omega\rangle \end{aligned} \tag{7.26}$$

and hence $H_\omega \geq 0$. This means that in its GNS representation a ground state is represented by an eigenvector of the Hamiltonian H_ω with eigenvalue 0, which corresponds to $\inf \mathrm{spec} H_\omega$.

For the readers's convenience, we include a statement of Stone's theorem here. See, e.g., [57] or [65] for a proof.

Theorem 7.3 (Stone's Theorem)**.** *For all $t \in \mathbb{R}$, let U_t be a bounded linear operator on a Hilbert space $\mathcal{H}$. Then, $\{U_t \mid t \in \mathbb{R}\}$ is a strongly continuous one-parameter group of unitary operators if and only if there exists a densely defined self-adjoint operator H with domain $D(H)$ such that*

$$U_t = e^{-itH}. \tag{7.27}$$

Moreover,

$$D(H) = \{\psi \in \mathcal{H} \mid \exists \phi \in \mathcal{H} \text{ such that } \lim_{t\to 0} \|t^{-1}(e^{-itH}\psi - \psi) - \phi\| = 0\}. \tag{7.28}$$

7.2. **Ground States and Equilibrium States for Infinite Systems.** Let us summarize the basic mathematical elements describing an infinite (or finite) quantum spin system. Associated with the points of a countable metric space (Γ, d), often referred to as the "lattice", are finite-dimensional complex Hilbert spaces $\mathcal{H}_x$. We introduced the algebra of local observables $\mathcal{A}_\Gamma^{\mathrm{loc}}$ and the C^*-algebra of quasi-local observables, $\mathcal{A}_\Gamma$, which is the norm completion of $\mathcal{A}_\Gamma^{\mathrm{loc}}$. We defined spaces, denoted by $\mathcal{B}_F(\Gamma$, of interactions $\Phi : \mathcal{P}_0(\Gamma) \to \mathcal{A}_\Gamma^{\mathrm{loc}}$, in terms of the so-called F-norms $\|\cdot\|_F$. For each such Φ there is a strongly continuous one-parameter group of automorphisms of $\mathcal{A}_\Gamma$, $\{\tau_t \mid t \in \mathbb{R}\}$, describing the dynamics of the system. There is a densely defined generator δ, for which $\mathcal{A}_\Gamma^{\mathrm{loc}}$ is a core, and such that $\tau_t = e^{it\delta}$.

Equilibrium states at inverse temperature $\beta \in [0, \infty)$, and ground states ($\beta = \infty$), can be characterized in terms of δ as follows. Let $\mathcal{S}_\beta$ be the set of states on $\mathcal{A}$ that satisfy the following conditions:

i. For $\beta = \infty$, the set of ground states $\mathcal{S}_\infty$ consists of those states ω such that

$$\omega(A^*\delta(A)) \geq 0, \quad \text{for all } A \in \mathcal{A}_{\mathrm{loc}}; \tag{7.29}$$

ii. For $\beta \in (0, \infty)$, the set of equilibium states at inverse temperature β, $\mathcal{S}_\beta$ consists of those states ω such that

$$\omega(A^*\delta(A)) \geq \frac{1}{\beta}\omega(A^*A)\ln\left[\frac{\omega(A^*A)}{\omega(AA^*)}\right], \quad \text{for all } A \in \mathcal{A}_{\mathrm{loc}}; \tag{7.30}$$

iii. For $\beta = 0$, describing infinite temperature, we have a unique state ω_0 such that

$$\omega_0(A^*A) = \omega_0(AA^*), \quad \text{for all } A \in \mathcal{A}_{\mathrm{loc}}. \tag{7.31}$$

Note that ω_0 does not depend on δ. It is called the tracial state and, in fact, satisfies $\omega_0(AB) = \omega(BA)$, for all $A, B \in \mathcal{A}_\Gamma$.

One can show that for all $\beta \in [0, \infty]$ the set $\mathcal{S}_\beta$ is a convex subset of the set of all states on $\mathcal{A}$, meaning that if $\omega_1, \omega_2 \in \mathcal{S}_\beta$, then $t\omega_1 + (1-t)\omega_2 \in \mathcal{S}_\beta$ for all $t \in [0, 1]$.

The following bit of terminology about convex sets will be useful.

Let C be a convex subset of a real vector space V. The point $c \in C$ is said to be an extreme point of C if it is not a non-trivial convex combination of points in C, i.e. if $c_1, c_2 \in C$ and there

is some $t \in (0,1)$ for which $c = tc_1 + (1-t)c_2$, then $c_1 = c_2 = c$. We will denote by $\mathcal{E}(C)$ the set of all extreme points in C.

If $c_1, c_2 \in C$ then the *segment* between c_1 and c_2 is the set

$$\{tc_1 + (1-t)c_2 : t \in [0,1]\} \subset C \tag{7.32}$$

C is said to be a *simplex* if for all $c \in C$, there exists a unique set of points $c_i \in \mathcal{E}(C)$, $i = 1, \ldots, n$, and $t_i \in (0,1)$ with $\sum_i t_i = 1$, such that $\sum_{i=1}^n t_i c_i = c$. Strictly speaking, this only defines finite-dimensional simplices. Working with infinite-dimensional simplices involves a choice of topology and possibly measure theory to generalize to convex combinations of infinite sets of points.

A set $F \subset C$ is said to be a *face* if it is convex and whenever $f \in F$ and $f = tc_1 + (1-t)c_2$ for some $c_1, c_2 \in C$ and $t \in (0,1)$, then $tc_1 + (1-t)c_2 \in F$ for all $t \in [0,1]$.

The set of all ground states of a given dynamics, $\mathcal{S}_\infty$, is a face in the set of all states. The extreme points of $\mathcal{S}_\infty$ are pure states, i.e., they are also extreme points in the set of all states.

In contrast, the set of all equilibrium states for a system at $\beta \in (0,\infty)$, $\mathcal{S}_\beta$, is a simplex in the set of all states. The extreme points are factor states, a notion we define in the next paragraph. They are not pure states.

Let ω be a state on a C^*-algebra $\mathcal{A}$. Consider the GNS triple associated to ω, namely $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$. Recall that

$$\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle \quad \text{for all } A \in \mathcal{A} \tag{7.33}$$

and $\pi_\omega(\mathcal{A}) \subset \mathcal{B}(\mathcal{H}_\omega)$ is a sub-algebra.

The commutant of $\pi_\omega(\mathcal{A})$ is defined by

$$\pi_\omega(\mathcal{A})' = \{B \in \mathcal{B}(\mathcal{H}_\omega) : [B, \pi_\omega(A)] = 0 \text{ for all } A \in \mathcal{A}\}. \tag{7.34}$$

The bi-commutant is then

$$\pi_\omega(\mathcal{A})'' = \left(\pi_\omega(\mathcal{A})'\right)'. \tag{7.35}$$

A famous theorem of von Neumann's states that

$$\pi_\omega(\mathcal{A})'' = \overline{\pi_\omega(\mathcal{A})}^{\mathrm{w}}, \tag{7.36}$$

i.e. the bi-commutant of $\pi_\omega(\mathcal{A})$ is the closure of $\pi_\omega(\mathcal{A})$ in the weak operator topology on $\mathcal{B}(\mathcal{H}_\omega)$.

The *center* of a representation π is:

$$Z_\pi = \pi(\mathcal{A})' \cap \pi(\mathcal{A})'' \tag{7.37}$$

A state ω is said to be a *factor state* (also know as a *primary state*) if and only if

$$Z_{\pi_\omega} = \pi_\omega(\mathcal{A})' \cap \pi_\omega(\mathcal{A})'' = \mathbb{C}\mathbb{1} \tag{7.38}$$

The GNS representation of a pure state ω is *irreducible*, meaning that $\pi_\omega(\mathcal{A})' = \mathbb{C}\mathbb{1}$. It follows that $\pi_\omega(\mathcal{A})'' = \mathcal{B}(\mathcal{H}_\omega)$.

8. Symmetry, Excitation Spectrum, and Correlations

As before, let (Γ, d) be a discrete metric space with an F-function F. Let $\{\tau_t \mid t \in \mathbb{R}\}$ be the dynamics generated by an interaction $\Phi \in \mathcal{B}_F(\Gamma)$ for a quantum spin system on Γ. An automorphism α on $\mathcal{A}_\Gamma$ is called a *symmetry* of the C^*-dynamical system $(\mathcal{A}_\Gamma, \tau_t)$ if it commutes with the dynamics, i.e., $\tau_t \circ \alpha = \alpha \circ \tau_t$, for all $t \in \mathbb{R}$. It is easy to see that the symmetries of $(\mathcal{A}_\Gamma, \tau_t)$ form a subgroup of the automorphism group of $\mathcal{A}_\Gamma$.

Two important classes of symmetries are the so-called *point symmetries*, or lattice symmetries, and *gauge symmetries*. As an example of the first class, consider quantum spin systems on $\Gamma = \mathbb{Z}^\nu$, with the lattice distance d, and with $\mathcal{H}_x = \mathbb{C}^n$, for all $x \in \mathbb{Z}^\nu$. In general, $\mathcal{A}_\Gamma^{\mathrm{loc}}$ is generated as an algebra by the collection of single-site algebras $\mathcal{A}_{\{x\}}$, $x \in \Gamma$. Automorphisms of $\mathcal{A}_\Gamma$ are therefore uniquely determined by their action on the one-site algebras. In the situation at hand, $\mathcal{A}_{\{x\}} \cong M_n$, for all $x \in \mathbb{Z}^\nu$. Then, given these identifications, there is a unique automorphism θ_x on $\mathcal{A}_{\mathbb{Z}^\nu}$ that maps $\mathcal{A}_{\{0\}}$ into $\mathcal{A}_{\{x\}}$. The automorphisms θ_x is called the translation by x, and $x \mapsto \theta_x$ is a representation of the additive group $\mathbb{Z}^\nu$ into the automorphisms on $\mathcal{A}_{\mathbb{Z}^\nu}$. In the same way, any bijection of Γ can in principle be a symmetry of a quantum spin system defined on Γ. E.g., $\mathbb{Z}^\nu$, in addition to the lattice translations, also has rotation and reflection symmetries that can be represented on $\mathcal{A}_\Gamma$ as automorphisms.

Continuing with the important example of $\Gamma = \mathbb{Z}^\nu$, we will say that an interaction $\Phi : \mathcal{P}_0(\mathbb{Z}^\nu) \to \mathcal{A}_\Gamma^{\mathrm{loc}}$, is *translation invariant* if for all $x \in \mathbb{Z}^\nu$, and $X \in \mathcal{P}_0(\mathbb{Z}^\nu)$, $\theta_x(\Phi(X)) = \Phi(X + x)$. It is easy to see that if τ_t is defined in terms of a translation invariant interaction, then the translations will be symmetries of the dynamics, i.e., $\tau_t \circ \theta_x = \theta_x \circ \tau_t$, for $t \in \mathbb{R}, x \in \mathbb{Z}^\nu$.

The second class, the gauge symmetries, are generated by unitaries acting on $\mathcal{H}_x$. For any quantum spin system with algebra of quasi-local observables $\mathcal{A}_\Gamma$, suppose we have a unitary $u_x \in \mathcal{A}_{\{x\}}$, for all $x \in \Gamma$. It is then straightforward to show that there is a unique automorphism α on $\mathcal{A}_\Gamma$ such that $\alpha(A) = u_x^* A u_x$, for all $A \in \mathcal{A}_{\{x\}}$. Given a group G, if for all x we have a unitary representation $g \mapsto u_x(g)$ of a group G on $\mathcal{H}_x$, the corresponding α_g give a representation of G as automorphisms of $\mathcal{A}_\Gamma$.

The Heisenberg model introduced in (2.55) has a gauge symmetry given by a representation of $SU(2)$. For the spin 1/2 model, $n = 2$, and $SU(2)$ acts on $\mathbb{C}^2$ by its fundamental representation: for every $u \in SU(2)$, $A \in M_2$, $\alpha_u(A) = u^* A u$. For the spin-S Heisenberg model, the unitaries are given by the $2S + 1$-dimensional irreducible representation of $SU(2)$. For a summary of the unitary representations of the Lie group $SU(2)$, see Appendix 9. Symmetries that are given by a representation of a Lie group (of dimension ≥ 1), are often referred to as continuous symmetries.

If α is a symmetry of $(\mathcal{A}_\Gamma, \tau_t)$, with the property that $\alpha(\mathcal{A}_\Gamma^{\mathrm{loc}}) \subset \mathcal{A}_\Gamma^{\mathrm{loc}}$, the generator δ of the dynamics $\tau_t = e^{it\delta}$ will also commute with α. Since under the above assumption, we have $\alpha(A) \in \mathrm{dom}(\delta)$, for all $A \in \mathcal{A}_\Gamma^{\mathrm{loc}}$, we can differentiate the identity $\alpha(\tau_t(A)) = \tau_t(\alpha(A))$ and obtain

$$\alpha \circ \tau_t(i\delta(A)) = \tau_t(i\delta(\alpha(A))). \tag{8.1}$$

After applying τ_{-t} to both sides of this equation and using the fact that α is a symmetry of the dynamics, we get

$$\alpha(\delta(A)) = \delta(\alpha(A)), \text{ for all } A \in \mathcal{A}_\Gamma^{\mathrm{loc}}. \tag{8.2}$$

Note that both point symmetries and gauge symmetries leave $\mathcal{A}_\Gamma^{\mathrm{loc}}$ invariant, hence (8.2) holds for these types of symmetries. Using this property it is easy to verify that the sets $\mathcal{S}_\beta$, $\beta \in [0, \infty]$, defined in Section 7.2 will be invariant under such symmetries of $(\mathcal{A}_\Gamma, \tau_t)$. That is, $\mathcal{S}_\beta$ is invariant as a set, meaning

$$\mathcal{S}_\beta = \{\omega \circ \alpha \mid \omega \in \mathcal{S}_\beta\}. \tag{8.3}$$

If, moreover, we have $\omega \circ \alpha = \omega$, for all $\omega \in \mathcal{S}_\beta$, we say that the symmetry α is unbroken. In the opposite case, i.e., if there exists $\omega \in \mathcal{S}_\beta$ such that $\omega \circ \alpha \neq \omega$, we say that the symmetry α is

spontaneously broken. Spontaneous symmetry breaking at some $\beta < \infty$ signals a phase transition. Spontaneous symmetry at any value of β has important physical consequences and it is a central concept to many phenomena in condensed matter and particle physics.

In the next section we will consider systems on $\mathbb{Z}^\nu$ with $\mathcal{H}_x = \mathbb{C}^n$, for all $x \in \mathbb{Z}^\nu$ and a continuous local symmetry that commutes with translations. Explicitly, this means that for all $s \in \mathbb{R}$, we α_s is of the form

$$\alpha_s(A) = \left(\bigotimes_{x\in X} u(s)^*\right) A \left(\bigotimes_{x\in X} u(s)\right), \text{ for all } A \in \mathcal{A}_X, \tag{8.4}$$

where $u(s) = e^{isJ}$, with $J = J^* \in M_n$. There may be more than one such continuous family of α_s. The $SU(2)$ symmetry of the Heisenberg model is an example of this situation.

Both the notion of gapped excitation spectrum and the concept of spontaneous symmetry breaking are most conveniently formulated for infinite systems. The spectrum of a finite quantum spin system is a finite set of eigenvalues. One usually associates the smallest eigenvalue with the ground states, but in some cases it is appropriate to consider one or more additional eigenvalues as corresponding to 'the ground state' as well. Also, there is no simple relationship between the degeneracy of the ground state eigenvalue and the number of distinct ground states in the thermodynamic limit. A illustrative example is the AKLT chain, which has a four-dimensional eigenspace belonging to the ground state eigenvalue, yet, there is a unique thermodynamic limit of those states [4]. Numerical calculations have shown that the spin-1 antiferromagnetic Heisenberg chain has a pair of eigenvalues corresponding to a very similar four-dimensional space of states that converge to a unique ground state in the thermodynamic limit [39]. For similar reasons, spontaneous symmetry breaking, which leads to multiple ground states in the thermodynamic limit, may be 'hidden' in a unique ground state in finite volume. This occurs in the antiferromagnetic Heisenberg models on finite volumes of even size in two and more dimensions [42].

All these ambiguities disappear in the thermodynamic limit. E.g., the excitation spectrum above a ground state ω is simply the spectrum of its GNS Hamiltonian H_ω, which is non-negative and the ground state is represented by an eigenvector with eigenvalue 0. The spectral gap γ can then be defined as follows:

$$\gamma = \sup\{\delta > 0 \mid (0, \delta) \cap \mathrm{spec} H_\omega = \emptyset\}, \tag{8.5}$$

with the convention that we put $\gamma = 0$ if the RHS is the empty set.

8.1. **The Goldstone Theorem.** The Goldstone's theorem in quantum field theory shows that the spontaneous breaking of a continuous symmetry breaking is always accompanied by the appearance of a massless particle, i.e., a gapless excitation or Goldstone mode [28, 29, 38]. As we explained before, spontaneous symmetry breaking is indicated by the existence of $\omega \in \mathcal{S}_\beta$ that are *not* invariant under the symmetry. In statistical mechanics, spontaneous breaking of a continuous symmetry in the ground state of a translation invariant system also implies a gapless excitation spectrum, while at positive temperature the symmetry breaking precludes fast (integrable) decay of correlations [43].

The Goldstone Theorem requires translation invariance. In order to keep the presentation of the basic argument here as simple as possible, we will limit the discussion to translation invariant quantum spin systems $\mathcal{A}_\Gamma$ with $\Gamma = \mathbb{Z}^\nu$ for some $\nu \geq 1$. It is possible to generalize Theorem 8.1: e.g. more general lattices can be considered, and it is also not crucial to assume full translation invariance. See the remarks following the proof of Theorem 8.1 for pointers to several generalizations.

Let $(\mathcal{A}_{\mathbb{Z}^\nu}, \tau_t)$ be a C^*-dynamical system with dynamics τ_t generated by $\Phi \in \mathcal{B}_F(\mathbb{Z}^\nu)$. Note: To be precise, translation invariance will be assumed of the ground state, however, the interaction Φ need not be translation invariant. Let α_s be a continuous, locally-generated symmetry on $\mathcal{A}_{\mathbb{Z}^\nu}$. In particular, this means that there is $J_0^* = J_0 \in \mathcal{A}_{\{0\}}$ and for any $x \in \mathbb{Z}^\nu$, one defines $J_x = \theta_x(J_0) \in$

$\mathcal{A}_{\{x\}}$ where θ_x denotes translation by x. In terms of these local operators, α_s is the one-parameter group of automorphisms of $\mathcal{A}_{\mathbb{Z}^\nu}$ defined by

$$\alpha_s(A) = e^{is\sum_x J_x} A e^{-is\sum_x J_x} \quad \text{for all } A \in \mathcal{A}_{\mathbb{Z}^\nu} \text{ and } s \in \mathbb{R}. \tag{8.6}$$

Let ω be a translation invariant ground state of $(\mathcal{A}_{\mathbb{Z}^\nu}, \tau_t)$, i.e. ω satisfies the ground state condition

$$\omega(A^*\delta(A)) \geq 0 \quad \text{for all } A \in D(\delta) \tag{8.7}$$

and also translation invariance

$$\omega(\theta_x(A)) = \omega(A) \quad \text{for every } A \in \mathcal{A}_{\mathbb{Z}^\nu} \text{ and } x \in \mathbb{Z}^\nu \tag{8.8}$$

In one formulation of the Goldstone's theorem one assumes that a translation-invariant ground state satisfies the following inequalities for a constant $\gamma > 0$:

$$\gamma\omega(A^*A) \leq \omega(A^*\delta(A)) \quad \text{for all } A \in \mathcal{D}(\delta) \text{ with } \omega(A) = 0\,, \tag{8.9}$$

This property implies that (i) ω is a ground state; (ii) that $\ker H_\omega = \mathbb{C}\mathbb{1}$; and (iii) there is a gap in the spectrum of H_ω above the ground state. If the ground state is unique, this property is actually *equivalent* to the existence of a spectral of size $\geq \gamma$. The theorem then states that these assumptions imply that the continuous symmetry is unbroken, which is the contrapositive of the more frequently encountered statement that continuous symmetry breaking implies gapless excitations (massless particles).

Theorem 8.1 (Goldstone for ground-states [43])**.** *Let $(\mathcal{A}_{\mathbb{Z}^\nu}, \tau_t)$ be C^*-dynamical system over $\mathbb{Z}^\nu$ with τ_t generated by an interaction $\Phi \in \mathcal{B}_F(\mathbb{Z}^\nu)$. Let α_s be a continuous gauge symmetry of the dynamics, i.e., α_s is of the form (**??**)*

$$\alpha_s \circ \tau_t = \tau_t \circ \alpha_s \quad \textit{for all } s, t \in \mathbb{R}\,. \tag{8.10}$$

Let ω be a translation invariant ground state of $(\mathcal{A}_{\mathbb{Z}^\nu}, \tau_t)$, for which there exists $\gamma > 0$ such that

$$\gamma \cdot \omega(A^*A) \leq \omega(A^*\delta(A)) \quad \textit{for all } A \in \mathcal{A}_\Gamma^{\mathrm{loc}} \textit{ with } \omega(A) = 0\,. \tag{8.11}$$

Then, ω is invariant with respect to α_s, i.e.

$$\omega(\alpha_s(A)) = \omega(A) \quad \textit{for all } A \in \mathcal{A}_{\mathbb{Z}^\nu} \textit{ and all } s \in \mathbb{R}. \tag{8.12}$$

Before we start the proof of this theorem, we derive a lemma that exploits the assumption that the interaction Φ has a finite F-norm.

Lemma 8.2. *Consider a C^*-dynamical system $(\mathcal{A}_{\mathbb{Z}^\nu}, \tau_t)$ with dynamics $\tau_t = e^{it\delta}$ generated by $\Phi \in B_F(\mathbb{Z}^\nu)$. For any $A \in \mathcal{A}_{\mathbb{Z}^\nu}^{\mathrm{loc}}$,*

$$\sup_{x\in\mathbb{Z}^\nu} \sum_{y\in\mathbb{Z}^\nu} \|[\theta_x(A), \delta(\theta_y(A))]\| \leq 4\|A\|^2 \|F\| \|\Phi\|_F |X| (2\mathrm{diam}(X) + 1)^\nu, \tag{8.13}$$

and moreover, for $d > \mathrm{diam}(X)$, we have the esitmate

$$\sup_{x\in\mathbb{Z}^\nu} \sum_{\substack{y\in\mathbb{Z}^\nu: \\ |y-x|\geq d}} \|[\theta_x(A), \delta(\theta_y(A))]\| \leq 4\|A\|^2 \|\Phi\| |X|^2 \sum_{\substack{y'\in\mathbb{Z}^\nu: \\ |y'|\geq d-\mathrm{diam}(X)}} F(|y'|), \tag{8.14}$$

which implies that the quantity vanishes as $d \to \infty$.

Proof. Let $A \in \mathcal{A}_{\mathbb{Z}^\nu}^{\mathrm{loc}}$ and denote by $X = \mathrm{supp}(A) \in \mathcal{P}_0(\mathbb{Z}^\nu)$. To ease notation, for any $y \in \mathbb{Z}^\nu$ we will set

$$A_y = \theta_y(A) \in \mathcal{A}_{X_y} \quad \text{where} \quad X_y = \{x + y : x \in X\} \in \mathcal{P}_0(\mathbb{Z}^\nu)\,. \tag{8.15}$$

Observe that for any fixed $x \in \mathbb{Z}^\nu$

$$\sum_{y\in\mathbb{Z}^\nu} \|[A_x, \delta(A_y)]\| \leq \sum_{y\in\mathbb{Z}^\nu} \sum_{\substack{Z\in\mathcal{P}_0(\mathbb{Z}^\nu):\\ Z\cap X_y\neq\emptyset}} \|[A_x, [\Phi(Z), A_y]]\| \tag{8.16}$$

For those $y \in \mathbb{Z}^\nu$ such that $X_y \cap X_x \neq \emptyset$, we estimate the above as

$$\begin{aligned} \sum_{\substack{y\in\mathbb{Z}^\nu:\\ X_y\cap X_x\neq\emptyset}} \sum_{\substack{Z\in\mathcal{P}_0(\mathbb{Z}^\nu):\\ Z\cap X_y\neq\emptyset}} \|[A_x, [\Phi(Z), A_y]]\| &\leq 4\|A\|^2 \sum_{\substack{y\in\mathbb{Z}^\nu:\\ X_y\cap X_x\neq\emptyset}} \sum_{z\in X_y} \sum_{\substack{Z\in\mathcal{P}_0(\mathbb{Z}^\nu):\\ z\in Z}} \|\Phi(Z)\| \\ &\leq 4\|A\|^2\|F\|\|\Phi\|_F|X|(2\mathrm{diam}(X)+1)^\nu, \end{aligned} \tag{8.17}$$

where we estimated the number of y such that $X_y \cap X_x \neq \emptyset$ by the cardinality of the ball, centered at the origin, having radius equal to the diameter of X.

For the remaining y, we have

$$\begin{aligned} \sum_{\substack{y\in\mathbb{Z}^\nu:\\ X_y\cap X_x=\emptyset}} \sum_{\substack{Z\in\mathcal{P}_0(\mathbb{Z}^\nu):\\ Z\cap X_y\neq\emptyset}} \|[A_x, [\Phi(Z), A_y]]\| &\leq 4\|A\|^2 \sum_{\substack{y\in\mathbb{Z}^\nu:\\ X_y\cap X_x=\emptyset}} \sum_{z_1\in X_y} \sum_{z_2\in X_x} \sum_{\substack{Z\in\mathcal{P}_0(\mathbb{Z}^\nu):\\ z_1,z_2\in Z}} \|\Phi(Z)\| \\ &\leq 4\|A\|^2\|\Phi\|_F \sum_{\substack{y\in\mathbb{Z}^\nu:\\ X_y\cap X_x=\emptyset}} \sum_{z_1\in X_y} \sum_{z_2\in X_x} F(|z_1-z_2|) \\ &\leq 4\|A\|^2\|\Phi\|_F \sum_{x_1\in X} \sum_{x_2\in X} \sum_{y\in\mathbb{Z}^\nu} F(|x_1-x_2+y-x|) \\ &\leq 4\|A\|^2\|\Phi\|_F\|F\||X|^2 \end{aligned} \tag{8.18}$$

Both estimates in (8.17) and (8.18) are independent of x, and it is straightforward to show they both are bounded above as in (8.13).

The proof of (8.14) is similar. In fact, let A be as above and take $d > \mathrm{diam}(X)$. In this case, any y with $|x-y| \geq d$ satisfies $X_x \cap X_y = \emptyset$. Hence, estimating as in (8.18) we find that

$$\begin{aligned} \sum_{\substack{y\in\mathbb{Z}^\nu:\\ |y-x|\geq d}} \|[A_x, \delta(A_y)]\| &\leq 4\|A\|^2\|\Phi\|_F \sum_{\substack{y\in\mathbb{Z}^\nu:\\ |y-x|\geq d}} \sum_{x_1\in X} \sum_{x_2\in X} F(|x_1-x_2+y-x|) \\ &\leq 4\|A\|^2\|\Phi\||X|^2 \sum_{\substack{y'\in\mathbb{Z}^\nu:\\ |y'|\geq d-\mathrm{diam}(X)}} F(|y'|) \end{aligned} \tag{8.19}$$

Since F is uniformly integrable, this proves (8.14). □

Proof of Theorem 8.1. We will prove that $\omega \circ \alpha_s = \omega$, for all $s \in \mathbb{R}$ by showing that, for all $A \in \mathcal{A}_\Gamma$

$$\frac{d}{ds}\omega(\alpha_s(A)) = 0, \text{ for all } s \in \mathbb{R}. \tag{8.20}$$

Since the strictly local observables are dense in $\mathcal{A}_\Gamma$, it suffices to show this for $A \in \mathcal{A}_\Gamma^{\mathrm{loc}}$. For local A, say $A \in \mathcal{A}_X$, $X \in \mathcal{P}_0(\Gamma)$, we have

$$\frac{d}{ds}\omega(\alpha_s(A)) = i\omega([J_x, (\alpha_s(A))]). \tag{8.21}$$

Since α_s is an automorphism leaving $\mathcal{A}_X$ invariant, it follows that it is sufficient to show

$$\omega([J_X, A)]) = 0, \text{ for all } X \in \mathcal{P}_0(\Gamma), \text{ and } A \in \mathcal{A}_X. \tag{8.22}$$

We prove (8.22) in two steps. First, by averaging over translations, we establish an upper bound, see (8.25) below. Next, we analyze the factors in our upper bound and see that this bound goes to zero as we average over more and more translations.

As a consequence of the translation invariance of ω and the commutation of the translations and the symmetry, for any finite $\Lambda \subset \mathbb{Z}^\nu$, we have that

$$\omega([J_X, A]) = \frac{1}{|\Lambda|}\sum_{x\in\Lambda}\omega([J_{X_x}, \theta_x(A)]) = \frac{1}{|\Lambda|}\sum_{x\in\Lambda}\omega([J_\Lambda, \theta_x(A)]) = \frac{1}{|\Lambda|}\omega([J_\Lambda, A_\Lambda]), \tag{8.23}$$

where we have set

$$A_\Lambda = \sum_{x\in\Lambda}\theta_x(A), \text{ and } J_\Lambda = \sum_{x\in\mathrm{supp}(A_\Lambda)} J_x\,. \tag{8.24}$$

We will now prove the upper bound

$$|\omega([J_X, A])|^2 = \frac{1}{|\Lambda|^2}|\omega([J_\Lambda, A_\Lambda])|^2 \leq \frac{4}{\gamma^2}\cdot\frac{1}{|\Lambda|}\omega([J_\Lambda, \delta(J_\Lambda)])\cdot\frac{1}{|\Lambda|}\omega([A_\Lambda, \delta(A_\Lambda)]) \tag{8.25}$$

valid for any $\Lambda \in \mathcal{P}_0(\mathbb{Z}^\nu)$, and $\gamma > 0$ is the constant appearing the in the assumptions of the theorem.

To prove (8.25), we start by noting that due to the commutator

$$\omega([J_\Lambda, A_\Lambda]) = \omega([\hat{J}_\Lambda, \hat{A}_\Lambda]) \tag{8.26}$$

where

$$\hat{B} = B - \omega(B)\mathbb{1} \quad \text{for any } B \in \mathcal{A}_{\mathbb{Z}^\nu} \tag{8.27}$$

Next, using Cauchy-Schwartz of both observables, we get

$$|\omega([J_\Lambda, A_\Lambda])|^2 \leq 4\omega(\hat{J}_\Lambda^*\hat{J}_\Lambda)\cdot\omega(\hat{A}_\Lambda^*\hat{A}_\Lambda) \tag{8.28}$$

For any local observable B, the time-invariance of the state implies

$$\omega(\delta(B)B^*) + \omega(B\delta(B^*)) = \omega(\delta(BB^*)) = 0. \tag{8.29}$$

For any local observable B, $\omega(\hat{B}) = 0$. Using the assumption (8.11), (8.29), and the ground state property, we obtain

$$\begin{aligned}
\omega(\hat{B}^*\hat{B}) \leq \frac{1}{\gamma}\omega(\hat{B}^*\delta(\hat{B})) &= \frac{1}{\gamma}\omega([\hat{B}^*, \delta(\hat{B})]) + \omega(\delta(\hat{B})\hat{B}^*) \\
&= \frac{1}{\gamma}\omega([\hat{B}^*, \delta(\hat{B})]) - \omega(\hat{B}\delta(\hat{B}^*)) \\
&\leq \frac{1}{\gamma}\omega([\hat{B}^*, \delta(\hat{B})]) = \frac{1}{\gamma}\omega([B^*, \delta(B)])
\end{aligned} \tag{8.30}$$

Using this bound for $B = J_\Lambda$ and $B = A_\Lambda$ in (8.28) yields (8.25) as claimed.

For the second step in the proof, we use Lemma 8.2 to further estimate the right-hand-side of (8.25). For the second factor in the right-hand-side of (8.25), note that

$$\begin{aligned}
\frac{1}{|\Lambda|}\omega([A_\Lambda, \delta(A_\Lambda)]) &\leq \frac{1}{|\Lambda|}\sum_{x\in\Lambda}\sum_{y\in\Lambda}|\omega\left([\theta_x(A), \delta(\theta_y(A))]\right)| \\
&\leq \sup_{x\in\mathbb{Z}^\nu}\sum_{y\in\mathbb{Z}^\nu}\|[\theta_x(A), \delta(\theta_y(A))]\|
\end{aligned} \tag{8.31}$$

which is finite by Lemma 8.2. This bound is independent of the set Λ and the support of the observable A.

Finally, we argue that the first factor in the right-hand-side of (8.25) tends to zero for a suitable choice of sets Λ which grow to $\mathbb{Z}^\nu$. To prove this we will need to use the assumption that the dynamics and the symmetry commute, i.e. (8.10).

Let us denote by $\mathcal{J}_\Lambda = \mathrm{supp}(J_\Lambda)$. It is clear that

$$\omega([J_\Lambda, \delta(J_\Lambda)]) = \sum_{x,y\in\mathcal{J}_\Lambda} \omega([J_x, \delta(J_y)]) = \sum_{x,y\in\mathbb{Z}^\nu} \chi_{\mathcal{J}_\Lambda}(x)\chi_{\mathcal{J}_\Lambda}(y)\omega([J_x, \delta(J_y)]) \tag{8.32}$$

with $\chi_{\mathcal{J}_\Lambda}$ being a characteristic function. Note that by using again the time-invariance of ω, we have $\omega(J_x\delta(J_y)) = -\omega(\delta(J_x)J_y)$. Therefore,

$$\omega([J_x, \delta(J_y)]) = \omega([J_y, \delta(J_x)]) \tag{8.33}$$

We now apply (8.2) to the observables J_y and once more the time-invariance of ω:

$$\omega(\alpha_s(\delta(J_y)) = \omega(\delta(\alpha_s(J_y)) = 0. \tag{8.34}$$

By taking the derivative with respect to s, in $s = 0$, of this equation, we obtain

$$\sum_{x\in\mathbb{Z}^\nu} \omega(J_x, \delta(J_y)]) = 0, \text{ for all } y \in \mathbb{Z}^\nu. \tag{8.35}$$

Note that Lemma 8.2 guarantees that the sum above is absolutely summable. Now, using (8.33) and (8.35), we can re-write (8.32) as

$$\omega([J_\Lambda, \delta(J_\Lambda)]) = -\frac{1}{2} \sum_{x,y\in\mathbb{Z}^\nu} |\chi_{\mathcal{J}_\Lambda}(x) - \chi_{\mathcal{J}_\Lambda}(y)|^2\omega([J_x, \delta(J_y)]) \tag{8.36}$$

from which we derive the following bound

$$|\omega([J_\Lambda, \delta(J_\Lambda)])| \leq \sum_{x\in\mathcal{J}_\Lambda} \sum_{y\in\mathcal{J}_\Lambda^c} |\omega([J_x, \delta(J_y)])|. \tag{8.37}$$

Up to this point, the support of the observables being considered has played a minor role. To complete the argument, we now make this more explicit. Recall that the original self-adjoint observable A was assumed local. Let us denote by $X = \mathrm{supp}(A)$. Without loss of generalty, we will assume that X is a cube with side-length $\ell > 0$, hence $|X| = (\ell + 1)^\nu$. It is convenient to choose the finite set Λ, as in (8.25) above, to also be a cube, e.g. with side-length $L > 0$. In this case,

$$\mathcal{J}_\Lambda = \mathrm{supp}(J_\Lambda) = \mathrm{supp}(A_\Lambda) \quad \text{satisfies} \quad |\mathcal{J}_\Lambda| = (L + \ell + 1)^\nu \,. \tag{8.38}$$

Consider $L \geq 1$ large and fix an integer d, independent of L, satisfying $\ell < 2d < L$. Set

$$\mathcal{J}_\Lambda^{\mathrm{int}} = \{x \in \mathcal{J}_\Lambda : \mathrm{dist}(x, \partial\mathcal{J}_\Lambda) \geq d\} \quad \text{and} \quad \mathcal{J}_\Lambda^{\mathrm{bd}} = \mathcal{J}_\Lambda \setminus \mathcal{J}_\Lambda^{\mathrm{int}} \,. \tag{8.39}$$

It is clear that

$$\sum_{x\in\mathcal{J}_\Lambda^{\mathrm{int}}} \sum_{y\in\mathcal{J}_\Lambda^c} |\omega([J_x, \delta(J_y)])| \leq |\mathcal{J}_\Lambda^{\mathrm{int}}| \cdot f(d) \quad \text{where} \quad f(d) = \sup_{x\in\mathbb{Z}^\nu} \sum_{\substack{y\in\mathbb{Z}^\nu: \\ |x-y|\geq d}} \|[J_x, \delta(J_y)]\| \tag{8.40}$$

For the remaining boundary terms, we have that

$$\sum_{x\in\mathcal{J}_\Lambda^{\mathrm{bd}}} \sum_{y\in\mathcal{J}_\Lambda^c} |\omega([J_x, \delta(J_y)])| \leq |\mathcal{J}_\Lambda^{\mathrm{bd}}| \cdot C \quad \text{with} \quad C = \sup_{x\in\mathbb{Z}^\nu} \sum_{y\in\mathbb{Z}^\nu} \|[J_x, \delta(J_y)]\| \tag{8.41}$$

C is guaranteed to be finite due Lemma 8.2. Combining these estimates, we have then that

$$\limsup_{L\to\infty} \frac{1}{|\Lambda|} |\omega([J_\Lambda, \delta(J_\Lambda)])| \leq f(d) \tag{8.42}$$

Taking now $d \to \infty$, we complete the proof. □

The set of ground states of the spin-1/2 ferromagnetic Heisenberg model on $\mathbb{Z}^\nu$ is spanned by the translation invariant pure product states, i.e., states determined by a unit vector $\phi \in \mathbb{C}^2$ through the formula,

$$\omega(A) = \langle \bigotimes_{x\in X} \phi, A \bigotimes_{x\in X} \phi\rangle, \text{ for all }, X \in \mathcal{P}_0(\mathbb{Z}^\nu), A \in \mathcal{A}_X. \tag{8.43}$$

Clearly, the $SU(2)$ symmetry of the model is spontaneously broken in the ground state. To illustrate the Goldstone Theorem, take for example $\phi = |+\rangle$, the unit eigenvector of σ^3 with eigenvalue 1. The GNS representation is easy to construct with $\mathcal{H}_\omega$ the separable Hilbert space with orthonormal basis $\{\xi_X \mid X \in \mathcal{P}_0(\mathbb{Z}^\nu)\}$. $\Omega_\omega = \xi_\emptyset$ and can be thought of as the formal tensor product $\bigotimes_{x\in\mathbb{Z}^\nu} |+\rangle$ and the representation π_ω can be constructed starting from

$$\pi_\omega(\sigma_x^-)\xi_X = \begin{cases} \xi_{X\cup\{x\}} & \text{if } x \notin X \\ 0 & \text{if } x \in X \end{cases}$$

It is then straightforward to show that $\mathcal{H}_1 = \text{span}\{\xi_{\{x\}} \mid x \in \mathbb{Z}^n u\}$ is an invariant subspace for H_ω. A simple calculation shows that $\text{spec}(H_\omega \restriction_{\mathcal{H}_1}) = [0, c]$, with $c > 0$, and hence H_ω is gappless.

8.2. **The Exponential Clustering Theorem.** let $(\mathcal{A}_\Gamma, \tau_t)$ be a C^*-dynamical system with $\mathcal{A}_\Gamma$ the quasi-local algebra corresponding to a quantum spin system over Γ and τ_t the dynamics generated by an interaction $\Phi \in \mathcal{B}_{F_a}(\Gamma)$, where $F_a(r) = e^{-ar}F(r)$, and $a > 0$.

The Exponential Clustering Theorem concerns a situation complementary to the gapless states associated with spontaneous breaking of a continuous symmetry considered, as implied by the Goldstone Theorem of the previous section. Briefly, The Exponential Clustering Theorem states that if there is a spectral gap above a ground states, then correlations in this state decay exponentially fast with the distance. The natural setting for this type of result is again systems on a infinite set (Γ, d). Translation invariance plays no direct role, however, and is not a condition of the theorem.

More precisely, let $(\mathcal{A}_\Gamma, \tau_t)$ be a C^*-dynamical system with $\mathcal{A}_\Gamma$ the quasi-local algebra corresponding to a quantum spin system over Γ and τ_t the dynamics generated by an interaction $\Phi \in \mathcal{B}_{F_a}(\Gamma)$. Assume that this system can be represented by a Hamiltonian H on a Hilbert space $\mathcal{H}$. This means that we assume there is a representation $\pi : \mathcal{A}_\Gamma \to \mathcal{B}(\mathcal{H})$ and a (densely defined) self-adjoint operator H on $\mathcal{H}$ for which

$$\pi(\tau_t(A)) = e^{itH}\pi(A)e^{-itH} \quad \text{for all} \quad A \in \mathcal{A}_\Gamma \text{ and } t \in \mathbb{R}. \tag{8.44}$$

We will further assume that $H \geq 0$ and has a spectral gap $\gamma > 0$ above 0, as defined in (8.5). Let P_0 denote the orthogonal projection onto $\ker H$. For the remainder of this section, we will always work in this representation and we simplify the notation by writing A instead of $\pi(A)$.

Theorem 8.3 (Exponential Clustering)**.** *Let $a > 0$ and take $\Phi \in \mathcal{B}_{F_a}(\Gamma)$. Suppose that the dynamics corresponding to Φ on Γ can be represented by a Hamiltonian H with a gap $\gamma > 0$ above the ground state energy, as described above. Let Ω be a normalized ground state vector for H; i.e. satisfy $H\Omega = 0$ with $\|\Omega\| = 1$. Then, there exists a constant $\mu > 0$ such that for any local observables $A \in \mathcal{A}_X$ and $B \in \mathcal{A}_Y$ with $X, Y \subset V$ and $d(X, Y) > 0$ satisfying $P_0 B\Omega = P_0 B^*\Omega = 0$, the bound*

$$|\langle \Omega, A\tau_{ib}(B)\Omega\rangle| \leq C(A, B, \gamma)\, e^{-\mu d(X,Y)\left(1+\frac{\gamma^2 b^2}{4\mu^2 d(X,Y)^2}\right)} \tag{8.45}$$

is valid for all non-negative b satisfying $0 \leq b\gamma \leq 2\mu d(X, Y)$. One may take

$$\mu = \frac{a\,\gamma}{4\|\Phi\|_a C_a + \gamma}, \tag{8.46}$$

as well as a constant

$$C(A,B,\gamma) \;=\; \|A\|\,\|B\| \left[1 \;+\; \sqrt{\frac{1}{\mu d(X,Y)}} \;+\; \frac{2\|F_0\|}{\pi C_a}\,\min\left(|\partial_\Phi X|, |\partial_\Phi Y|\right)\right]. \tag{8.47}$$

Note that in the case of a non-degenerate ground state, the condition on B is equivalent to $\langle \Omega, B\Omega\rangle = 0$. In this case, the theorem with $b = 0$ becomes

$$|\langle \Omega, AB\Omega\rangle - \langle \Omega, A\Omega\rangle \langle \Omega, B\Omega\rangle| \leq C(A,B,\gamma)\, e^{-\mu d(X,Y)}, \tag{8.48}$$

which is the standard (equal-time) correlation function. For small $b > 0$, the estimate (8.45) can be viewed as a perturbation of (8.48). Moreover, for $b > 0$ large, there is a trivial bound

$$|\langle \Omega, A\tau_{ib}(B)\Omega\rangle| \;\leq\; \|A\|\,\|B\|\, e^{-b\gamma}. \tag{8.49}$$

Proof. The proof of this result has two main steps. First, using techniques from complex analysis, we reduce an estimate on the quantity of interest to that of an integral over the real line. Next, we carefully analyze the resulting integral.

Step 1: We begin by noting that for any $z \in \mathbb{C}$ with $\mathrm{Im}[z] \geq 0$, the function f with

$$f(z) \;:=\; \langle \Omega, A\tau_z(B)\Omega\rangle \;=\; \int_\gamma^\infty e^{izE}\, d\,\langle A^*\Omega, P_E B\Omega\rangle \tag{8.50}$$

The final equality above uses the spectral theorem for the self-adjoint operator H and the fact that that B projects off the ground state, i.e. $P_0 B\Omega = 0$. This integral representation of f clearly demonstrates that f is analytic in $\mathbb{C}^+$, i.e. those $z \in \mathbb{C}$ with $\mathrm{Im}[z] > 0$, and moreover, f has a continuous (and bounded) boundary value on the real axis. Our first goal is to now estimate $|f(ib)|$ for $b > 0$ as in the statement above. The case $b = 0$ will follow by a limiting argument.

Let $b > 0$. For any $T > b$, denote by Γ_T the semi-circular contour in the upper-half plane which passes through the points $-T$, T, and iT. A simple limiting argument, using that f has a continuous boundary value, shows that

$$f(ib) \;=\; \frac{1}{2\pi i}\int_{\Gamma_T} \frac{f(z)}{z - ib} dz\,. \tag{8.51}$$

The first step in the proof is completed when we demonstrate that the piece of this contour integral that extends into the upper half plane is vanishingly small, i.e. we claim that

$$|\langle \Omega, A\tau_{ib}(B)\Omega\rangle| \;=\; |f(ib)| \;\leq\; \limsup_{T\to\infty} \left|\frac{1}{2\pi i}\int_{-T}^{T} \frac{f(t)}{t - ib} dt\right|. \tag{8.52}$$

This follows from two observations. First, given (8.50), it is clear that

$$|f(e^{i\theta}T)| \leq \|A\|\|B\| e^{-T\gamma\sin(\theta)} \quad \text{for all } \theta \in [0,\pi]\,. \tag{8.53}$$

Lastly, the integral over the arc, e.g. when $T > 2b$, can be bounded by

$$\frac{\|A\|\|B\|}{\pi}\int_0^\pi e^{-T\gamma\sin(\theta)}\, d\theta \tag{8.54}$$

which clearly goes to zero as $T \to \infty$ by dominated convergence. This proves (8.52). We note that while (8.52) is true for any value of $b > 0$, we will have to choose $b > 0$ sufficiently small later in the proof; see the comments following (8.70) below.

Step 2: We now estimate the integral over the real line. Let $\alpha > 0$; this is a free parameter which will be judiciously chosen later. It is convenient to write

$$f(t) \;=\; e^{-\alpha b^2}\,\left[f(t)e^{-\alpha t^2} \;+\; f(t)\left(e^{\alpha b^2} - e^{-\alpha t^2}\right)\right]. \tag{8.55}$$

With this in mind, the pre-limit integral on the right-hand-side of (8.52) can be estimated by

$$e^{-\alpha b^2}\left|\frac{1}{2\pi i}\int_{-T}^{T}\frac{f(t)e^{-\alpha t^2}}{t-ib}dt\right| + e^{-\alpha b^2}\left|\frac{1}{2\pi i}\int_{-T}^{T}\frac{f(t)\left(e^{\alpha b^2}-e^{-\alpha t^2}\right)}{t-ib}dt\right|. \tag{8.56}$$

We will bound the absolute value of each of the integrals appearing in (8.56) separately; the prefactor $e^{-\alpha b^2}$ will be an additional damping made explicit by the choice of α.

To bound the first integral appearing in (8.56), we further divide the integrand into two terms. Note that

$$f(t)\,e^{-\alpha t^2} = \langle\Omega,\tau_t(B)A\Omega\rangle e^{-\alpha t^2} + \langle\Omega,[A,\tau_t(B)]\,\Omega\rangle e^{-\alpha t^2}. \tag{8.57}$$

Appealing again to the spectral theorem, we have that

$$\frac{1}{2\pi i}\int_{-T}^{T}\frac{\langle\Omega,\tau_t(B)A\Omega\rangle\,e^{-\alpha t^2}}{t-ib}dt = \int_{\gamma}^{\infty}\frac{1}{2\pi i}\int_{-T}^{T}\frac{e^{-itE}e^{-\alpha t^2}}{t-ib}dt\,d\langle P_E B^*\Omega, A\Omega\rangle, \tag{8.58}$$

using that $P_0 B^*\Omega = 0$ as well. An application of Lemma 8.4, stated below, now yields that

$$\lim_{T\to\infty}\frac{1}{2\pi i}\int_{-T}^{T}\frac{e^{-itE}\,e^{-\alpha t^2}}{t-ib}dt = \frac{1}{2\sqrt{\pi\alpha}}\int_0^{\infty}e^{-bw}e^{-\frac{(w+E)^2}{4\alpha}}dw \leq \frac{1}{2}e^{-\frac{\gamma^2}{4\alpha}}, \tag{8.59}$$

since each of $E\geq\gamma>0$, $\alpha>0$, and $b>0$ hold. Altogether, this proves that

$$\limsup_{T\to\infty}\left|\frac{1}{2\pi i}\int_{-T}^{T}\frac{\langle\Omega,\tau_t(B)A\Omega\rangle\,e^{-\alpha t^2}}{t-ib}dt\right| \leq \frac{\|A\|\,\|B\|}{2}e^{-\frac{\gamma^2}{4\alpha}}. \tag{8.60}$$

For the integral corresponding to the second term in (8.57), we use the bound

$$\left|\frac{1}{2\pi i}\int_{-T}^{T}\frac{\langle\Omega,[A,\tau_t(B)]\,\Omega\rangle\,e^{-\alpha t^2}}{t-ib}dt\right| \leq \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\|[A,\tau_t(B)]\|}{|t|}e^{-\alpha t^2}dt, \tag{8.61}$$

which takes advantage of the fact that $b>0$. To complete the estimate of the integral on the right-hand-side of (8.61), we introduce another free parameter $s>0$. For values of $|t|\leq s$, we estimate with the Lieb-Robinson bound, i.e. Theorem **??**, and for $|t|>s$ the gaussian factor dominates the integral. A short calculation shows that the right-hand-side of (8.61) is bounded from above by

$$\frac{2\,\|A\|\,\|B\|}{\pi\,\|\Phi\|_a\,C_a}D_a(X,Y)\left(e^{2\|\Phi\|_a C_a s}-1\right) + \frac{\|A\|\,\|B\|}{s\sqrt{\pi\alpha}}e^{-\alpha s^2}. \tag{8.62}$$

This completes the bound of the first integral appearing in (8.56) in terms of two free parameters $s>0$ and $\alpha>0$.

We now turn to the second integral in (8.56) and claim that if $2\alpha b\leq\gamma$, then

$$\limsup_{T\to\infty}\left|\frac{1}{2\pi i}\int_{-T}^{T}\frac{f(t)\left(e^{\alpha b^2}-e^{-\alpha t^2}\right)}{t-ib}dt\right| \leq \frac{\|A\|\,\|B\|}{2}e^{-\frac{\gamma^2}{4\alpha}}. \tag{8.63}$$

To prove this, first insert (8.50) into the integrand above and see that

$$\frac{1}{2\pi i}\int_{-T}^{T}\frac{f(t)\left(e^{\alpha b^2}-e^{-\alpha t^2}\right)}{t-ib}dt = \int_{\gamma}^{\infty}\frac{1}{2\pi i}\int_{-T}^{T}\frac{e^{itE}\left(e^{\alpha b^2}-e^{-\alpha t^2}\right)}{t-ib}dt\,d\langle A^*\Omega, P_E B\Omega\rangle \tag{8.64}$$

The inner integral on the right-hand-side above can be re-written

$$\begin{aligned}\frac{1}{2\pi i}\int_{-T}^{T}\frac{e^{itE}\left(e^{\alpha b^2}-e^{-\alpha t^2}\right)}{t-ib}dt &= e^{\alpha}b^2 H_T(E;ib)-\frac{1}{2\pi i}\int_{-T}^{T}\frac{e^{itE}\,e^{-\alpha t^2}}{t-ib}dt \\ &= e^{\alpha b^2}e^{-Eb}-\frac{1}{2\sqrt{\pi\alpha}}\int_0^{\infty}e^{-bw}e^{-\frac{(w-E)^2}{4\alpha}}dw \\ &\quad +e^{\alpha b^2}\left(H_T(E;ib)-e^{-Eb}\right)-R_1-R_2 \end{aligned} \tag{8.65}$$

where we have introduced the notation of Lemma 8.4. For positive E, α, and b, the equality

$$\frac{1}{2\sqrt{\pi\alpha}}\int_{-\infty}^{\infty}e^{-wb}e^{-\frac{(w-E)^2}{4\alpha}}\,dw=e^{-Eb}e^{\alpha b^2} \tag{8.66}$$

holds; this can be seen e.g. by continuation and evaluation of (8.73) at $t=ib$. Moreover, since $E\geq\gamma$, the first two terms on the right-hand-side of (8.65) can be estimated by

$$\frac{1}{2\sqrt{\pi\alpha}}\int_{-\infty}^{0}e^{-bw}e^{-\frac{(w-E)^2}{4\alpha}}dw\leq\frac{1}{2}e^{-\frac{\gamma^2}{4\alpha}} \tag{8.67}$$

if $2\alpha b\leq\gamma$. Using the bounds established in Lemma 8.4, (8.63) now follows by an application of dominated convergence.

All of our estimates above combine to demonstrate that the right hand side of (8.52) is bounded by

$$\|A\|\,\|B\|\,\left[e^{-\frac{\gamma^2}{4\alpha}}+\frac{2\,D_a(X,Y)}{\pi\,\|\Phi\|_a\,C_a}\left(e^{2\,\|\Phi\|_a\,C_a\,s}-1\right)+\frac{1}{s\sqrt{\pi\alpha}}e^{-\alpha s^2}\right] \tag{8.68}$$

if α satisfies $\gamma\geq 2\alpha b$. The choice $\alpha=\gamma/2s$ yields:

$$\|A\|\,\|B\|\,e^{-\frac{\gamma s}{2}}\,\left[1+\sqrt{\frac{2}{\pi\gamma s}}+\frac{2\,D_a(X,Y)}{\pi\,\|\Phi\|_a\,C_a}e^{\left(2\,\|\Phi\|_a\,C_a+\frac{\gamma}{2}\right)s}\right] \tag{8.69}$$

As is demonstrated in (**??**), $D_a(X,Y)$ decays exponentially as $e^{-ad(X,Y)}$. In this case, if we choose s to be the solution of the equation

$$s\,(\,2\,\|\Phi\|_a\,C_a\,+\,\gamma/2\,)\,=\,a\,d(X,Y), \tag{8.70}$$

then we have proven the result. Notice that we have chosen α in terms of s, which is defined independently of b, thus the condition $\gamma\geq 2\alpha b$ will be satisfied for sufficiently small $b>0$. □

In the proof above we used the following lemma. We use the following notation.

$$\mathbb{C}^+=\{z\in\mathbb{C}:\mathrm{Im}[z]>0\}\,. \tag{8.71}$$

Lemma 8.4. *Fix $\alpha>0$, $E\in\mathbb{R}$, and $z\in\mathbb{C}^+$. One has that*

$$\lim_{T\to\infty}\frac{1}{2\pi i}\int_{-T}^{T}\frac{e^{iEt}\,e^{-\alpha t^2}}{t-z}\,dt\,=\,\frac{1}{2\sqrt{\pi\alpha}}\int_0^{\infty}e^{iwz}\,e^{-\frac{(w-E)^2}{4\alpha}}\,dw. \tag{8.72}$$

Moreover, the convergence is uniform with respect to z in compact subsets of $\mathbb{C}^+$.

Proof. For any $\alpha>0$, it is easy to check that

$$\frac{1}{2\sqrt{\pi\alpha}}\int_{-\infty}^{\infty}e^{iwt}\,e^{-\frac{(w-E)^2}{4\alpha}}\,dw=e^{iEt}\,e^{-\alpha t^2}\quad\text{for all } t,E\in\mathbb{R}\,. \tag{8.73}$$

Up to appropriate normalizations, this is just the observation that the Fourier transform of a gaussian is a gaussian. Given $z\in\mathbb{C}^+$, it is now clear that for any $T>0$,

$$\frac{1}{2\pi i}\int_{-T}^{T}\frac{e^{iEt}\,e^{-\alpha t^2}}{t-z}\,dt=\frac{1}{2\sqrt{\pi\alpha}}\int_{-\infty}^{\infty}H_T(w;z)\,e^{-\frac{(w-E)^2}{4\alpha}}\,dw \tag{8.74}$$

where we have denoted by $H_T(w;z)$ the function

$$H_T(w;z) \,=\, \frac{1}{2\pi i}\int_{-T}^{T} \frac{e^{iwt}}{t-z}\,dt \quad \text{for any } T>0 \text{ and } z\in\mathbb{C}^+. \tag{8.75}$$

Rewriting the integral on the right-hand-side of (8.74), we find that

$$\frac{1}{2\sqrt{\pi\alpha}}\int_{-\infty}^{\infty} H_T(w;z)\,e^{-\frac{(w-E)^2}{4\alpha}}\,dw = \frac{1}{2\sqrt{\pi\alpha}}\int_{0}^{\infty} e^{iwz}\,e^{-\frac{(w-E)^2}{4\alpha}}\,dw \,+\, R_1 \,+\, R_2$$

where we have labeled by R_1 and R_2 the integrals

$$\frac{1}{2\sqrt{\pi\alpha}}\int_{0}^{\infty} \left(H_T(w;z)-e^{iwz}\right)\,e^{-\frac{(w-E)^2}{4\alpha}}\,dw \quad \text{and} \quad \frac{1}{2\sqrt{\pi\alpha}}\int_{-\infty}^{0} H_T(w;z)\,e^{-\frac{(w-E)^2}{4\alpha}}\,dw \tag{8.76}$$

respectively.

We now show that: for fixed $\alpha>0$ and $E\in\mathbb{R}$, the above integrals R_1 and R_2 go to zero as $T\to\infty$. To see this, we inspect the function $H_T(w;z)$. There are two cases to consider.

Let $w>0$, i.e. we estimate R_1. With $z\in\mathbb{C}^+$ fixed, take $T>0$ large enough so that $0<2|z|<T$. In this case, integration about the rectangular contour Γ_T with corners:$-T$, T, $T+iT$, and $-T+iT$ produces:

$$\frac{1}{2\pi i}\int_{\Gamma_T} \frac{e^{iwz'}}{z'-z}\,dz' \,=\, e^{iwz} \tag{8.77}$$

and consequently the bound

$$\left|H_T(w;z)-e^{iwz}\right| \,\le\, \frac{2}{\pi}\left[\frac{1}{wT}\left(1-e^{-wT}\right)\,+\,e^{-wT}\right]. \tag{8.78}$$

For $w<0$, a similar rectangular contour, now in the lower half plane, can be integrated to yield

$$|H_T(w;z)| \,\le\, \frac{2}{\pi}\left[\frac{1}{|w|T}\left(1-e^{-|w|T}\right)\,+\,e^{-|w|T}\right]. \tag{8.79}$$

The claimed result, including the statement regarding uniformity, now follows from an application of dominated convergence. □

9. Appendix: Lie Groups and Lie Algebras

A *Lie Group* G is a group G with a compatible structure of a smooth (real or complex) manifold. For compatibility, it is assumed that the product and inversion mappings are smooth.

Many interesting Lie Groups, and the focus for most of these notes, are matrix Lie Groups which are subgroups of $GL(n,\mathbb{R})$, resp. $GL(n,\mathbb{C})$, here denoting the set of real, resp. complex, $n \times n$ invertible matrices. Two key examples are

$$SO(n) = \{A \in GL(n,\mathbb{R}) : AA^t = \mathbb{1} \text{ and } \det(A) = 1\} \tag{9.1}$$

and

$$SU(n) = \{A \in GL(n,\mathbb{C}) : AA^* = \mathbb{1} \text{ and } \det(A) = 1\} \tag{9.2}$$

both defined for any integer $n \geq 2$.

A Lie Group G is *compact* if G is compact as a manifold. A Lie Group G is *connected* if any two points in G can be linked together by a continuous curve in G.

In general, a *Lie Algebra* $\mathfrak{g}$ is a vector space $\mathfrak{g}$, over a field $\mathbb{F} \in \{\mathbb{R},\mathbb{C}\}$, equipped with a mapping $[\cdot,\cdot] : g \times g \to g$ which satisfies:
i) $[\alpha x + \beta y, z] = \alpha[x,z] + \beta[y,z]$ for all $x,y,z \in g$ and all $\alpha,\beta \in \mathbb{F}$.
ii) $[x,y] = -[y,x]$ for all $x,y \in g$.
iii) $[[x,y],z] + [[y,z],x] + [[z,x],y] = 0$ for all $x,y,z \in g$.

If $\mathfrak{g}$ is a Lie Algebra, then the mapping $[\cdot,\cdot]$ described above is called the *Lie bracket* associated with $\mathfrak{g}$.

If G is a Lie Group, then the Lie Algebra $\mathfrak{g}$ associated to G is, $T_{\mathbb{1}}(G)$, i.e. the tangent space of G at the identity $\mathbb{1} \in G$. The corresponding Lie bracket, i.e. $[x,y]$ for $x,y \in T_{\mathbb{1}}(G)$, is the standard vector field commutator of the vectors x and y pushed forward by left-multiplication, i.e.

$$[x,y] = [Lx, Ly]_{\mathbb{1}} \quad \text{for all } x,y \in T_{\mathbb{1}}(G)\,. \tag{9.3}$$

It will be important to keep the following examples in mind.

$$SU(2) = \{A \in GL(2,\mathbb{C}) : AA^* = \mathbb{1} \text{ and } \det(A) = 1\} \tag{9.4}$$

One readily checks that

$$SU(2) = \left\{ A = \begin{pmatrix} z & -w \\ \overline{w} & \overline{z} \end{pmatrix} : (z,w) \in \mathbb{C}^2 \text{ and } |z|^2 + |w|^2 = 1 \right\} \tag{9.5}$$

In fact, it is easy to see that any matrix A with form given by (9.5) is in SU(2). Conversely, if $A \in SU(2)$, then

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = A^{-1} = A^* = \begin{pmatrix} \overline{a} & \overline{c} \\ \overline{b} & \overline{d} \end{pmatrix} \tag{9.6}$$

and thus A has the form of (9.5). With (9.5), it is clear that SU(2) is equivalent to the unit sphere in $\mathbb{C}^2$. Since the unit sphere in $\mathbb{C}^2$ is equivalent to the real 3-sphere, i.e. the unit sphere in $\mathbb{R}^4$, the same is true for SU(2). In fact, let us define the Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{9.7}$$

Observe that any $A \in SU(2)$ can be written as:

$$A = x_0 \mathbb{1} + i \sum_{j=1}^{3} x_j \sigma^j \quad \text{for some real } x_j \text{ satisfying } 1 = \sum_{j=0}^{3} x_j^2\,, \tag{9.8}$$

where we have taken A with the form of (9.5) and written $z = x_0 + ix_3$ and $w = -x_2 - ix_1$. This smooth invertible map between SU(2) and the 3-sphere demonstrates that SU(2) is connected. It is also clearly compact.

Let us now consider SO(3). The group SO(3) is easily seen to be generated by the following three matrices:

(9.9)

$$R_1(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) \\ 0 & \sin(\theta) & \cos(\theta) \end{pmatrix}, R_2(\theta) = \begin{pmatrix} \cos(\theta) & 0 & \sin(\theta) \\ 0 & 1 & 0 \\ -\sin(\theta) & 0 & \cos(\theta) \end{pmatrix}, R_3(\theta) = \begin{pmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with $\theta \in [0, 2\pi)$. This can be argued as follows. As a matrix over the complex field, any $A \in SO(3)$ can be diagonalized, since every such A is normal. By orthogonality, any eigenvalue of A must have unit modulus. If all eigenvalues are real, then there are only two choices: all are 1 or 2 are -1. As the entries of A are real valued, any complex eigenvalues must come in conjugate pairs. Since the product of all the eigenvalues is 1, we conclude that A must have an eigenvector corresponding to eigenvalue one. Using the standard basis vectors to extend this normalized vector to an orthonormal basis, we see that any $A \in SO(3)$ is unitarily equivalent to a matrix as in (9.9) above.

Consider the mapping $f : SU(2) \to SO(3)$ given by

$$f(A)_{ij} = \frac{1}{3}\mathrm{Tr}[\sigma^i A \sigma^j A^*] \tag{9.10}$$

One can check that this mapping is indeed into SO(3). In fact, it is onto, $f(-A) = f(A)$, and this mapping is in fact 2 to 1. Moreover, $f(AB) = f(A)f(B)$, i.e. f is a group homomorphism.

Note: we have parametrized the matrices in (9.9) above so that $R_j(0) = \mathbb{1}$ for all $j = 1, 2, 3$. It is easy to see that

$$R_1'(0) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, R_2'(0) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, R_3'(0) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{9.11}$$

The matrices form a basis for the corresponding Lie Algebra so(3) .

9.1. **Representations of Lie Groups and Lie Algebras.** In this section, we will consider some of the general theory of finite dimensional representations of both Lie Groups and Lie Algebras. Again, most of the focus will be on matrix Lie Groups and their associated Lie Algebras. Throughout this section, we will denote by V a finite dimensional vector space over a field $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. By $L(V)$, we will denote the set of all linear transformations from V to V. By $GL(V)$, we will denote the set of all invertible linear transformations from V to V.

Definition 9.1. Let G be a Lie Group and V be a finite dimensional vector space over $\mathbb{K}$. A representation Π of G acting on V is a mapping $\Pi : G \to GL(V)$ which satisfies

$$\Pi(g_1 g_2) = \Pi(g_1)\Pi(g_2) \quad \text{for all } g_1, g_2 \in G\,. \tag{9.12}$$

The dimension of the representation Π is defined by $\dim(\Pi) = \dim(V)$.

It follows immediately from this definition that:

i) $\Pi(\mathbb{1}) = \mathrm{id}$, where id is the identity map on V.

ii) $\Pi(g^{-1}) = (\Pi(g))^{-1}$ for all $g \in G$.

iii) If $\Pi : G \to L(V)$ satisfying $\Pi(\mathbb{1}) = \mathrm{id}$ and (9.12), then Π is a representation of G acting on V.

The definition of representation for a Lie Algebra corresponding to a Lie Group is similar.

Definition 9.2. Let g be a Lie Algebra and V a finite dimensional vector space over $\mathbb{K}$. A representation π of g acting on V is a mapping $\pi : g \to L(V)$ which satisfies

$$\pi([x, y]) = [\pi(x), \pi(y)] \quad \text{for all } x, y \in g\,. \tag{9.13}$$

The dimension of the representation π is defined by $\dim(\pi) = \dim(V)$.

Examples:

1) For any Lie Group G and any vector space V, the trivial representation is the mapping $\Pi(g) = \mathrm{id}$ for all $g \in G$. For $\mathfrak{g}$ a Lie Algebra, the trivial representation of $\mathfrak{g}$ is defined by $\pi(x) = 0$ for all $x \in g$.

2) If G is a matrix Lie Group, i.e. a sub-group of $GL(n, \mathbb{R})$, resp. $GL(n, \mathbb{C})$, then with $V = \mathbb{R}^n$, resp. $V = \mathbb{C}^n$, the mapping $\Pi(g) = g$ for all $g \in G$ is called the fundamental representation of G. In this case, one can also define the fundamental representation of the corresponding Lie Algebra, and it is $\pi(x) = x$ for all $x \in g$.

3) Let G be a matrix Lie Group and $\mathfrak{g}$ the corresponding Lie Algebra. The mapping $\mathrm{Ad} : G \to GL(g)$ defined by

$$\mathrm{Ad}(g)x = gxg^{-1} \quad \text{for all } g \in G \text{ and } x \in g \tag{9.14}$$

is a representation of G on $\mathfrak{g}$. This is called the adjoint representation of the Lie Group G. There is an analogous representation of the Lie Algebra $\mathfrak{g}$ acting on $\mathfrak{g}$ which is the mapping $\mathrm{ad} : g \to L(g)$ given by

$$(\mathrm{ad}x)(y) = [x, y] \quad \text{for all } x, y \in g. \tag{9.15}$$

Proposition 9.3. *Let G be a matrix Lie Group. If Π is a representation of G acting on V, then there exists a representation π of the corresponding Lie Algebra g, also acting on V, defined via*

$$\pi(x) = \frac{d}{dt}\left(\Pi\left(\exp(tx)\right)\right)|_{t=0} \quad \textit{for all } x \in g\,. \tag{9.16}$$

π is said to be the representation of g induced by Π.

Example:

For any matrix Lie Group G, the adjoint representation Ad, see (9.14), induces the adjoint representation ad, see (9.15). In fact,

$$\frac{d}{dt}\left(\mathrm{Ad}(e^{tx})\right)|_{t=0} = \mathrm{ad}(x) \quad \text{for all } x \in g\,. \tag{9.17}$$

There is a (partial) converse of Proposition 9.3.

Proposition 9.4. *Let G be a matrix Lie Group, and let π be a representation of the corresponding Lie Algebra g acting on V. The mapping*

$$\Pi(g) = e^{\pi(x)} \quad \textit{defined for all } g \in G \textit{ with } g = e^x\,, \tag{9.18}$$

defines a representation Π of G on V.

Since $\mathbb{1} \in G$ satisfies $\mathbb{1} = e^0$, it is clear that the above is well-defined for all x near 0. For this reason, the mapping Π is said to be the representation locally induced by π.

The following is an important definition.

Definition 9.5. Let Π be a representation of a Lie Group G on a finite dimensional vector space V over $\mathbb{C}$. If $\Pi(g)\Pi(g)^* = \mathrm{id}$ for all $g \in G$, then Π is said to be a unitary representation. Similarly, let π be a representation of a Lie Algebra $\mathfrak{g}$ on a finite dimensional vector space V over $\mathbb{C}$. If $\pi(x)^* = -\pi(x)$ for all $x \in g$, then π is said to be an anti-hermitian representation.

Proposition 9.6. *Let G be a matrix Lie Group and g the corresponding Lie Algebra.*
a) If Π is a unitary representation of G on V, then the induced representation π of g on V is anti-hermitian.
b) If π is an anti-hermitian representation of g on V, then the (locally) induced representation Π of G on V is unitary.

The following definition applies to representations of Lie Groups and Lie Algebras. In general, we will denote such a representation by ρ.

Definition 9.7. Let ρ be a representation of G, which may either be a Lie Group or a Lie Algebra, acting on a finite dimensional vector space V. If $W \subset V$ is a subspace and $\rho(g)w \in W$ for all $g \in G$ and $w \in W$, then W is said to be a ρ-invariant subspace. A representation ρ is said to be reducible if there exists a non-trivial ρ-invariant subspace, i.e. a ρ-invariant subspace $W \subset V$ with $W \neq \{0\}$ and $W \neq V$. If the only ρ-invariant subspaces of V are $\{0\}$ and V, then ρ is said to be irreducible.

Proposition 9.8. *Let G be a matrix Lie Group and $\mathfrak{g}$ the associated Lie Algebra.*
a) If Π is a representation of G acting on V and W is a Π-invariant subspace, then W is also an π-invariant subspace of V, where π is the induced representation of $\mathfrak{g}$ acting on V.
b) If π is a representation of $\mathfrak{g}$ acting on V and W is a π-invariant subspace, then W is also an Π-invariant subspace of V, where Π is the (locally) induced representation of G acting on V.

Definition 9.9. Let ρ be a representation of G, which may either be a Lie Group or a Lie Algebra, acting on a finite dimensional vector space V. ρ is said to be totally reducible if there exists a direct sum decomposition of V into subspaces $\{W_j\}_{j=1}^k$, i.e.,

$$V = W_1 \oplus W_2 \oplus \cdots \oplus W_k \tag{9.19}$$

with each W_j being a ρ-invariant subspace for which $\rho_j = \rho|_{W_j}$ is irreducible.

Note that if ρ is a totally reducible representation on a finite dimensional vectors space V, then there is a basis of V for which

$$\rho(g) = \begin{pmatrix} \rho_1(g) & 0 & 0 & 0 \\ 0 & \rho_2(g) & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & \cdots & \rho_k(g) \end{pmatrix} \tag{9.20}$$

i.e. ρ acts block-diagonally.

Proposition 9.10. *Any finite dimensional unitary representation is totally reducible.*

Proof. Let Π be a unitary representation of a Lie Group G acting on a finite dimensional vector space V over $\mathbb{C}$. If Π is irreducible, we are done. Otherwise, there exists a non-trivial Π-invariant subspace $W \subset V$. We can write $V = W \oplus W^\perp$ and note that if $x \in W^\perp$, $y \in W$, and $g \in G$, then

$$\langle \Pi(g)x, y\rangle = \langle x, \Pi(g)^* y\rangle = \langle x, \Pi(g)^{-1} y\rangle = \langle x, \Pi(g^{-1})y\rangle = 0 \tag{9.21}$$

where the last equality follows since W is Π-invariant. This proves that $W^\perp$ is also a Π-invariant subspace. Iterating this argument to the restrictions of Π to these (finite dimensional) subspaces produces the desired result. □

On equivalent representations:

Definition 9.11. Let ρ_1 be a representation of G, which may either be a Lie Group or a Lie Algebra, acting on finite dimensional vector spaces V_1. For any invertible linear transformation $T : V_1 \to V_2$, then the mapping

$$\rho_2(g) = T\rho_1(g)T^{-1} \tag{9.22}$$

defines a representation of G on V_2. Representations of this type are said to be equivalent representations.

It is easy to check that if Π_1 and Π_2 are equivalent representations, then the corresponding induced representations π_1 and π_2 are equivalent as well. Similarly, if π_1 and π_2 are equivalent, then the locally induced representations Π_1 and Π_2 are also equivalent.

Lemma 9.12. *Let ρ_1 and ρ_2 be two irreducible representations of G acting on vector spaces V_1 and V_2 respectively. If there exists a linear transformation $T : V_1 \to V_2$ for which*

$$T\rho_1(g) = \rho_2(g)T \quad \text{for all } g \in G, \tag{9.23}$$

then either ρ_1 and ρ_2 are equivalent representations or $T = 0$.

Proof. It is easy to check that $\ker(T) \subset V_1$ is a ρ_1-invariant subspace and similarly $\mathrm{ran}(T) \subset V_2$ is a ρ_2-invariant subspace. The claimed result follows. □

Lemma 9.13. *Let ρ be an irreducible representation of G on a finite dimensional vector space V over $\mathbb{C}$. If $T : V \to V$ is linear and*

$$T\rho(g) = \rho(g)T \quad \text{for all } g \in G, \tag{9.24}$$

then $T = \lambda \mathrm{id}$ for some $\lambda \in \mathbb{C}$.

Proof. As a linear operator on a finite dimensional vector space over $\mathbb{C}$, T has at least one eigenvalue $\lambda \in \mathbb{C}$. The non-empty eigenspace U_λ is clearly a ρ-invariant subspace. □

On tensor products. Fix a Lie Group G. For $j = 1, 2$, let Π_j be a representation of G acting on a vector space V_j. Consider the vector space

$$V = V_1 \otimes V_2 \tag{9.25}$$

For any $g \in G$, we define a linear mapping $\Pi(g) : V \to V$ by setting

$$\Pi(g)v_1 \otimes v_2 = (\Pi_1(g)v_1) \otimes (\Pi_2(g)v_2) \ , \tag{9.26}$$

e.g. on a collection of basis vectors, and extending by linearity. The mapping Π is a representation G, it is called the tensor product representation, and it is often denoted by $\Pi = \Pi_1 \otimes \Pi_2$. Similarly, if π_1 and π_2 are representations of g acting on vector spaces V_1 and V_2 respectively, then π defined by setting

$$\pi = \pi_1 \otimes \mathrm{id} + \mathrm{id} \otimes \pi_2 \tag{9.27}$$

is a representation of g acting on $V = V_1 \otimes V_2$. In fact, if Π_1 and Π_2 are representations of a matrix Lie Group acting on V_1 and V_2 respectively, then the induced representation of $\Pi = \Pi_1 \otimes \Pi_2$ acting on $V = V_1 \otimes V_2$ is given by $\pi = \pi_1 \otimes \mathrm{id} + \mathrm{id} \otimes \pi_2$.

9.2. **Irreducible Representations of SU(2).** The Lie Algebra corresponding to $SU(2)$, which we denote by $\mathrm{SU(2)}$, has as basis vectors:

$$T_1 = -\frac{i}{2}\sigma^1 = \begin{pmatrix} 0 & -\frac{i}{2} \\ -\frac{i}{2} & 0 \end{pmatrix}, \quad T_2 = -\frac{i}{2}\sigma^2 = \begin{pmatrix} 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}, \quad \text{and} \quad T_3 = -\frac{i}{2}\sigma^3 = \begin{pmatrix} -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} \end{pmatrix}. \tag{9.28}$$

Let π be an irreducible representation of $\mathrm{SU(2)}$ on a finite dimensional vector space V with $\dim(V) = n$. Define linear mappings

$$J_3 = i\pi(T_3) \quad \text{and} \quad J_\pm = \frac{i}{\sqrt{2}} \left(\pi(T_1) \pm i\pi(T_2)\right) \ . \tag{9.29}$$

The commutation relations

$$[J_3, J_\pm] = \pm J_\pm \quad \text{and} \quad [J_+, J_-] = J_3 \tag{9.30}$$

are easily checked.

Since V is a complex vector space, it is clear that J_3 has at least one eigenvalue $\lambda \in \mathbb{C}$. Let us denote a corresponding (non-zero) eigenvector by ϕ. One readily calculates that

$$J_3(J_\pm)^k\phi = (\lambda \pm k)(J_\pm)^k\phi \quad \text{for any integer } k \geq 0. \tag{9.31}$$

The mappings $J_\pm$ are called raising and lowering operators. The eigenvalues of J_3 are called weights. The above calculation shows that either $(J_\pm)^k\phi = 0$ or it is an eigenvector of J_3 with eigenvalue $\lambda \pm k$.

Consider the sequence of vectors $\{(J_+)^k\phi\}_{k=0}^\infty \subset V$. The non-zero vectors in this sequence are eigenvectors of J_3 corresponding to distinct eigenvalues, and therefore, linearly independent. Since the vector space V is finite dimensional, there must exist a number $j \geq 0$ for which $(J_+)^j\phi \neq 0$ but $(J_+)^{j+1}\phi = 0$. The corresponding eigenvalue of J_3, which we denote by λ_j, is called the highest weight of the representation π. It is convenient to relabel $\psi = (J_+)^j\phi \neq 0$.

Mimicking the above calculation, we find that

$$J_3(J_-)^k\psi = (\lambda_j - k)(J_-)^k\psi \quad \text{for all integers } k \geq 0. \tag{9.32}$$

Again, these are either 0 or linearly independent eigenvectors of J_3. Using again that V is finite dimensional, there is a number $m \geq 0$ such that $0 \neq (J_-)^m\psi$, but $(J_-)^{m+1}\psi = 0$. For $k = 0, \cdots, m$, denote by $\psi_k = (J_-)^k\psi$. Note that $\psi_0 = \psi$, and for all $0 \leq k \leq m$, $\psi_k \neq 0$ and $J_3\psi_k = (\lambda_j - k)\psi_k$.

We will now prove that $2\lambda_j = m$. Recall the integer $m \geq 0$. Consider the case $m = 0$. In this case, there is a non-zero vector $\psi = \psi_0$ that satisfies $J_+\psi = 0 = J_-\psi$. As a result,

$$\lambda_j\psi = J_3\psi = [J_+, J_-]\psi = 0 \quad \Rightarrow \quad 2\lambda_j = 0 = m. \tag{9.33}$$

Now, if $m \geq 1$, then it is easy to see that for $1 \leq k \leq m$

$$\begin{aligned} J_+\psi_k = J_+(J_-)^k\psi_0 &= ([J_+, J_-] + J_-J_+)\,(J_-)^{k-1}\psi_0 \\ &= J_3(J_-)^{k-1}\psi_0 + J_-\left([J_+, J_-] + J_-J_+\right)(J_-)^{k-2}\psi_0 \\ &= \sum_{\ell=0}^{k-1}(J_-)^\ell J_3(J_-)^{k-1-\ell}\psi_0 \\ &= k\left(\lambda_j - \frac{1}{2}(k-1)\right)\psi_{k-1} \end{aligned} \tag{9.34}$$

where we have used (9.32) and that, by construction, $J_+\psi_0 = J_+\psi = 0$. Since we also have that $J_-\psi_m = 0$, we find that

$$\begin{aligned} 0 = J_+J_-\psi_m = ([J_+, J_-] + J_-J_+)\,\psi_m &= (\lambda_j - m)\psi_m + J_-J_+\psi_m \\ &= \left[(\lambda_j - m) + m\left(\lambda_j - \frac{1}{2}(m-1)\right)\right]\psi_m \\ &= \frac{1}{2}(m+1)(2\lambda_j - m)\psi_m \end{aligned} \tag{9.35}$$

Since $\psi_m \neq 0$, we have then that $2\lambda_j = m$ as claimed.

We now claim that the vectors $\{\psi_k\}_{k=0}^m$ form a basis of V and that the highest weight vector $\psi_0 = \psi$ is unique up to normalization. Consider the subspace $V' \subset V$ spanned by these vectors. This is easily checked to be a non-empty π-invariant subspace, and hence $V' = V$ since π is irreducible. As a consequence, we have also proven that J_3 is diagonalizable on V and that each eigenspace is one-dimensional. Moreover, $n = \dim(V) = m + 1 = 2\lambda_j + 1$.

To see that the highest weight vector is unique, suppose that φ is an eigenvector of J_3 with $J_3\varphi = \mu\varphi$ and $J_+\varphi = 0$. As the vectors $\{\psi_k\}_{k=0}^m$ form a basis of V, it is clear that

$$\varphi = \sum_{k=0}^m c_k\psi_k \tag{9.36}$$

We also showed above that the eigenspaces of J_3 are one-dimensional. Thus there is some $0 \leq k_0 \leq m$ for which $\varphi = c_{k_0}\psi_{k_0}$. If $k_0 = 0$, we are done. Otherwise, we have that

$$\mu\varphi = J_3\varphi = c_{k_0}(\lambda_j - k_0)\psi_{k_0} = (\lambda_j - k_0)\varphi \quad \Rightarrow \quad \mu = \lambda_j - k_0 \tag{9.37}$$

We also know that

$$0 = J_+\varphi = c_{k_0} J_+ \psi_{k_0} = c_{k_0} k_0 \left(\lambda_j - \frac{1}{2}(k_0 - 1)\right)\psi_{k_0 - 1} \quad \Rightarrow \quad \lambda_j = \frac{1}{2}(k_0 - 1) \tag{9.38}$$

But we know that $k_0 \leq m = 2\lambda_j$. Thus $2\lambda_j = k_0 - 1 \leq 2\lambda_j - 1$ an obvious contradiction. We conclude $k_0 = 0$ and we are done.

9.3. **Tensor products of representations.** Let π_1 and π_2 be two irreducible representations of $SU(2)$ on vector spaces $V^{(1)}$ and $V^{(2)}$. We will consider the representation

$$\pi = \pi_1 \otimes \mathbb{1} + \mathbb{1} \otimes \pi_2 \tag{9.39}$$

acting on $V = V^{(1)} \otimes V^{(2)}$. Our goal is to decompose V into irreducible representations of π, i.e. write V as a direct sum of π-invariant subspaces with the property that on each π acts as an irreducible representation.

We begin with some notation. As before, for $k = 1, 2$, set

$$J_3^{(k)} = i\pi_k(T_3) \quad \text{and} \quad J_\pm^{(k)} \frac{i}{\sqrt{2}} \left(\pi_k(T_1) \pm i\pi_k(T_2)\right) \tag{9.40}$$

On V we define

$$J_3 = J_3^{(1)} \otimes \mathbb{1} + \mathbb{1} \otimes J_3^{(2)} \quad \text{and} \quad J_\pm = J_\pm^{(1)} \otimes \mathbb{1} + \mathbb{1} \otimes J_\pm^{(2)} \tag{9.41}$$

The commutation relations

$$[J_3, J_\pm] = \pm J_\pm \quad \text{and} \quad [J_+, J_-] = J_3 \tag{9.42}$$

are easily checked.

Let us now suppose that $\dim(V^{(k)}) = 2j_k + 1$ for $k = 1, 2$. Denote by $\{\psi_m^{(k)}\}$ the sequences of eigenvectors of $J_3^{(k)}$ constructed previously, i.e.

$$J_3^{(k)} \psi_m^{(k)} = m\psi_m^{(k)} \quad \text{for all } -j_k \leq m \leq j_k\,. \tag{9.43}$$

It is clear that vectors of the form

$$\Psi_{m,n} = \psi_m^{(1)} \otimes \psi_n^{(2)} \tag{9.44}$$

form a basis of V and moreover, one readily checks that

$$J_3 \Psi_{m,n} = (m + n)\Psi_{m,n} \tag{9.45}$$

Let us denote by E_λ the eigen-subspace of V corresponding to the operator J_3 and the eigenvalue λ. By construction, it is clear that $\dim(E_{j_1+j_2}) = 1$. In fact, one also sees that

$$\dim(E_{j_1+j_2-k}) = k + 1 \quad \text{for all } 0 \leq k \leq j_1 + j_2 - |j_1 - j_2| \tag{9.46}$$

This is because there are $k+1$ ways to write the vectors above in such a way that the sum of their eigenvalues is this number . . . The collection of these eigenspaces does not exhaust the whole of V, but they will be sufficient for our purposes.

We find this direct sum decomposition algorithmically. We start with the highest weight vector, i.e. Ψ_{j_1,j_2}. This vector is the unique vector, up to normalization, in the eigenspace of J_3 corresponding to $j_1 + j_2$. Iteratively applying J_- to this vector, we produce $2(j_1 + j_2) + 1$ vectors in V that are eigenvectors of J_3 with eigenvalues m with $-(j_1 + j_2) \leq m \leq j_1 + j_2$. The subspace spanned by these orthogonal vectors, which we will denote by $V_{j_1+j_2}$, is a π-invariant subspace of V on which π acts an irreducible representation. Take $V' = V_{j_1+j_2}^{\perp}$.

Now consider $\lambda_1 = j_1 + j_2 - 1$. If $1 \leq j_1 + j_2 - |j_1 - j_2|$, then the dimension of the eigenspace of J_3 corresponding to λ_1 is 2, using (9.46). One of these vectors was constructed in the previous argument and hence it lies in $V_{j_1+j_2}$. Since the dimension of the eigenspace is 2, we are guaranteed that there exists a linearly independent vector in V' which is also an eigenvector of J_3 with eigenvalue λ_1. Using it and iteratively applying J_-, we find $2(j_1 + j_2 - 1) + 1$ orthogonal vectors in V' - each

eigenvectors of J_3 with prescribed eigenvalues. The subspace spanned by these vectors, which we will denote by $V_{j_1+j_2-1}$ is π-invariant and π acts on this subspace as an irreducible representation. Relabel $V' = (V_{j_1+j_2} \oplus V_{j_1+j_2-1})^{\perp}$.

Now, by way of induction, let $\lambda_k = j_1 + j_2 - k$ and assume that we have continued as above k times. If $k \leq j_1 + j_2 - |j_1 - j_2|$, then the eigenspace associated to J_3 and eigenvalue λ_k is $k+1$ dimensional by (9.46). By way of induction, we have already selected k linearly independent vectors in this subspace. In this step, we select the remaining vector. We apply J_- iteratively and obtain $2\lambda_k + 1$ orthogonal vectors which span the π-invariant subspace V_{λ_k}.

This procedure cannot be continued beyond $k = j_1 + j_2 - |j_1 - j_2|$. At that point, we have a subspace of V with dimension

$$\begin{aligned} \sum_{k=|j_1-j_2|}^{j_1+j_2} \dim(V_k) = \sum_{k=|j_1-j_2|}^{j_1+j_2} 2k+1 &= \sum_{\ell=0}^{j_1+j_2-|j_1-j_2|} (2(|j_1-j_2|+\ell)+1) \\ &= (2j_1+1)(2j_2+1) = \dim(V) \end{aligned} \tag{9.47}$$

and therefore, we have decomposed all of V.

10. Four Examples

The phenomena we studied in the general theorems and discussion in the previous chapters, spontaneaous symmetry breaking and long-range order, gapped versus gapless excitation spectrum, and the decay of correlations, are well-illustrated by the ground states of the isotropic ferromagnetic Heisenberg model (Example 1), the ferromagnetic XXZ model (Example 2), and the AKLT chain (Example 3). Later we will also discuss the Toric Code model to illustrate the concept of topological order (Example 4). All these models are examples of so-called Frustration-Free models, a property we will exploit in more detail in the next chapter on Matrix Product States and their Hamiltonians.

10.1. **Example 1: the isotropic Heisenberg model.** We start with the isotropic ferromagnetic spin 1/2 Heisenberg model on $\mathbb{Z}^\nu$, introduced by Heisenberg [35], which presents a good illustration of the gapless excitation spectrum implied by Goldstone's Theorem in the presence of spontaneous breaking of a continuous symmetry, in this case $SU(2)$.

At each $x \in \mathbb{Z}^2$, we have a spin 1/2 system with Hilbert space $\mathcal{H}_{\{x\}} \cong \mathbb{C}^2$. The interaction is between nearest neighbors only and is given in terms of the Pauli matrices by

$$h = -(\sigma^1 \otimes \sigma^1 + \sigma^2 \otimes \sigma^2 + \sigma^3 \otimes \sigma^3) = (\mathbb{1} - 2T) \in M_2 \otimes M_2, \tag{10.1}$$

where T denotes the transposition operator determined by $T(u \otimes v) = v \otimes u$, for all $u, v \in \mathbb{C}^2$. For every finite $\Lambda \subset \mathbb{Z}^\nu$, the Hamiltonian is given by

$$H_\Lambda = \sum_{\substack{x,y \in \Lambda \\ |x-y|=1}} (\mathbb{1} - 2T_{x,y}). \tag{10.2}$$

For example, one can take $\Lambda = [a_1, b_1] \times \cdots \times [a_\nu, b_\nu]$, with $a_i < b_i \in \mathbb{Z}$, $i = 1, \ldots, \nu$. It is quite obvious from the form Hamiltonian that all states symmetric under arbitrary permutations of the sites in Λ, will be a ground state of H_Λ. If Λ is connected (in the nearest neighbor sense), the set of transpositions $T_{x,y}$ for all nearest neighbor pairs $x, y \in \Lambda$, generate the full permutation group. In this case the ground state space of H_Λ is exactly the subspace of $\mathcal{H}_\Lambda$ consisting of all symmetric vectors. Let $E_0(H)$ denote the smalled eigenvalue of H. Then,

$$E_0(H_\Lambda) = -\#\{\{x, y\} \mid x, y \in \Lambda, |x - y|\}. \tag{10.3}$$

It will be slightly simpler to work with the non-negative definite Hamiltonian

$$0 \leq \tilde{H}_\Lambda = \frac{1}{2}(H_\Lambda - E_0(H_\Lambda)\mathbb{1}) = \sum_{\substack{x,y \in \Lambda \\ |x-y|=1}} (\mathbb{1} - T_{x,y}), \tag{10.4}$$

which obviously has the same ground state space and has H_Λ.

For all $u \in SU(2)$, we have $[T, u \otimes u] = 0$, and hence H_Λ (and $\tilde{H}_\Lambda$) commute with

$$U_\Lambda = \bigotimes_{x \in \Lambda} u. \tag{10.5}$$

As a consequence, the Hamiltonians also commute with the third component of the total magnetization or, equivalently, with the following operator N_Λ which counts the number of down spins (minus signs):

$$N_\Lambda = \sum_{x \in \Lambda} (\mathbb{1} - \sigma_x^3)/2. \tag{10.6}$$

$\mathrm{spec} N_\Lambda = \{0, 1, \ldots, |\Lambda|\}$, and there is one symmetric state in each eigenspace of N_Λ. Hence, $\dim \ker(\tilde{H}_\Lambda) = |\Lambda| + 1$. For $n = 0, \ldots, |\Lambda|$, let $\mathcal{H}^{(n)}$ denote the eigenspace of N_Λ belonging to the

eigenvalue n. This is the space of states with n down spins. A basis for this spaces can therefore be labeled by the possible sets of n sites (the positions of the down spins) in Λ. Hence,

$$\dim(\mathcal{H}_\Lambda^{(n)}) = \binom{|\Lambda|}{n}. \tag{10.7}$$

$\mathcal{H}_\Lambda^{(0)}$ is one-dimensional and spanned by the vector $\bigotimes_{x\in\Lambda}|+\rangle$. Let ω_+ denote the corresponding vector state. On each $\mathcal{A}_\Lambda$, ω_+ is uniquely determined by the property $\omega(\sigma_x^3)=1$, for all $x\in\Lambda$. It follows that this also determines ω_+ uniquely on $\mathcal{A}_{\mathbb{Z}^\nu}$.

Since ω_+ is a product state its GNS representation is easy to construct. As GNS Hilbert space we can take $\ell^2(\mathcal{P}_0(\mathbb{Z}^\nu))$. Let $\{\xi_X \mid x\in\mathcal{P}_0(\mathbb{Z}^\nu)\}$ denote the standard orthonormal basis of $\ell^2(\mathcal{P}_0(\mathbb{Z}^\nu))$ given by Kronecker delta functions. The finite subsets $X\in\mathcal{P}_0(\mathbb{Z}^\nu)$ are the locations of a finite number of down spins. In ω_+, the are zero down spins and this state should therefore represented by $\Omega=\xi_\emptyset$. This can be verified with the following defintion of the representation π:

$$\pi_\omega(\sigma_x^-)\xi_X = \begin{cases} \xi_{X\cup\{x\}} & \text{if } x\notin X \\ 0 & \text{if } x\in X \end{cases}. \tag{10.8}$$

The morphism property of π implies that it is uniquely determined by its action on σ_x^-, $x\in\mathbb{Z}^\nu$, and one can easily derive its action on arbitrary local observables. For instance, $\pi(\sigma_x^+)=\pi(\sigma_x^-)^*$, $\pi(\sigma_x^3)=\pi(\sigma_x^+)\pi(\sigma_x^-)-\pi(\sigma_x^-)\pi(\sigma_x^+)$, etc.. Since we have $\pi(\prod_{x\in X}\sigma_x^-)\Omega=\xi_X$, it is clear that $\pi(\mathcal{A}_{\mathbb{Z}^\nu}^{\rm loc})\Omega$ is dense in $\mathcal{H}$. Therefore $(\mathcal{H},\pi,\Omega)$ is the GNS triple for ω_+.

In the GNS representation of ω_+, the number of down spins of the infinite system is represented by the densely defined self-adjoint operator N, for which $\pi(\mathcal{A}_{\mathbb{Z}^\nu}^{\rm loc})\Omega$ is a core, and for which the standard basis vectors ξ_X are eigenvectors with eigenvalue $n=|X|$. The corresponding eigenspaces $\mathcal{H}^{(n)}$ are invariant subspaces of the GNS Hamiltonian H_{ω_+}. The latter is easily see from the explicit definition of H_{ω_+} on $\pi(\mathcal{A}_{\mathbb{Z}^\nu}^{\rm loc})\Omega$ as follows. For each $X\in\mathbb{Z}$, define $\overline{X}=\{y\in\mathbb{Z}^\nu \mid d(y,X)\le 1\}$. Then, for all finite X, $\overline{X}$ is finite, and for all $A\in\mathcal{A}_X$, we have

$$H_{\omega_+}\pi(A)\Omega = \lim_{\Lambda\to\mathbb{Z}^\nu}[\pi(H_\Lambda),\pi(A)]\Omega = [\pi(H_{\overline{X}}),\pi(A)]\Omega = \sum_{\substack{x,y\in\overline{X}\\ |x-y|=1}} 2(\mathbb{1}-T_{x,y})\pi(A)\Omega, \tag{10.9}$$

where, by slight abuse of notation, $T_{x,y}=\pi(T_{x,y})$ is the transposition of the states at x and y acting as a unitary operator on $\mathcal{H}$, and we have used $T_{x,y}\Omega=\Omega$, for all $x,y\in\mathbb{Z}^\nu$. Clearly, the spaces $\mathcal{H}^{(n)}$ are invariant under the $T_{x,y}$, and therefore also invariant subspaces of H_{ω_+}. So, we have $\mathrm{spec}(H_{\omega_+}\restriction_{\mathcal{H}^{(1)}})\subset\mathrm{spec}(H_{\omega_+})$. Now, $\mathcal{H}^{(1)}=\overline{\mathrm{span}\{\xi_{\{x\}}\mid x\in\mathbb{Z}^\nu\}}\cong\ell^2(\mathbb{Z}^\nu)$, and it turns out that $H_{\omega_+}\restriction_{\mathcal{H}^{(1)}}$ can be represented as a familiar operator on $\ell^2(\mathbb{Z}^\nu)$. To see this, calculate the matrix elements in the orthonormal basis $\{\xi_{\{x\}}\}$:

$$\langle\xi_{\{x\}},H_{\omega_+}\xi_{\{y\}}\rangle = \begin{cases} -2 & \text{if } |x-y|=1 \\ 4\nu & \text{if } x=y \\ 0 & \text{else} \end{cases}. \tag{10.10}$$

Up to trivial constants, these are the matrix elements of the discrete Laplacian on $\mathbb{Z}^\nu$. Its spectrum is the interval $[0,8\nu]$, and is absolutely continuous. Therefore, H_{ω_+} has no gap above the ground state, as implied by the Goldstone Theorem. The generalized eigenfunction corresponding this part of the spectrum are called *spin waves*. Considering the positions of the single down spin in the subspace $\mathcal{H}^{(1)}$ as the coordinate of a particle, the corresponding generalized eigenfunctions are plane waves on $\mathbb{Z}^\nu$. Dyson pointed out that the generalized eigenstates of the Heisenberg ferromagnet in the subspace $\mathcal{H}^{(n)}$ can be regarded as describing n such particles with boson statistics which satisfy a hard-core condition (at most one particle can occupy any give site) and a nearest neighbor interaction. He also showed that the spin-S Heisenberg ferromagnet in the ground state

representation can be described in a similar way as bosons and that the interaction would become weaker with increasing S [18,19]. Recently, Correggi, Giuliani, and Seiringer gave a rigorous proof that the approximation by free bosons is at least sufficiently good to predict correct low-temperature asymptotics of the free energy density of the Heisenberg model for any S [16].

10.2. **Example 2: the XXZ model.** The spin 1/2 ferromagnetic XXZ model depends on a real parameter, Δ, which is often called the anisotropy. It is defined in terms of a nearest neighbor interaction and coincides with the isotropic Heisenberg model for $\Delta = 1$. The XXZ nearest neighbor interaction is given by

$$h^{(\Delta)} = -(\sigma^1 \otimes \sigma^1 + \sigma^2 \otimes \sigma^2 + \Delta\sigma^3 \otimes \sigma^3) = h^{(1)} - (\Delta - 1)\sigma^3 \otimes \sigma^3. \tag{10.11}$$

We already studied the ground states of the isotropic model with interaction $h^{(1)}$ in the previous section. It is quite immediate that, for all $\Delta > 1$, there are exactly two of the ground states of the isotropic model that are simultaneous eigenstates belonging to the smallest each of the additional terms of the form $-(\Delta - 1)\sigma^3 \otimes \sigma^3$, namely the states with all spins up and all spins down. Let ω_+ and ω_- denote the corresponding states on $\mathcal{A}_{\mathbb{Z}^\nu}$. The XXZ model has a continuous symmetry, given by the rotations about the third axis, described by the group $U(1)$ (or $SO(2)$). This symmetry is, however not broken in the ground states of the model. The model has a discrete symmetry that is spontaneously broken: a $\mathbb{Z}_2$ symmetry represented by the automorphism α defined by

$$\alpha(A) = (\bigotimes_{x\in X} \sigma^1) A (\bigotimes_{x\in X} \sigma^1), \text{ for all } A \in \mathcal{A}_X, X \in \mathcal{P}_0(\mathbb{Z}^\nu). \tag{10.12}$$

One can show that the GNS Hamiltonian of $\omega_\pm$ have a spectral gap above their ground state equal to $2(\Delta - 1)$. As the Goldstone Theorem predicts, the continuous $U(1)$ is unbroken.

10.3. **Example 3: the AKLT model.** The AKLT model was introduced by Affleck, Kennedy, Lieb, and Tasaki [3, 4]. It is a spin-1 chain, so $\mathcal{H}_x = \mathbb{C}^3$, for all $x \in \mathbb{Z}$, with an $SU(2)$-invariant nearest neighbor interaction. Its Hamiltonian for a finite chain of length $L \geq 2$ is given by

$$H_{[1,L]} = \sum_{x=1}^{L-1} \left(\frac{1}{3}\mathbb{1} + \frac{1}{2}\mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6}(\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2 \right) = \sum_{x=1}^{L-1} P^{(2)}_{x,x+1}. \tag{10.13}$$

Here, $\mathbf{S} = (S^1, S^2, S^3)$ is the vector of standard spin-1 matrices, and $P^{(2)}_{x,x+1} \in \mathcal{A}_{\{x,x+1\}}$ is the orthogonal projection onto the 5-dimensional subspace of $\mathbb{C}^3 \otimes \mathbb{C}^3$ corresponding to the spin-2 irreducible representation of $SU(2)$ contained in the tensor product of the two spin-1 representations acting on the sites x and $x + 1$.

In the limit of the infinite chain, the AKLT chain has a unique frustration-free ground state and there is a non-vanishing gap in the spectrum above the ground state. The correlation length, which is guaranteed to be finite by the Exponential Clustering Theorem, can be compute explicitly: $\xi = 1/\log 3$. Affleck, Kennedy, Lieb, and Tasaki proved these properties are proved in [4] model and thus demonstrated the existence of the so-called Haldane phase in quantum spin chains, predicted by Haldane based on his analysis of the large spin limit [31].

The exact ground state of the AKLT model has a special structure in which the correlations are generated by entangled nearest neighbor pairs and were called Valence Bond Solid states (VBS) in [3]. The construction of the ground state of the AKLT chain shows a close similarity with the Quantum Markov Chains constructed by Accardi [1]. Inspired by this similarity Fannes, Nachtergaele, and Werner introduced Finitely Correlated States (FCS) [21] and proved that FCS provide the exact ground state of a large family of spin chains, including the AKLT model, with similar properties. Matrix Product States (MPS) are a special case of FCS, and have proved to be a very useful tool in the study of quantum spin chains. Because of the matrix product structure of the formulas for the AKLT ground state given in [23], the name Matrix Product States was proposed in [41].

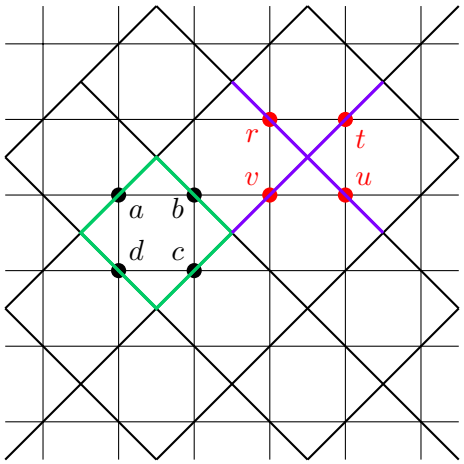

FIGURE 1. The distinction between stars and plaquettes becomes obvious by considering the spins to reside on the edges than rather than the vertices of a square lattice.

The ground state of the AKLT chain has only short-range correlations and no long-range order. Nevertheless, this state has a long-range structure that can be regarded as the one-dimensional analogue of Topological Order (see Example 4). This structure was discovered by den Nijs and Rommelse, who called it String Order [17].

There are several interesting generalizations of the AKLT model and its MPS ground state, including to higher dimensions, some of which we will discuss later on.

10.4. **Example 4: the Toric Code model.** The following example of a two-dimensional model which exhibits Topological Order was introduced by Kitaev [40]. One can associate the variables with the sites of the standard square lattice, but it turns out to be more convenient for the discussion of this model to associate the variables with the edges of a (different) square lattice. See Figure 10.4. The Hamiltonian contains two different types of four-body terms:

$$H_\Lambda = \sum_{s\subset\Lambda} (\mathbb{1} - A_s) + \sum_{p\subset\Lambda} (\mathbb{1} - B_p), \tag{10.14}$$

where s stands for 'star', meaning the four edges, labeled r, t, u, v, meeting a vertex, and p stands for 'plaquette', meaning four edges, labeled a, b, c, d, forming an square (see Figure). The corresponding terms in the Hamiltonian are defined as follows:

$$\begin{aligned} A_s &= \sigma_r^1 \sigma_t^1 \sigma_u^1 \sigma_v^1 \\ B_p &= \sigma_a^3 \sigma_b^3 \sigma_c^3 \sigma_d^3. \end{aligned}$$

This model has the remarkable property that when defined on a finite lattice embedded in a closed two-dimensional manifold (e.g., a 2-torus) the ground state space has dimension 4^g, where g is the genus of the manifold ($g = 1$ for the 2-torus).

11. Frustration free models

In the past decade, much of the progress in our understanding of the ground state problem of quantum spin models was achieved by studying so-called frustration free interactions. An interaction $\Phi : \mathcal{P}_0(\Gamma) \to \mathcal{A}_{\rm loc}$, is *frustration free* if for all $\Lambda \in \mathcal{P}_0(\Gamma)$ we have

$$\inf \mathrm{spec} \left(\sum_{X \subset \Lambda} \Phi(X) \right) = \sum_{X \subset \Lambda} \inf \mathrm{spec}(\Phi(X)). \tag{11.1}$$

Equivalently, the frustration free property can be expressed by stating that the finite-volume Hamiltonians $H_\Lambda = \sum_{X \subset \Lambda} \Phi(X)$ and each of the terms $\Phi(X)$ appearing in it, have a common eigenvector belonging to their respective smallest eigenvalues. While this requirement is generically *not* fulfilled, there is a remarkable range of quantum spin models, which model interesting physics, that do satisfy it. The frustration free property has turned out to be very helpful in the study of a range of problems. General results about the existence of a non-vanishing spectral gap in the thermodynamic limit and proving that a spectral gap above the ground state is stable under arbitrary perturbations of the interaction Φ, have so far only been proved for frustration free models. Understanding these questions first in the frustration free context, we expect, will prove to be an important step toward obtaining more general results.

Although the ferromagnetic Heisenberg model, introduced by Heisenberg in 1928 [35], is frustration-free, and other frustration-free models have been introduced a long time ago (e.g., the Majumdar-Ghosh model in 1969 [46–48]), frustration-free models as a class have been considered only more recently. The starting point for a wave of new developments was the introduction of the AKLT model by Affleck, Kennedy, Lieb, and Tasaki [3, 4], which is frustration free. The AKLT model played a pivotal role in more than one way. Not only was it a breakthrough by itself in establishing rigorously the existence of the so-called Haldane phase of quantum spin chains, it allso set in motion a series of fruitful new directions in the mathematics and physics research on quantum lattice models.

The AKLT model is a translation-invariant spin-1 chain with an $SU(2)$-invariant nearest neighbor interaction. For a finite chain of L spins the Hamiltonian of the AKLT model is given by

$$H_{[1,L]} = \sum_{x=1}^{L} \left(\frac{1}{3}\mathbb{1} + \frac{1}{2}\mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6}(\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2 \right), \tag{11.2}$$

where $\mathbf{S}_x$ denotes the vector of the 3×3 spin-1 matrices acting at the xth site of the chain, which generate the three-dimensional unitary irreducible representation of $SU(2)$. See Appendix 9 for the definitions and elementary properties of representations of $SU(2)$. In [4] the authors prove that, the limit of the infinite chain, the ground state is unique, has a finite correlation length, and that there is a non-vanishing gap in the spectrum above the ground state, thereby demonstrating the existence of the Haldane phase of the isotropic spin-1 chain predicted by Haldane [30,31]. This was a milestone result but the impact if this work and the AKLT model in particular, turned out to reach much further. Soon, it was realized that the exact ground state of the AKLT chain could be viewed as an example of a suitable generalization of the Quantum Markov Chains introduced by Accardi [1, 2]. This led to the introduction of Finitely Correlated States (FCS) [21, 23, 24], and the definition of a large class of frustration-free quantum spin models in one and more dimensions. Matrix Product States (MPS) is the name given to the subclass of Finitely Correlated States most relevant for the ground state problem in one dimension. An alternative representation goes under the name Valence Bond States (VBS), which is the term used in [4] for the particular $SU(2)$ invariant states constructed in that work. Examples of higher-dimensional VBS states already in the same paper and a general construction was given in [21]. Later, the construction was applied with considerable success to the study of concrete problems in two dimensions and renamed Products of Entangled Pairs (PEPS) in [63] which are, in turn, a special case of Tensor Networks [54].

Around the same time with the development of Matrix Product Sates, Steven White introduced his Density Matrix Renormalization Group method for the numerical computation of the ground state and low-lying excitations of quantum spin chains [68, 69]. The method immediately yielded very accurate results, e.g., for the spectral gap of the spin-1 antiferromagnetic Heisenberg chain and the AKLT chain [67]. The latter is easily understood since the exact ground state of the AKLT chain is a fixed point of the DMRG iteration [55]. By now we also understand why the DMRG method works well for one-dimensional problems more generally, especially for models with a non-vanishing gap, as is in the case for any Hamiltonian in the Haldane phase [5, 20, 32, 55].

The AKLT chain is frequently used as a testing ground for new concepts in many-body physics and quantum information theory. Well-known examples are string order [17], localizable entanglement [56], and symmetry-protected topological order [14,27,59,62]. The model has been generalized in different directions: from spin 1 to higher spin [6], from one to two and more dimensions, from $SU(2)$ and $O(3)$ to $SU(n)$ and $O(2n+1)$ [61], etc. As already mentioned, the construction of the exact ground state of the AKLT chain led to the study of a large class of frustration-free models, which in turn provided a fruitful starting point for understanding gapped ground states, entanglement in many-body states (including the so-called Area Law), the development of numerical algorithms for calculating correlations, the spectrum of excitations, the dynamics, form factors etc., and the study of the complexity of the computational problem of finding the ground state of a quantum spin system and of estimating the spectral gap above it.

In the next section, we present the ground state of the AKLT chain in some detail. This will serve as a solid foundation for the general discussion of frustration free modes in the rest of this chapter.

11.1. **The AKLT chain.** The most general translation invariant spin-1 chain with an $SU(2)$-invariant nearest neighbor interaction is of the following form

$$H_{[1,L]} = \sum_{x=1}^{L} \left(J_0 \mathbb{1} + J_1 \mathbf{S}_x \cdot \mathbf{S}_{x+1} + J_2 (\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2 \right). \tag{11.3}$$

By a shift and a scaling of the energy, which has no consequences for the ground states, the three coupling constants can be taken to be $J_0 = 0, J_1 = \cos\theta, J_2 = \sin\theta$, with $\theta \in [0, 2\pi)$. The conjectures ground state phase diagram is depicted in Figure 11.1. The angle θ corresponding to the AKLT chain is given by $\tan\theta = 1/3$.

It is simple exercise using the irreducible representations of $SU(2)$ to show that the AKLT interaction is the orthogonal projections onto the spin-2 subspace of a pair of spins:

$$\frac{1}{3}\mathbb{1} + \frac{1}{2}\mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6}(\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2 = P^{(2)}_{x,x+1}.$$

It follows that $\ker H_{[1,2]} = D^{(0)} \oplus D^{(1)} \subset \mathbb{C}^3 \otimes \mathbb{C}^3$. Therefore the space of ground state of the AKLT chain of length 2 is 4-dimensional and is given by the spin 0 and spin 1 vectors in the tensor product of two spins. It will turn out that $\ker H_{[1,2]}$ is 4-dimensional for all $L \geq 2$. In particular the ground state energy vanishes for all finite chains and the model is frustration free. To construct the ground states of the AKLT chain, one has the choice between the VBS, FCS, and MPS constructions mentioned above. As we will demonstrate below, these are three equivalent approaches that each highlight particular features of theses states.

From the decomposition $D^{(1)} \otimes D^{(1/2)} \cong D^{(1/2)} \oplus D^{(3/2)}$, it follows that there is an isometry $V : \mathbb{C}^2 \to \mathbb{C}^3 \otimes \mathbb{C}^2$, unique up to a phase, such that

$$V D^{(1/2)}(g) = (D^{(1)}(g) \otimes D^{(1/2)}(g)) V, \text{ for all } g \in SU(2). \tag{11.4}$$

One says that V *intertwines* the $SU(2)$ representations $D^{(1/2)}$ and $D^{(1)} \otimes D^{(1/2)}$. With respect to the standard orthonormal basis of $\mathbb{C}^2$ and $\mathbb{C}^3 \otimes \mathbb{C}^2$ consisting of eigenvectors of the third component

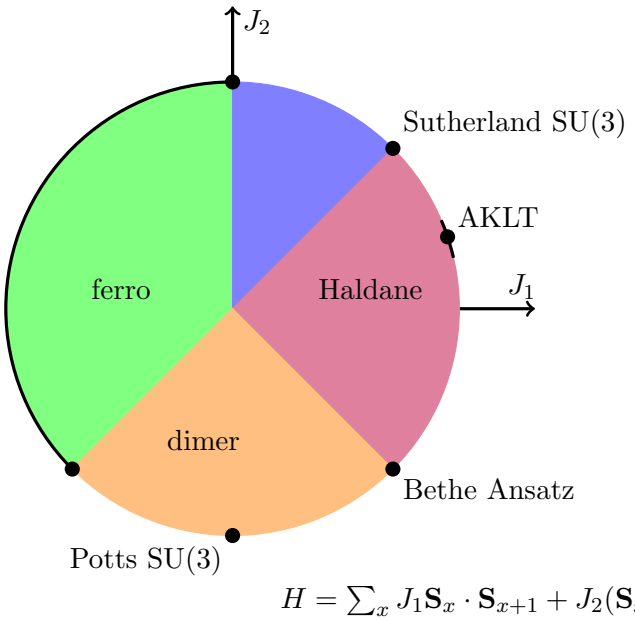

FIGURE 2. The conjectured phase diagram of the translation invariant spin 1 chains with $SU(2)$-invariant nearest neighbor interactions.

of the spin: $|1/2; m\rangle$, and $|1, 1/2; m_1, m_2\rangle$, the matrix elements of V are given by the familiar Clebsch-Gordan coefficients:

$$V|m\rangle = \sum_{\substack{m_1,m_2 \\ m_1+m_2=m}} \langle 1, 1/2; m_1, m_2 \mid 1/2; m\rangle |1, 1/2; m_1, m_2\rangle.$$

With the standard normalizations, $V^*V = \mathbb{1}$, i.e., V is an isometry.

For $\alpha, \beta \in \mathbb{C}^2$, and $n \geq 2$, define $\psi^{(n)}_{\alpha\beta} \in \mathcal{H}_{[1,n]}$ by

$$\psi^{(n)}_{\alpha\beta} = (\mathbb{1}_3^{\otimes n} \otimes \langle \beta\, |)(\underbrace{\mathbb{1}_3 \otimes \cdots \mathbb{1}_3}_{n-1} \otimes V) \cdots (\mathbb{1}_3 \otimes V)V|\alpha\rangle. \tag{11.5}$$

By using the interwining property of V n times, we find

$$\begin{aligned} & (D^{(1)})^{\otimes n} \psi^{(n)}_{\alpha\beta} \\ = \; & (\mathbb{1}_3^{\otimes n} \otimes \langle D^{(1/2)}\beta\, |)(\underbrace{D^{(1)} \otimes \cdots D^{(1)}}_{n} \otimes D^{(1/2)}V) \cdots V|\alpha\rangle \\ = \; & (\mathbb{1}_3^{\otimes n} \otimes \langle D^{(1/2)}\beta\, |)(\underbrace{\mathbb{1}_3 \otimes \cdots \mathbb{1}_3}_{n-1} \otimes V) \cdots (\mathbb{1}_3 \otimes V)V|D^{(1/2)}\alpha\rangle. \end{aligned} \tag{11.6}$$

This means that $SU(2)$ acts on the space $\{\psi^{(n)}_{\alpha\beta} \mid \alpha, \beta \in \mathbb{C}^2\}$ by the representation $(D^{(1/2)})^* \otimes D^{(1/2)} \cong D^{(0)} \oplus D^{(1)}$. In particular this proves that

$$P^{(2)}\psi^{(2)}_{\alpha\beta} = 0, \tag{11.7}$$

for all $\alpha, \beta \in \mathbb{C}^2$. Next, we will derive the MPS representation of the states $\psi^{(n)}_{\alpha\beta}$ and use it to show, in Proposition 11.1 below, that

$$\operatorname{span}\{\psi^{(n)}_{\alpha\beta} \mid \alpha, \beta \in \mathbb{C}^2\} = \ker H_{[1,n]}, \tag{11.8}$$

thus determining the ground state space of finite chains.

Given the standard basis $|1\rangle, |0\rangle, |-1\rangle$ of $\mathbb{C}^3$, we can define 2×2 matrices v_i, $i=1,0,-1$, by

$$V|\alpha\rangle = \sum_i |i\rangle \otimes v_i|\alpha\rangle.$$

Explicitly:

$$V = \begin{bmatrix} v_1 \\ v_0 \\ v_{-1} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \sqrt{\frac{2}{3}} & 0 \\ -\sqrt{\frac{1}{3}} & 0 \\ 0 & \sqrt{\frac{1}{3}} \\ 0 & -\sqrt{\frac{2}{3}} \\ 0 & 0 \end{bmatrix}. \tag{11.9}$$

One easily checks:

$$\langle i_1,\dots,i_n \mid \psi^{(n)}_{\alpha\beta}\rangle = \langle \beta \mid v_{i_n}\cdots v_{i_1}|\alpha\rangle = \mathrm{Tr}|\alpha\rangle\langle\beta|\, v_{i_n}\cdots v_{i_1}. \tag{11.10}$$

In other words

$$\psi^{(n)}_{\alpha\beta} = \sum_{i_1,\dots,i_n} \mathrm{Tr}[|\alpha\rangle\langle\beta|v_{i_n}\cdots v_{i_1}]|i_1,\dots,i_n\rangle. \tag{11.11}$$

It therefore makes sense to extend the vectors $\psi^{(n)}$ linearly to a map $\psi^{(n)}: M_2 \to \mathcal{H}_{[1,n]}$:

$$\psi^{(n)}(B) = \sum_{i_1,\dots,i_n} \mathrm{Tr}[Bv_{i_n}\cdots v_{i_1}]|i_1,\dots,i_n\rangle,\ B\in M_2. \tag{11.12}$$

The following is then obvious:

$$\mathrm{span}\{\psi^{(n)}_{\alpha\beta} \mid \alpha,\beta\in\mathbb{C}^2\} = \{\psi^{(n)}(B) \mid B\in M_2\},$$

and we define $\mathcal{G}_n = \{\psi^{(n)}(B) \mid B\in M_2\}$. We can now prove the inclusion

$$\mathcal{G}_n \subset \ker H_{[1,n]}, \tag{11.13}$$

by a direct computation. Let $x=1,\dots,n-1$, and compute the expectation of $P^{(2)}_{x,x+1}\in\mathcal{A}_{[1,n]}$ in a state $\psi^{(n)}(B)$:

$$\begin{aligned}
&\langle \psi^{(n)}(B), P^{(2)}_{x,x+1}\psi^{(n)}(B)\rangle \\
&\quad= \sum_{\substack{i_1,\dots,j_n \\ j_1,\dots,j_n}} \overline{\mathrm{Tr}[Bv_{i_n}\cdots v_{i_1}]}\mathrm{Tr}[Bv_{j_n}\cdots v_{j_1}] \\
&\qquad\quad \times\langle i_1,\dots,i_n|\mathbb{1}_{[1,x-1]}\otimes P^{(2)}\otimes\mathbb{1}_{x+2,n]}|j_1,\dots,j_n\rangle \\
&\quad= \sum_{\substack{i_1,\dots,i_{x-1} \\ i_{x+2},\dots,i_n}} \langle \psi^{(2)}(v_{i_{x-1}}\cdots v_{i_1}Bv_{i_n}\cdots v_{i_{x+2}}), P^{(2)}\psi^{(2)}(v_{i_{x-1}}\cdots v_{i_1}Bv_{i_n}\cdots v_{i_{x+2}})\rangle
\end{aligned}$$

By linear extension we see from (11.7) that $P^{(2)}\psi^{(2)}(C)=0$, for all $C\in M_2$. Hence, each term in the sum above vanishes. This proves (11.13). The other inclusion is proved as part of the following proposition.

Proposition 11.1. *For all $n\geq 2$ we have*

$$\ker H_{[1,n]} = \{\psi^{(n)}(B) \mid B\in M_2\}$$

Proof. We start by showing that

$$\dim\{\psi^{(2)}(B) \mid B \in M_2\} = 4.$$

To see this, recall the action of $SU(2)$ on the MPS vectors (11.7):

$$(D^{(1)} \otimes D^{(1)})\psi^{(2)}(B) = \psi^{(2)}((D^{(1/2)})^* B D^{(1/2)}).$$

Therefore, unless these vectors turn out to vanish, $\psi^{(2)}(\mathbb{1})$ is a singlet and $\psi^{(2)}(\sigma^i)$, $i = 1, 2, 3$, is a triplet representation of $SU(2)$. These are mutually orthogonal and the claim can be proved by showing they are non-zero. This follows by a straightforward computation using the definitions. E.g.,

$$\begin{aligned}\psi^{(2)}(\mathbb{1}) &= \mathrm{Tr}(v_{-1}v_1)|1,-1\rangle + \mathrm{Tr}(v_0)^2|0,0\rangle + \mathrm{Tr}(v_1 v_{-1})|-1,1\rangle \\ &= -\frac{2}{3}(|1,-1\rangle - |0,0\rangle + |-1,1\rangle.\end{aligned}$$

Therefore the singlet vector is non-zero. A similar computation shows that the triplet vectors are non-vanishing too. This also shows that the map $B \mapsto \psi^{(2)}(B)$ is injective. Furthermore, we can now show, by induction on n, that the maps $\psi^{(n)} : M_2 \to \mathcal{H}_{[1,n]}$ are injective for all $n \geq 2$. To do this, note that if $\psi^{(n)}$ is in injective, there exists a constant $c_n > 0$ such that $\|\psi^{(n)}(B)\|^2 \geq c_n \mathrm{Tr} B^* B$. Using the definition (11.12) we can then estimate $\|\psi^{(n+1)}(B)\|$ as follows:

$$\begin{aligned}\|\psi^{(n+1)}(B)\|^2 &= \sum_{i_{n+1}} \sum_{i_1,\ldots,i_n} |\mathrm{Tr} B v_{i_{n+1}} v_{i_n} \cdots v_{i_1}|^2 \\ &= \sum_{i_{n+1}} \|\psi^{(n)}(B v_{i_{n+1}})\|^2 \\ &\geq c_n \sum_{i_{n+1}} \mathrm{Tr}(B v_{i_{n+1}})^* B v_{i_{n+1}} \\ &= c_n \mathrm{Tr}\left[\sum_{i_{n+1}} v_{i_{n+1}} v_{i_{n+1}}^*\right] B^* B.\end{aligned}$$

Using the explicit form of the matrices v_i, (11.9), one easily checks that the sum in the square brackets equals $\mathbb{1}$. Since $c_n > 0$ by the induction hypothesis, this proves that $\psi^{(n+1)}$ is injective.

As the next step in the proof we show that

$$\ker H_{[1,3]} = (\mathcal{G}_2 \otimes \mathbb{C}^3) \cap (\mathbb{C}^3 \otimes \mathcal{G}_2) = \mathcal{G}_3. \tag{11.14}$$

The first identity follows directly from what we have proved so far and we already proved the inclusion of $\mathcal{G}_3 \subset \ker H_{[1,3]}$ in (11.13). We have shown above that $\psi^{(3)}$ is injective and, hence, $\dim \mathcal{G}_3 = 4$. Therefore, we will have proved our claim if we show that $\dim \ker H_{[1,3]} \leq 4$. We do this by considering the decomposition of $\mathcal{G}_2 \otimes \mathbb{C}^3$ into irreducible representations of $SU(2)$, and the fact that for any $\phi \in \ker H_{[1,3]}$, we have $\phi \in \mathcal{G}_2 \otimes \mathbb{C}^3$ and $\mathbb{1} \otimes P^{(2)}\phi = 0$. $\mathcal{G}_2 = W_0 \oplus W_1$, where W_0 is a singlet and W_1 is a triplet for $SU(2)$. Therefore, in the decompostion of $\mathcal{G}_2 \otimes \mathbb{C}^3$ into irreducibles, we will have two triplets, one singlet, and one copy of the spin 2 representation. Using the methods explained in Appendix 9, one easily finds that the highest weight vector in that spin 2 representation is given by $\xi_{22} = |1,0,1\rangle - |0,1,1\rangle$. One easily checks that $(\mathbb{1} \otimes P^{(2)})\xi_{22} \neq 0$. Since there is only one spin 2 representation in the subspace $\mathcal{G}_2 \otimes \mathbb{C}^3$, it must therefore be orthogonal to $\ker H_{[1,3]}$. Similarly, one shows that the spin 1 highest weight vector $\xi_{11} = |1,-1,1\rangle - |0,0,1\rangle + |-1,1,1\rangle$ satisfies $(\mathbb{1} \otimes P^{(2)})\xi_{11} \neq 0$. Therefore, since there are only two copies of the spin 1 representation on $\mathcal{G}_2 \otimes \mathbb{C}^3$, at most one can belong to $\ker H_{[1,3]}$. Taking this together, we see that $\ker H_{[1,3]}$ can contain at most one singlet and one triplet representation and no representations of higher spin. It follows that $\dim \ker H_{[1,3]} \leq 4$, thus completing the proof of (11.14).

For the final step in the proof of the proposition, we will show the following intersection property of the spaces $\mathcal{G}_n$: for $\ell, r \geq 0, m \geq 2$,

$$(\mathcal{G}_{\ell+m} \otimes \mathcal{H}_{[1,r]}) \cap (\mathcal{H}_{[1,\ell]} \otimes \mathcal{G}_{m+r}) = \mathcal{G}_{\ell+m+r}. \tag{11.15}$$

It will be convenient to use multi-indices $\mathbf{i} = (i_1, \ldots, i_\ell)$, $\mathbf{j} = (j_1, \ldots, j_m)$, $\mathbf{k} = (k_1, \ldots, j_r)$, and to let $v_\mathbf{i}$ denote the product $v_{i_\ell} \cdots v_{i_1}$ etc. Then, for $\phi \in (\mathcal{G}_{\ell+m} \otimes \mathcal{H}_{[1,r]}) \cap (\mathcal{H}_{[1,\ell]} \otimes \mathcal{G}_{m+r})$, we have $C_\mathbf{i}, D_\mathbf{k} \in M_2$, such that

$$\phi = \sum_\mathbf{i} |\mathbf{i}\rangle \otimes \psi^{(m+r)}(C_\mathbf{i}) = \sum_\mathbf{k} \psi^{(\ell+m)}(D_\mathbf{k}) \otimes |\mathbf{k}\rangle. \tag{11.16}$$

By expanding both expressions using (11.12) and equating coefficients, one finds

$$0 = \mathrm{Tr} C_\mathbf{i} v_\mathbf{j} v_\mathbf{k} - \mathrm{Tr} D_\mathbf{k} v_\mathbf{i} v_\mathbf{j} = \mathrm{Tr}\left[v_\mathbf{k} C_\mathbf{i} - D_\mathbf{k} v_\mathbf{i}\right] v_\mathbf{j}.$$

This means that for all $\mathbf{i}, \mathbf{k}$ $\psi^{(m)}(v_\mathbf{k} C_\mathbf{i} - D_\mathbf{k} v_\mathbf{i}) = 0$. By the assumption $m \geq 2$, hence $\psi^{(m)}$ is injective and hence

$$v_\mathbf{k} C_\mathbf{i} - D_\mathbf{k} v_\mathbf{i} = 0, \text{ for all } \mathbf{i}, \mathbf{k}. \tag{11.17}$$

Multiplying this relation from the left by $v_\mathbf{k}^*$ and summing over $\mathbf{k}$, we find

$$\sum_\mathbf{k} (v_\mathbf{k}^* v_\mathbf{k}) C_\mathbf{i} = (\sum_\mathbf{k} v_\mathbf{k}^* D_\mathbf{k}) v_\mathbf{i}.$$

By the isometry property of V, we have $\sum_\mathbf{k} (v_\mathbf{k}^* v_\mathbf{k}) = \mathbb{1}$, and therefore

$$C_\mathbf{i} = B v_\mathbf{i}, \text{ with } B = \sum_\mathbf{k} v_\mathbf{k}^* D_\mathbf{k}.$$

Inserting this expression for $C_\mathbf{i}$ into (11.16) gives

$$\phi = \psi^{(\ell+m+r)}(B),$$

which completes the proof of (11.15).

We can now finish the proof of the proposition by combining the properties proved above:

$$\begin{aligned}
\ker H_{[1,n]} &= \bigcap_{x=1}^{n-1} \mathcal{H}_{[1,x-1]} \otimes \mathcal{G}_2 \otimes \mathcal{H}_{[x+2,n]} \\
&= \bigcap_{x=1}^{n-2} \mathcal{H}_{[1,x-1]} \otimes (\mathcal{G}_2 \otimes \mathbb{C}^3 \cap \mathbb{C}^3 \otimes \mathcal{G}_2) \otimes \mathcal{H}_{[x+3,n]} \\
&= \bigcap_{x=1}^{n-2} \mathcal{H}_{[1,x-1]} \otimes \mathcal{G}_3 \otimes \mathcal{H}_{[x+3,n]} \\
&= \bigcap_{x=1}^{n-3} \mathcal{H}_{[1,x-1]} \otimes \mathcal{G}_4 \otimes \mathcal{H}_{[x+4,n]} \\
&\vdots \\
&= \mathcal{G}_n
\end{aligned}$$

where we have used (11.14), (11.15), and the conventions that $\mathcal{H}_\emptyset = \mathbb{C}$ and $[a, b] = \emptyset$ if $a > b$. □

The intersection property (11.15) is 'visualized' in the Valence Bond Solid representation of the ground states of the AKLT chain. This representation can be derived from the expression (11.5) by noting that, up to a normalization constant C, the intertwining isometry V can be expressed as follows: for all $u \in \mathbb{C}^2$

$$Vu = (P^+ \otimes \mathbb{1})(u \otimes \phi),$$

where $\phi \in \mathbb{C}^2 \otimes \mathbb{C}^2$ is the antisymmetric vector (i.e., the singlet state) and $P^+ : \mathbb{C}^2 \otimes \mathbb{C}^2 \to \mathbb{C}^3$ is the projection onto the symmetric states, which represent the triplet of spin-1 states.

$$\begin{aligned}
\psi^{(n)}_{\alpha\beta} &= \left[\underbrace{P^+ \otimes \cdots \otimes P^+}_{n} \otimes \langle\beta|\right] \left[|\alpha\rangle \otimes \underbrace{\phi \otimes \phi \cdots \otimes \phi}_{n}\right] \\
&= \pm \left[\underbrace{P^+ \otimes \cdots \otimes P^+}_{n}\right] \left[|\alpha\rangle \otimes \underbrace{\phi \otimes \phi \cdots \otimes \phi}_{n-1} \otimes |-\beta\rangle\right] \\
&= VBS
\end{aligned}$$

Remark by bxn: VBS should be replaced by a visual representation of the VBS state as it routinely appears in the literature *End of Remark.*

To study correlation functions and the thermodynamic limit, the representation of the ground states as Finitely Correlated States is very convenient.

Since

$$\psi^{(n)}_{\alpha\beta} = \sum_{i_1,\ldots,i_n} \langle \beta \mid v_{i_n} \cdots v_{i_1} |\alpha\rangle |i_1, \ldots, i_n\rangle,$$

we have for $A_1, \ldots, A_n \in M_3$:

$$\begin{aligned}
&\langle \psi^{(n)}_{\alpha\beta} | A_1 \otimes \cdots \otimes A_n \psi^{(n)}_{\alpha\beta}\rangle \\
= &\sum_{\substack{i_1,\ldots,i_n \\ j_1,\ldots,j_n}} (A_1)_{i_1 j_1} \cdots (A_n)_{i_n j_n} \overline{\langle \beta \mid v_{i_n} \cdots v_{i_1} |\alpha\rangle} \langle \beta \mid v_{j_n} \cdots v_{j_1} |\alpha\rangle \\
= &\sum_{\substack{i_1,\ldots,i_n \\ j_1,\ldots,j_n}} (A_1)_{i_1 j_1} \cdots (A_n)_{i_n j_n} \langle \alpha \mid v^*_{i_1} \cdots v^*_{i_n} |\beta\rangle \langle \beta \mid v_{j_n} \cdots v_{j_1} |\alpha\rangle \\
= &\sum_{\substack{i_1,\ldots,i_{n-1} \\ j_1,\ldots,j_{n-1}}} (A_1)_{i_1 j_1} \cdots (A_n)_{i_{n-1} j_{n-1}} \\
&\quad \times \langle \alpha \mid v^*_{i_1} \cdots v^*_{i_{n-1}} \left[\sum_{i_n, j_n} (A_n)_{i_n j_n} v^*_{i_n} |\beta\rangle\langle\beta| v_{j_n}\right] v_{j_{n-1}} \cdots v_{j_1} |\alpha\rangle.
\end{aligned}$$

It is now convenient to define for all $A \in M_3$, a map $\mathbb{E}_A : M_2 \to M_2$ by

$$\mathbb{E}_A(B) = \sum_{ij} A_{ij} v^*_i B v_j = V^*(A \otimes B)V.$$

In terms of these maps we can write the expectations of general tensor product observables in a compact form:

$$\begin{aligned}
&\langle \psi^{(n)}_{\alpha\beta} | A_1 \otimes \cdots \otimes A_n \psi^{(n)}_{\alpha\beta}\rangle \\
= &\sum_{\substack{i_1,\ldots,i_{n-1} \\ j_1,\ldots,j_{n-1}}} (A_1)_{i_1 j_1} \cdots (A_n)_{i_{n-1} j_{n-1}} \langle \alpha \mid v^*_{i_1} \cdots v^*_{i_{n-1}} [\mathbb{E}_{A_n}(|\beta\rangle\langle\beta|)] v_{j_{n-1}} \cdots v_{j_1} |\alpha\rangle \\
= &\langle \alpha \mid \mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n}(|\beta\rangle\langle\beta|) |\alpha\rangle.
\end{aligned}$$

This expression makes the calculation of the thermodynamic limit very transparent. Adding $\ell + 1$ sites to the left and r to the right of the interval $[1, n]$ gives the following expression for the

expectation of $A = \mathbb{1}^{\otimes \ell} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{\otimes r} \in \mathcal{A}_{[-\ell+1,n+r]}$ in the vector state $\psi_{\alpha\beta}^{(\ell+n+r)}$:

$$\begin{aligned}
&\langle \psi_{\alpha\beta}^{(\ell+n+r)} | A \psi_{\alpha\beta}^{(\ell+n+r)} \rangle \\
&\quad = \langle \alpha \mid \mathbb{E}_{\mathbb{1}}^{\ell} \circ \mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n} \circ \mathbb{E}_{\mathbb{1}}^{r}(|\beta\rangle\langle\beta|)|\alpha\rangle \\
&\quad = \mathrm{Tr}|\alpha\rangle\langle\alpha| \mathbb{E}_{\mathbb{1}}^{\ell} \circ \mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n} \circ \mathbb{E}_{\mathbb{1}}^{r}(|\beta\rangle\langle\beta|) \\
&\quad = \mathrm{Tr}(\mathbb{E}_{\mathbb{1}}^{T})^{\ell}(|\alpha\rangle\langle\alpha|)\mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n} \circ \mathbb{E}_{\mathbb{1}}^{r}(|\beta\rangle\langle\beta|)
\end{aligned}$$

Here, $(\mathbb{E}_{\mathbb{1}}^{T})$ denotes the transpose of $\mathbb{E}_{\mathbb{1}}^{T}$ with respect to the Hilbert-Schmidt inner product on M_2.

The map $\mathbb{E}_{\mathbb{1}}$ is called the *transfer operator* and its spectral properties control the limits $\lim_{\ell\to\infty}$ and $\lim_{r\to\infty}$. Using (11.9) or (11.4) it is straightforward to verify the following diagonalization of $\mathbb{E}_{\mathbb{1}}$:

$$\mathbb{E}(\mathbb{1}) = \mathbb{1}, \quad \mathbb{E}_{\mathbb{1}}(\sigma^i) = -\frac{1}{3}\sigma^i, \ i = 1, 2, 3.$$

Since, for $B \in M_2$

$$B = \frac{1}{2}(\mathrm{Tr}B)\mathbb{1} + \frac{1}{2}\sum_{i=1}^{3}(\mathrm{Tr}B\sigma^i)\sigma^i,$$

we have

$$\mathbb{E}_{\mathbb{1}}(B) = \frac{1}{2}(\mathrm{Tr}B)\mathbb{1} - \frac{1}{3}[B - \frac{1}{2}(\mathrm{Tr}B)\mathbb{1}],$$

and therefore

$$\mathbb{E}_{\mathbb{1}}^{p}(|\beta\rangle\langle\beta|) = \frac{1}{2}\|\beta\|^2\mathbb{1} + \left(-\frac{1}{3}\right)^{p}[|\beta\rangle\langle\beta| - \frac{1}{2}\|\beta\|^2\mathbb{1}]. \tag{11.18}$$

This implies

$$\begin{aligned}
&\lim_{\ell\to\infty, r\to\infty} \langle \alpha \mid \mathbb{E}_{\mathbb{1}}^{\ell} \circ \mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n} \circ \mathbb{E}_{\mathbb{1}}^{r}(|\beta\rangle\langle\beta|)|\alpha\rangle \\
&\quad = \frac{\|\alpha\|^2\|\beta\|^2}{2}\mathrm{Tr}(\frac{1}{2}\mathbb{1})\mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n}(\mathbb{1}) \\
&\quad = \omega(A_1 \otimes \cdots \otimes A_n), \qquad (11.19)
\end{aligned}$$

where ω is a translation invariant pure state on $\mathcal{A}_{\mathbb{Z}}$ uniquely determined by the above expression for simple tensor observables.

Define $Q : M_2 \to M_2$ by

$$Q(B) = \frac{1}{2}(\mathrm{Tr}B)\mathbb{1}.$$

(11.18) then implies

$$\|\mathbb{E}_{\mathbb{1}}^{p} - Q\| \leq \frac{2}{3^p}.$$

By taking $A_2 = \cdots A_{n-1} = \mathbb{1}$ in (11.19), we obtain the following estimate for the two-point correlation function of ω:

$$\begin{aligned}
|\omega(A_1 \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes A_n) - \omega(A_1)\omega(A_n)| &= \left|\frac{1}{2}\mathrm{Tr}\mathbb{E}_{A_1} \circ (\mathbb{E}_{\mathbb{1}}^{n-2} - Q) \circ \mathbb{E}_{A_n}\right| \\
&\leq \|A_1\|\|A_n\|\frac{C}{3^n}.
\end{aligned}$$

Thus we have shown exponential decay of correlations in the state ω. Next, we show that ω is the unique zero-energy ground state of the AKLT chain.

Proposition 11.2. *ω defined by (11.19) is the unique state on $\mathcal{A}_{\mathbb{Z}}$ such that $\omega(P_{x,x+1}^{(2)}) = 0$, for all $x \in \mathbb{Z}$.*

Proof. Any state η on $\mathcal{A}_{\mathbb{Z}}$ is uniquely determined by its restrictions to the subalgebras $\mathcal{A}_{[a,b]}$, $a < b$. Let $\rho_{[a,b]}$ denote the density matrices of η restricted to $\mathcal{A}_{[a,b]}$. $\eta(P^{(2)}_{x,x+1}) = 0$, for $x = a, \ldots, b-1$, implies that $\mathrm{ran}\rho_{[a,b]} \subset \mathcal{G}_{b-a+1}$. From (11.19) and Proposition 11.1 it then follows that, for all $a_1 < b_1 \in \mathbb{Z}$, $A_{a_1}, \ldots, A_{b_1} \in M_3$, we have

$$\begin{aligned}
&\eta(A_{a_1} \otimes \cdots \otimes A_{b_1}) \\
&\quad = \lim_{\substack{a \to -\infty \\ b \to \infty}} \mathrm{Tr}\rho_{[a,b]} \mathbb{1}_{[a,a_1-1]} \otimes A_{a_1} \otimes \cdots \otimes A_{b_1} \otimes \mathbb{1}_{[b_1+1,b]} \\
&\quad = \omega(A_{a_1} \otimes \cdots \otimes A_{b_1}),
\end{aligned}$$

proving the claim. □

So far, we have proved that the AKLT model has two of the three characterizing properties of the Haldane phase: it has a unique ground state and a finite correlation length. The third property, the non-vanishing spectral gap above the ground state, can be proved by further exploiting the structure of the ground states of the model. In order to avoid too much repetition, we will do this in the more general context of arbitrary quantum spin chains with a finite number of ground states that are of the MPS form (11.11).

11.2. **Frustration free spin chains with a unique Matrix Product ground state.** We begin our discussion of general frustration free models in one dimension by stating a result about the structure of the ground states of frustration free spin chains. This will serve as motivation to analyzing in some detail the spin chains with unique MPS ground states and also set the stage for studying some interesting generalizations, such as models with multiple ground states, examples of frustration free chains for which the product structure is not expressed in terms of matrices but in terms of operators on an infinite-dimensional Hilbert space, and frustration free models in more than one dimension.

We start by considering spin systems on $\mathbb{Z}^+ = \{1, 2, \cdots\}$, i.e., a half-infinite chain, with a d-dimensional Hilbert space $\mathcal{H}_x = \mathbb{C}^d$, at each site $x \in \mathbb{Z}^+$. We assume that $0 \leq h \in \mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^d)$ is a frustration free nearest neighbor interaction. By this we mean that the finite-volume Hamiltonians

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

where $h_{x,x+1} = h \in \mathcal{A}_{[x,x+1]}$, have a non-trivial kernel for all $L \geq 2$. Let $\mathcal{G} = \ker h \subset \mathbb{C}^d \otimes \mathbb{C}^d$. Then the frustration free property is equivalent to

$$\bigcap_{x=1}^{L-1} \underbrace{\mathbb{C}^d \otimes \cdots \otimes \mathbb{C}^d}_{x-1} \otimes \mathcal{G} \otimes \underbrace{\mathbb{C}^d \otimes \cdots \otimes \mathbb{C}^d}_{L-1-x} \neq \{0\}, \text{ for all } L \geq 2. \tag{11.20}$$

The set of states η on $\mathcal{A}_{\mathbb{Z}^+}$ such that $\eta(h_{x,x+1}) = 0$, for $x = 1, \ldots, L-1$, has weak-$*$ limit points. Any such limiting state ω satisfies $\omega(h_{x,x+1}) = 0$ for all $x \in \mathbb{Z}^+$. We will call such states zero-energy states and, since they are defined as limits of finite-volume ground states, they are ground states in the sense of Definition 6.2. The set of zero-energy states is a face in the set of all states, meaning that any pure states appearing in the decomposition of a zero-energy state are also zero-energy states. This shows that the set of pure zero-energy states on $\mathcal{A}_{\mathbb{Z}^+}$ for a nearest neighbor interaction $h \geq 0$ such that $\mathcal{G} = \ker h$ satisfies (11.20), is non-empty. We have the following theorem about the structure of such states.

Theorem 11.3 ([22]). *Let $0 \leq h \in \mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^d)$ such that $\mathcal{G} = \ker h$ satisfies (11.20), and suppose ω is a pure state on $\mathcal{A}_{\mathbb{Z}^+}$ such that $\omega(h_{x,x+1}) = 0$, for all $x \geq 1$. Then, given an orthonormal basis $\{|i\rangle \mid i = 1, \ldots, d\}$ of $\mathbb{C}^d$, there exists a Hilbert space $\mathcal{K}$, a unit vector $\Omega \in \mathcal{K}$, and a set of operators $V_1, \cdots, V_d \in \mathcal{B}(\mathcal{K})$ for which:*
i) $\mathcal{K}$ is the closed linear span of

$$\{V_{i_1} \cdots V_{i_n}\Omega \mid i_1, \cdots i_n \in \{1, \cdots, d\} \text{ and } n \geq 0\}$$

ii) $\sum_{\alpha=1}^d V_\alpha^* V_\alpha = \mathbb{1}$.
iii) For all $n \geq 1, i_1, \ldots, i_n, j_1, \ldots, j_n \in \{1, \ldots, d\}$, we have

$$\omega\left(|i_1, \cdots, i_n\rangle\langle j_1, \cdots, j_n|\right) = \langle V_{i_n} \cdots V_{i_1}\Omega, V_{j_n} \cdots V_{j_1}\Omega\rangle \tag{11.21}$$

iv) For every $\psi = \sum_{i,j=1}^d \psi_{i,j}|i,j\rangle \in \mathcal{G}^\perp$, we have

$$\sum_{i,j=1}^d \overline{\psi_{i,j}} V_j V_i = 0. \tag{11.22}$$

v) Define the operator $\hat{\mathbb{E}} : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{K})$ by

$$\hat{\mathbb{E}}(X) = \sum_{i=1}^d V_i^* X V_i, \quad \text{for all } X \in \mathcal{B}(\mathcal{K}). \tag{11.23}$$

Then, for any $X \in \mathcal{B}(\mathcal{K})$, $\hat{\mathbb{E}}(X) = X$ if and only if $X = \lambda \mathbb{1}$ for some $\lambda \in \mathbb{C}$.

In order to make the connection with the structure of the ground states we found for the AKLT model in the previous section, consider $\mathcal{K} = \mathbb{C}^2$, and define the maps $E_A : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{K})$, for $A \in M_d$, by

$$\mathbb{E}_A(X) = \sum_{i,j=1}^{d} \langle i|A|j\rangle V_i^* X V_i = V^*(A \otimes X)V, \quad \text{for all } X \in \mathcal{B}(\mathcal{K}),$$

where $V : \mathcal{K} \to \mathbb{C}^d \otimes \mathcal{K}$ is the isometry defined by

$$V\varphi = \sum_{i=1}^{d} |i\rangle \otimes V_i \varphi.$$

Then,

$$\omega(A_1 \otimes \cdots \otimes A_n) = \mathrm{Tr}|\Omega\rangle\langle\Omega|\mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n}(\mathbb{1}). \tag{11.24}$$

Since the space $\mathcal{K}$ for the AKLT model is finite-dimensional, the operators V_i and and the transfer operator $\hat{\mathbb{E}}$ are represented by matrices. Properties very similar to the ones we proved for the AKLT model in Section 11.1, follow from the product structure whenever $\dim \mathcal{K} < \infty$ without further assumptions. This will be shown in the next section. We will also prove a general result about the spectral gap of models with matrix product ground state.

11.3. **Some properties of translation invariant matrix product states.** In this section we derive some general properties of states of a form very similar to (11.24) under the additional assumption that $k = \dim \mathcal{K} < \infty$. This is the case of Matrix Product States (MPS). The operators V_i are now $k \times k$ matrices. Under the assumptions of Theorem 11.3 the transfer matrix $\hat{\mathbb{E}}$ has a simple eigenvalue 1. Its transpose, $\hat{\mathbb{E}}^T$ then also has a simple eigenvalue 1 and the Perron-Frobenius theory for completely positive maps (see Appendix **??**) then implies that there is a unique density matrix $\rho \in M_k$ such that $\hat{\mathbb{E}}^T(\rho) = \rho$. Regarding ρ as a positive linear functional on M_k, we can express this by the relation

$$\rho(\hat{\mathbb{E}}(B)) = \rho(B), \quad B \in M_k. \tag{11.25}$$

By replacing $|\Omega\rangle\langle\Omega|$ by ρ in (11.24), we get expectations $\omega(A_1 \otimes \cdots A_n)$ that are translation invariant. Indeed, using $\hat{\mathbb{E}}(\mathbb{1}) = \mathbb{1}$ and (11.25) it is straighforward to verify that

$$\omega(A_1 \otimes \cdots \otimes A_n) = \omega(\mathbb{1} \otimes A_1 \otimes \cdots \otimes A_n) = \omega(A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}). \tag{11.26}$$

The positivity and normalization also follow directly from the definition. Therefore, the finite chain expressions

$$\omega(A_1 \otimes \cdots \otimes A_n) = \mathrm{Tr}\rho\mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n}(\mathbb{1}). \tag{11.27}$$

define a unique translation invariant state on $\mathcal{A}_{\mathbb{Z}}$.

In addition to the assumption that 1 is a simple eigenvalue of $\hat{\mathbb{E}}$, we will also assume in this section that all other eigenvalues of $\hat{\mathbb{E}}$ have modulus strictly less than one. This situation is referred as a transfer matrix with *trivial peripheral spectrum* or, equivalently, that $\hat{\mathbb{E}}$ is *primitive*. (see [70]). Eigenvalues of absolute value 1 other than a simple eigenvalue 1, in general correspond to states that are not pure but have a non-trivial decomposition into pure states.

If ρ is not faithful and has support projection P, then one can construct the same translation-invariant pure state by replacing V_i with Pv_iP, $i = 1, \ldots, d$ (see [21]). In the sequel we will assume that $P = \mathbb{1}$, i.e., that $\rho > 0$, or work with the modified v_i if, originally, $P \neq \mathbb{1}$. In particular, the smallest eigenvalue of ρ is then strictly positive.

For any faithful state ρ, i.e., a density matrix with trivial kernel, we can define a non-degenerate inner product on M_k by

$$\langle A, B\rangle_\rho = \mathrm{Tr}\rho A^* B \quad \text{for all } A, B \in M_k\,, \tag{11.28}$$

and let $\|\cdot\|_\rho$ denote the corresponding norm. Let $\rho_{\min} = \min \mathrm{spec}(\rho)$. Since ρ is finite-dimensional, we have $\rho_{\min} > 0$. It follows that the norm $\|\cdot\|_\rho$ is equivalent to the Hilbert-Schmidt norm on M_k, $\|A\|_2 = \sqrt{\mathrm{Tr}A^*A}$, i.e.

$$\|A\|_2^2 = \mathrm{Tr}[A^*A] \leq \mathrm{Tr}\left[\frac{\rho}{\rho_{\min}} A^*A\right] = \frac{1}{\rho_{\min}}\|A\|_\rho^2 \quad \text{for any } A \in M_k\,. \tag{11.29}$$

As in the case of the AKLT model, the trivial peripheral spectrum of $\hat{\mathbb{E}}$ implies that there exists $C > 0$ and $\lambda \in (0,1)$ such that

$$a(n) := \left\|\hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho|\right\| \leq C\lambda^n. \tag{11.30}$$

Since $\hat{\mathbb{E}}(\mathbb{1}) = \mathbb{1}$, we have

$$\left\|\hat{\mathbb{E}}^{n+1} - |\mathbb{1}\rangle\langle\rho|\right\| = \left\|\hat{\mathbb{E}} \circ (\hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho|)\right\| \leq \left\|\hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho|\right\| \tag{11.31}$$

and therefore $a(n)$ is monotone decreasing in n.

The following maps $\Gamma_n : M_k \to \mathcal{H}_{[1,n]}$ generalize the maps $\psi^{(n)}(\cdot)$ of the AKLT model:

$$\Gamma_n(B) = \sum_{i_1,\ldots,i_n} \mathrm{Tr}[Bv_{i_n}\cdots v_{i_1}]|i_1,\ldots,i_n\rangle,\ B \in M_k. \tag{11.32}$$

These are the Matrix Product Ground states for finite chains of length n. We will now study the vectors $\Gamma_n(B)$ and the linear subspace spanned by them in some detail. We begin with a lemma that estmates the inner product of two such vectors.

Lemma 11.4. *For any $B, C \in M_k$,*

$$|\langle\Gamma_n(B), \Gamma_n(C)\rangle - \langle B, C\rangle_\rho| \leq ka(n)\|B^*\|_2\|C^*\|_2 \leq \frac{k}{\rho_{\min}} a(n)\|B\|_\rho\|C\|_\rho \tag{11.33}$$

Proof. Recall (11.32).

$$\begin{aligned}
\langle\Gamma_n(B), \Gamma_n(C)\rangle &= \sum_{i_1,\cdots,i_n} \overline{\mathrm{Tr}[Bv_{i_n}\cdots v_{i_1}]}\cdot \mathrm{Tr}[Cv_{i_n}\cdots v_{i_1}] \\
&= \sum_{i_1,\cdots,i_n} \mathrm{Tr}[v_{i_1}^*\cdots v_{i_n}^* B^*]\mathrm{Tr}[Cv_{i_n}\cdots v_{i_1}] \\
&= \sum_{\alpha,\beta}\sum_{i_1,\cdots,i_n} \langle\alpha|v_{i_1}^*\cdots v_{i_n}^* B^*|\alpha\rangle\cdot\langle\beta|Cv_{i_n}\cdots v_{i_1}|j\beta\rangle \\
&= \sum_{\alpha,\beta}\langle\alpha|\,\hat{\mathbb{E}}^n\left(B^*|\alpha\rangle\langle\beta|C\right)|\beta\rangle \\
&= \sum_{\alpha,\beta}\langle\alpha|\,|\mathbb{1}\rangle\langle\rho|\left(B^*|\alpha\rangle\langle\beta|C\right)|\beta\rangle + \sum_{\alpha,\beta}\langle\alpha|\,\left(\hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho|\right)\left(B^*|\alpha\rangle\langle\beta|C\right)|\beta\rangle,
\end{aligned} \tag{11.34}$$

where we have used the indices α and β to denote summation over the orthonormal basis of $\mathbb{C}^k$. Now the first term above is clearly

$$\sum_{\alpha,\beta}\langle\alpha|\mathbb{1}|\beta\rangle\mathrm{Tr}[\rho(B^*|\alpha\rangle\langle\beta|C)] = \mathrm{Tr}[\rho B^* C] = \langle B, C\rangle_\rho \tag{11.35}$$

and the remainder can then be estimated by

$$\sum_{\alpha,\beta} \left\| \hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho| \right\| \, \|B^*|\alpha\rangle\| \, \|C^*|\beta\rangle\| \leq a(n)k\|B\|_2\|C\|_2 \leq \frac{a(n)k}{\rho_{\min}}\|B\|_\rho\|C\|_\rho \tag{11.36}$$

where we have used both (11.29) and (11.42). □

It is clear that in the special case of $C = B$, the above lemma yields:

$$\left| \|\Gamma_n(B)\|^2 - \|B\|_\rho^2 \right| \leq \frac{k}{\rho_{\min}} a(n) \|B\|_\rho^2 \tag{11.37}$$

and if $\|B\|_\rho \neq 0$, then

$$\left| \frac{\|\Gamma_n(B)\|^2}{\|B\|_\rho^2} - 1 \right| \leq \frac{k}{\rho_{\min}} a(n) \tag{11.38}$$

Thus, if $k\rho_{\min}^{-1} a(n) < 1$, Γ_n is injective. Let us set $b(n) = k\rho_{\min}^{-1} a(n)$.

Let n_0 be the smallest integer such that Γ_n is injective for all $n \geq n_0$. We will refer to n_0 as the *injectivity length*.

As the ρ inner product is non-degenerate, a simple consequence of this bound is that Γ_n is eventually injective. In fact, the following corollary is immediate.

Corollary 11.5. *For any $B \in M_k$, the bound*

$$\|B\|_\rho \sqrt{1 - b(n)} \leq \|\Gamma_n(B)\| \leq \|B\|_\rho \sqrt{1 + b(n)} \tag{11.39}$$

holds for n sufficiently large. Here $\rho_{\min} b(n) = ka(n)$ and n large means $b(n) < 1$.

Proof of Corollary 11.5. The bound

$$\left| \|\Gamma_n(B)\|^2 - \|B\|_\rho^2 \right| \leq b(n) \|B\|_\rho^2 \tag{11.40}$$

follows immediately from (11.38). If $B = 0$, there is nothing to prove. Otherwise, this bound can be re-written as

$$-b(n) \leq \frac{\|\Gamma_n(B)\|^2}{\|B\|_\rho^2} - 1 \leq b(n) \tag{11.41}$$

from which the above claim readily follows. □

This result shows that Γ_n is injective for sufficiently large n, *i.e.* that there exists n_0 such that for all $n \geq n_0$, we have $\dim \mathrm{ran}\Gamma_n = k^2$. One can also show that, if $\hat{\mathbb{E}}$ is primitive, regardless of the values of λ and $\rho_{\min}$, Γ_n is injective for $n \geq k^4$ [70].

Let $\alpha_1, \ldots, \alpha_k$ be an orthonormal basis of $\mathbb{C}^k$. Using Cauchy-Schwarz, we then have the following pair of inequalities, which we will use to prove the next lemma:

$$\sum_{j=1}^{k} \|B^*\alpha_j\| \leq \sqrt{k} \sqrt{\sum_j \|B^*\alpha_j\|^2} = \sqrt{k}\|B^*\|_2 = \sqrt{k}\|B\|_2 \leq \sqrt{\frac{k}{\rho_{\min}}}\|B\|_\rho \tag{11.42}$$

for any $B \in M_k$.

Now consider three consecutive intervals (organized left-middle-right) with lengths ℓ, m, and r respectively. We wish to estimate the inner product of vectors $\varphi \in \mathcal{G}_{\ell+m} \otimes (\mathbb{C}^d)^{\otimes r}$ and $\psi \in (\mathbb{C}^d)^{\otimes \ell} \otimes \mathcal{G}_{m+r}$. If $m \geq n_0$, the maps Γ_{m+r} and $\Gamma_{\ell+m}$ are injective. Therefore there exist unique matrices $B_\varphi(k_1, \ldots, k_r), B_\psi(i_1, \ldots, i_\ell) \in M_k$, such that

$$\varphi = \sum_{k_1,\ldots,k_r} \Gamma_{\ell+m}(B_\varphi(k_1, \ldots, k_r)) \otimes |k_1, \ldots, k_r\rangle \tag{11.43}$$

and similarly,

$$\psi = \sum_{i_1,\ldots,i_\ell} |i_1,\ldots,i_\ell\rangle \otimes \Gamma_{m+r}(B_\psi(i_1,\ldots,i_\ell)). \tag{11.44}$$

It will be convenient to define

$$C_\varphi = \sum_{k_1,\ldots,k_r} B_\varphi(k_1,\ldots,k_r)\rho v_{k_1}^* \cdots v_{k_r}^* \rho^{-1} \tag{11.45}$$

and

$$D_\psi = \sum_{i_1,\ldots,i_\ell} v_{i_1}^* \cdots v_{i_\ell}^* B_\psi(i_1,\ldots,v_\ell) \tag{11.46}$$

It will be useful to use the following notations: $\mathbf{i} = (i_1,\ldots,i_\ell), \mathbf{j} = (j_1,\ldots,j_m), \mathbf{k} = (k_1,\ldots,k_r)$, where each individual index takes value in $\{1,\ldots,k\}$. We also define $v_\mathbf{i} = v_{i_\ell}\cdots v_{i_1}$, $v_\mathbf{i}^* = v_{i_1}^*\cdots v_{i_\ell}^*$, etc.

Lemma 11.6. *Suppose that m is large enough so that $b(m) < 1$. (Thus $m \geq n_0$.) Let $\ell \geq 0$ and $r \geq 0$. For every $\varphi \in \mathcal{G}_{\ell+m} \otimes (\mathbb{C}^d)^{\otimes^r}$ and $\psi \in (\mathbb{C}^d)^{\otimes^\ell} \otimes \mathcal{G}_{m+r}$, we have the estimate*

$$|\langle\varphi,\psi\rangle - \langle C_\varphi, D_\psi\rangle_\rho| \leq \frac{b(m)}{1-b(m)}\|\varphi\|\|\psi\|. \tag{11.47}$$

Proof.

$$\begin{aligned}\langle\varphi,\psi\rangle &= \sum_{\mathbf{i},\mathbf{j},\mathbf{k}} \mathrm{Tr}[v_\mathbf{i}^* v_\mathbf{j}^* B_\varphi(\mathbf{k})^*]\mathrm{Tr}[B_\psi(\mathbf{i})v_\mathbf{k}v_\mathbf{j}] \\ &= \sum_{\mathbf{i},\mathbf{k}} \langle\Gamma_m(v_\mathbf{i}B_\varphi(\mathbf{k})), \Gamma_m(B_\psi(\mathbf{i})v_\mathbf{k})\rangle \qquad (11.48)\end{aligned}$$

Now we apply Lemma 11.4. See that

$$\begin{aligned}\left|\langle\varphi,\psi\rangle - \sum_{\mathbf{i},\mathbf{k}}\langle v_\mathbf{i}^* B_\varphi(\mathbf{k}), B_\psi(\mathbf{i})v_\mathbf{k}\rangle_\rho\right| &\leq b(m)\sum_{\mathbf{i},\mathbf{k}}\|v_\mathbf{i}B_\varphi(\mathbf{k})\|_\rho\|B_\psi(\mathbf{i})v_\mathbf{k}\|_\rho \\ &\leq b(m)\sqrt{\sum_{\mathbf{i},\mathbf{k}}\|v_\mathbf{i}B_\varphi(\mathbf{k})\|_\rho^2}\sqrt{\sum_{\mathbf{i},\mathbf{k}}\|B_\psi(\mathbf{i})v_\mathbf{k}\|_\rho^2} \qquad (11.49)\end{aligned}$$

by an application of Cauchy-Schwarz.

One now sees that

$$\begin{aligned}\sum_{\mathbf{i},\mathbf{k}}\|v_\mathbf{i}B_\varphi(\mathbf{k})\|_\rho^2 &= \sum_{\mathbf{i},\mathbf{k}}\mathrm{Tr}\left[\rho B_\varphi(\mathbf{k})^* v_\mathbf{i}^* v_\mathbf{i} B_\varphi(\mathbf{k})\right] \\ &= \sum_{\mathbf{k}}\mathrm{Tr}\left[\rho B_\varphi(\mathbf{k})^* B_\varphi(\mathbf{k})\right] = \sum_{\mathbf{k}}\|B_\varphi(\mathbf{k})\|_\rho^2 \qquad (11.50)\end{aligned}$$

where we have used that

$$\sum_\mathbf{i} v_\mathbf{i}^* v_\mathbf{i} = \mathbb{1} \tag{11.51}$$

By (11.38), it is clear that

$$\sum_{\mathbf{k}}\|B_\varphi(\mathbf{k})\|_\rho^2 \leq \frac{1}{1-b(\ell+m)}\sum_{\mathbf{k}}\|\Gamma_{m+\ell}(B_\varphi(\mathbf{k}))\|^2 \tag{11.52}$$

and by the orthonormality of the basis $|\mathbf{k}\rangle$, we have

$$\sum_{\mathbf{k}} \|\Gamma_{m+\ell}(B_\varphi(\mathbf{k}))\|^2 = \|\varphi\|^2 \tag{11.53}$$

The other factor is seen to be:

$$\begin{aligned}
\sum_{\mathbf{i},\mathbf{k}} \|B_\psi(\mathbf{i})v_\mathbf{k}\|_\rho^2 &= \sum_{\mathbf{i},\mathbf{k}} \mathrm{Tr}\left[\rho v_\mathbf{k}^* B_\psi(\mathbf{i})^* B_\psi(\mathbf{i}) v_\mathbf{k}\right] \\
&= \sum_{\mathbf{i}} \mathrm{Tr}\left[\left(\hat{\mathbb{E}}^t\right)^r(\rho) B_\psi(\mathbf{i})^* B_\psi(\mathbf{i})\right] \\
&= \sum_{\mathbf{i}} \|B_\psi(\mathbf{i})\|_\rho^2 \\
&\leq \frac{1}{1-b(m+r)} \sum_{\mathbf{i}} \|\Gamma_{m+r}(B_\psi(\mathbf{i}))\|^2 = \frac{\|\psi\|^2}{1-b(m+r)} \qquad (11.54)
\end{aligned}$$

where we used that $\hat{\mathbb{E}}^t(\rho) = \rho$.

Thus the right-hand-side of (11.49) is bounded by

$$b(m)\frac{1}{\sqrt{1-b(\ell+m)}}\frac{1}{\sqrt{1-b(m+r)}}\|\varphi\|\|\psi\| \leq \frac{b(m)}{1-b(m)}\|\varphi\|\|\psi\| \tag{11.55}$$

where we have used the monotonicity property that follows from (11.31).

Note also that

$$\begin{aligned}
\sum_{\mathbf{i},\mathbf{k}} \langle v_\mathbf{i} B_\varphi(\mathbf{k}), B_\psi(\mathbf{i}) v_\mathbf{k}\rangle_\rho &= \sum_{\mathbf{i},\mathbf{k}} \mathrm{Tr}\left[\rho B_\varphi(\mathbf{k})^* v_\mathbf{i}^* B_\psi(\mathbf{i}) \rho \rho^{-1} v_\mathbf{k}\right] \\
&= \mathrm{Tr}\left[\rho \left(\sum_{\mathbf{k}} \rho^{-1} v_\mathbf{k} \rho B_\varphi(\mathbf{k})^*\right)\left(\sum_{\mathbf{i}} v_\mathbf{i}^* B_\psi(\mathbf{i})\right)\right] \\
&= \langle C_\varphi, D_\psi\rangle_\rho \qquad (11.56)
\end{aligned}$$

as claimed. □

11.4. **The commutation property.** Consider a frustration free quantum spin chain with MPS ground states such as, e.g., the AKLT chain. To start, we assume that $\hat{\mathbb{E}}$ is primitive with a unique density matrix ρ that is an eigenvector with eigenvalue 1 of $\hat{\mathbb{E}}^T$, and WLOG we can assume that $\ker\rho = \{0\}$, the smallest eigenvalue of ρ, $\rho_{\min}$, is non-zero. Let $G_n \in M_d^{\otimes n}$ denote the orthogonal projections onto $\mathcal{G}_n$.

Proposition 11.7 (Commutation Property)**.** *For all $m \geq 1, \ell \geq 0, r \geq 0$, we have*

$$\left\|(G_{\ell+m} \otimes \mathbb{1}^{\otimes r})(\mathbb{1}^{\otimes \ell} \otimes G_{m+r}) - G_{\ell+m+r}\right\| \leq \epsilon_m, \tag{11.57}$$

where

$$\epsilon_m = \frac{b(m)}{(1-b(m))^2}. \tag{11.58}$$

Proof. Since $G_{\ell+m+r}$ projects onto a subspace of the ranges of both $G_{\ell+m} \otimes \mathbb{1}^{\otimes r}$ and $\mathbb{1}^{\otimes \ell} \otimes G_{m+r}$, we have the identity

$$(G_{\ell+m} \otimes \mathbb{1}^{\otimes r})(\mathbb{1}^{\otimes \ell} \otimes G_{m+r}) - G_{\ell+m+r} = (G_{\ell+m} \otimes \mathbb{1}^{\otimes r} - G_{\ell+m+r})(\mathbb{1}^{\otimes \ell} \otimes G_{m+r} - G_{\ell+m+r}).$$

From this it is easy to see that to prove (11.57) is equivalent to showing that for all $\varphi \in \mathcal{G}_{\ell+m} \otimes (\mathbb{C})^{\otimes r}, \psi \in \mathbb{C}^{\otimes \ell} \otimes \mathcal{G}_{m+r}$, such that $G_{\ell+m+r}\varphi = G_{\ell+m+r}\psi = 0$, the have the following bound

$$|\langle\varphi, \psi\rangle| \leq \epsilon_m \|\varphi\| \, \|\psi\|. \tag{11.59}$$

The inner product can be estimated by applying Lemma 11.6 and using the extra information we have about the vectors φ and ψ. Since $\varphi \in \mathcal{G}_{\ell+m} \otimes (\mathbb{C})^{\otimes r}$, there exists $A \in M_k$ such that $B_\varphi(\mathbf{k}) = Av_{\mathbf{k}}$, which allows us to determine C_φ:

$$C_\varphi = \sum_{\mathbf{k}} Av_{\mathbf{k}} \rho v_{\mathbf{k}}^* \rho^{-1} = A(\hat{\mathbb{E}}^T)^r(\rho)\rho^{-1} = A. \tag{11.60}$$

Now, $G_{\ell+m+r}\psi = 0$ implies

$$\langle \Gamma_{\ell+m+r}(A), \psi \rangle = 0, \text{ for all } A \in M_k. \tag{11.61}$$

In combination with Lemma 11.6 this gives

$$|\langle A, D_\psi \rangle_\rho| \leq \frac{b(m)}{1-b(m)} \|\psi\| \, \|A\|_\rho, \tag{11.62}$$

and hence

$$\|D_\psi\|_\rho \leq \frac{b(m)}{1-b(m)} \|\psi\|. \tag{11.63}$$

By a similar reasoning, we find

$$\|C_\varphi\|_\rho \leq \frac{b(m)}{1-b(m)} \|\varphi\|. \tag{11.64}$$

Combining this information with Lemma 11.6 proves the proposition. □

Proposition 11.7 is referred to as the Commutation Property of the the ground states projections because it directly implies a bound on the commutator:

$$\begin{aligned} \left\| [G_{\ell+m} \otimes \mathbb{1}^{\otimes r}, \mathbb{1}^{\otimes \ell} \otimes G_{m+r}] \right\| &\leq \left\| (G_{\ell+m} \otimes \mathbb{1}^{\otimes r})(\mathbb{1}^{\otimes \ell} \otimes G_{m+r}) - G_{\ell+m+r} \right\| \\ &\quad + \left\| G_{\ell+m+r} - (\mathbb{1}^{\otimes \ell} \otimes G_{m+r})(G_{\ell+m} \otimes \mathbb{1}^{\otimes r}) \right\| \\ &\leq 2\epsilon_m. \end{aligned}$$

This property is closely related to the Factorization Property proved in [36] which, in turn, can be seen to underly the Area Law for the entanglement entropy [33].

11.5. **The martingale method and proof of non-vanishing spectral gap for quantum chains with MPS ground states.** The Commutation Property of Proposition 11.7 in combination with the frustration freeness of the spin chains with MPS ground states we are considering in this chapter, can be seen to imply a uniform lower bound for the spectral gap of these models. See, e.g., [21] or [64]. The martingale method is a simple argument that relates the quantity ϵ_m to a lower bound for the spectral gap in an efficient way [49] and is based on an idea that has been very useful in the context of classical interacting particle models [45] and other many-body systems [12, 13].

To present the martingale method in a transparant way, it is useful to identify the crucial properties that make it work in the context of quantum spin systems.

The ground state space of a finite chain is the intersection of the ground state spaces of shorter chains. We will describe this as a sequence of decreasing subspaces $\mathcal{H}_N \supset \mathcal{G}_1 \supset \mathcal{G}_2 \cdots \supset \mathcal{G}_N$, which are the null spaces of a corresponding increasing sequence of non-negative Hamiltonians. For $n = 1, \ldots, N$, $H_n \in \mathcal{B}(\mathcal{H}_N), \mathcal{G}_n = \ker H_n$, $H_1 \leq H_2 \cdots \leq H_N$. Note however, that although the sequence H_n, $n = 1, \ldots, N$, will typically be associated with the system on an increasing sequence of finite volumes, the H_n do not have to coincide with the finite-volume Hamiltonians in terms of which the model is defined. In general, we will have constants $c, C > 0$ such that

$$cH_N \leq H_{\Lambda_N} \leq CH_N, \tag{11.65}$$

where H_{Λ_N} is the finite-volume Hamiltonian of which we want the estimate the spectral gap.

Define

$$h_n = \begin{cases} H_1 & \text{if } n = 1 \\ H_n - H_{n-1} & \text{if } n = 2, \dots, N \end{cases} \tag{11.66}$$

and let G_n and $g_n \in \mathcal{B}(\mathcal{H})_N$ be the orthogonal projection onto $\ker H_n$ and $\ker h_n$, respectively. Of course, (11.66) is equivalent to assuming that $H_n = \sum_{k=1}^{n} h_k$, and H_n will be increasing if we require $h_k \geq 0$. Furthermore, define

$$E_n = \begin{cases} \mathbb{1} - G_1 & \text{if } n = 0 \\ G_n - G_{n+1} & \text{if } 1 \leq n \leq N-1 \\ G_N & \text{if } n = N \end{cases} . \tag{11.67}$$

It is easily verified that the E_n are mutually orthogonal orthogonal projections forming a resolution of the identity: $\sum_{n=0}^{N} E_n = \mathbb{1}$ and $E_n E_m = \delta_{n,m} E_n$.

Assumptions for the Martingale Method:

(i) There is a constant $\gamma > 0$ such that $h_n \geq \gamma(\mathbb{1} - g_n)$, $n = 1 \dots N$.

(ii) There are integers $\ell \geq 0, r \geq 1$, such that $E_k g_n = g_n E_k$, if $k \notin [n - \ell, n + r]$.

(iii) There exists $\epsilon \in [0, \sqrt{\ell + r}]$, such that $E_n g_{n+1} E_n \leq \epsilon^2 E_n$, $n = 1, \dots, N-1$.

Theorem 11.8. *In the setup described immediately here above, assume the Assumption (i)–(iii) hold. Let $\psi \in \mathcal{H}_N$ such that $G_N \psi = 0$. Then*

$$\langle \psi, H_N \psi \rangle \geq \frac{\gamma}{2} (1 - \epsilon \sqrt{1 + \ell + r})^2 \|\psi\|^2.$$

Proof. By assumption $E_N \psi = G_N \psi = 0$. Hence

$$\|\psi\|^2 = \sum_{n=0}^{N-1} \|E_n \psi\|^2. \tag{11.68}$$

Using this, for all $n = 0, \dots, N-1$, we have

$$\begin{aligned} \|E_n \psi\|^2 &= \langle \psi, (\mathbb{1} - g_{n+1}) E_n \psi \rangle + \langle \psi, g_{n+1} E_n \psi \rangle \\ &= \langle \psi, (\mathbb{1} - g_{n+1}) E_n \psi \rangle + \langle \psi, \left(\sum_{m=0}^{N-1} E_m \right) g_{n+1} E_n \psi \rangle. \end{aligned} \tag{11.69}$$

By Assumption (ii) and the mutual orthogonality of the projections E_m, the summation in the last term can be reduced and we obtain

$$\|E_n \psi\|^2 \leq \langle \psi, (\mathbb{1} - g_{n+1}) E_n \psi \rangle + \langle \psi, \left(\sum_{k=n-\ell}^{n+r} E_k \right) g_{n+1} E_n \psi \rangle. \tag{11.70}$$

After applying the inequality

$$|\langle \varphi_1, \varphi_2 \rangle| \leq \frac{1}{2c} \|\varphi_1\|^2 + \frac{c}{2} \|\varphi_2\|^2, \ \varphi_1, \varphi_2 \in \mathcal{H}, c > 0, \tag{11.71}$$

two each of the two terms in (11.70), we find

$$\begin{aligned} \|E_n \psi\|^2 \leq\ & \frac{1}{2c_1} \langle \psi, (\mathbb{1} - g_{n+1}) \psi \rangle + \frac{c_1}{2} \langle \psi, E_n \psi \rangle \\ & + \frac{1}{2c_2} \langle \psi, E_n g_{n+1} E_n \psi \rangle + \frac{c_2}{2} \langle \psi, \left(\sum_{k=n-\ell}^{n+r} E_k \right)^2 \psi \rangle. \end{aligned}$$

To estimate the first term of the RHS, we use Assumption (i). The second term can be combined with the LHS. For the third term we use Assumption (iii). In the fourth term we can use the mutual orthogonality of the E_m. This gives

$$(1-\frac{c_1}{2}-\frac{\epsilon^2}{2c_2})\|E_n\psi\|^2-\frac{c_2}{2}\sum_{k=n-\ell}^{n+r}\|E_k\psi\|^2\leq\frac{1}{2c_1\gamma}\langle\psi,h_{n+1}\psi\rangle. \tag{11.72}$$

We now sum over $n=0,\ldots,N-1$, use the fact the $\{E_n\mid n=0,\ldots,N\}$ is a resolution of the identity, and recall that $E_N\psi=G_N\psi=0$. The result is

$$\langle\psi,H_N\psi\rangle\geq 2c_1\gamma\left[1-\frac{c_1}{2}-\frac{\epsilon^2}{2c_2}-\frac{c_2(1+\ell+r)}{2}\right]\|\psi\|^2. \tag{11.73}$$

We can maximize the constant in the RHS by choosing $c_1=1-\epsilon\sqrt{1+\ell+r}$ and $c_2=\epsilon/\sqrt{1+\ell+r}$. This yields the inequality stated in the theorem. □

Let us now apply this theorem to the spin chains with a unique pure MPS ground state, such as the AKLT chain. For simplicity of the notation, assume that the model is defined in terms of a frustration-free nearest neighbor interaction $0\leq h\in M_d\otimes M_d$. Then, let $m\geq 1$ and define

$$h_n=\sum_{x=(n-1)m+1}^{(n+1)m-1}h_{x,x+1}. \tag{11.74}$$

Then, we have

$$\begin{aligned}
H_n &= \sum_{k=1}^{n}h_k\\
H_{[1,(n+1)m]} &\leq H_n\leq 2H_{[1,(n+1)m]}\\
E_n &= G_{(n+1)m}\otimes\mathbb{1}^{\otimes(N-n)m}-G_{(n+2)m}\otimes\mathbb{1}^{\otimes(N-n-1)m}\\
g_n &= \mathbb{1}^{\otimes(n-1)m}\otimes G_{2m}\otimes\mathbb{1}^{\otimes(N-n)m}.
\end{aligned}$$

Assumption (i) is satisfied with γ given by the spectral gap of $H_{[(n-1)m+1,(n+1)m]}$. Since m is fixed, and the model is translation invariant this gap is positive and independent of n. Assumption (ii) is satisfied with $\ell=0,r=1$. For the spin chains with a unique pure MPS ground states (iii) follows from the Commutation Property (Proposition 11.7). To see this, it suffices to express the quantities E_n and g_{n+1} in terms of the ground state projection operators:

$$\|g_{n+1}E_n\|=\|(\mathbb{1}^{\otimes(n-1)m}\otimes G_{2m})(G_{(n+1)m}\otimes\mathbb{1}^{\otimes m}-G_{(n+2)m})\|\leq\epsilon_m \tag{11.75}$$

where ϵ_m is the quantity estimate in Proposition 11.7. It then suffices to note that, for two orthogonal projections G and E, one has

$$\|GE\|\leq\epsilon\Leftrightarrow EGE\leq\epsilon^2E. \tag{11.76}$$

Other choices for the sequence H_n are possible and may provide more precise information in some cases. E.g., if one is interested in estimating the spectral gap for finite systems with periodic boundary conditions, it is useful to let H_{N-1} be comparable to the Hamiltonian of the chain with open boundary conditions and H_N the Hamiltonian for the system with the same Hilbert space but with the additional term(s) that corresponds to considering periodic boundary conditions. Further refinements of the method exist. See, e.g., [60].

The method can also be applied to some quantum spin models in higher dimensions as long as one can find sequences of finite volumes and associate Hamiltonians such that the Assumptions (i)-(iii) are satisfied. See, e.g., [7, 9] for a few examples in two and more dimensions.

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