PhD Thesis

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To my Family

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Introduction

Quantum statistical mechanics is concerned with the properties of quantum systems with an infinite number of degrees of freedom. Lattice fermion models belong to the most popular topics of this field. They can serve as toy models for studying general properties of fermionic systems. Furthermore, many continuum models can be reduced to such lattice models under some appropriate assumptions. The big technical advantage that makes both the analytical and the numerical study of lattice fermion models very effective is that the algebra describing the fermionic creation and annihilation operators belonging to a finite region of the lattice is finite dimensional. Although in quantum statistical mechanics we study states on the infinite dimensional algebra belonging to the whole lattice, these states are entirely determined by their restrictions to the finite dimensional algebras corresponding to the finite regions.

The von Neumann entropy serves as a measure of how mixed a state defined on such a finite dimensional algebra is. For finite temperature states the von Neumann entropy of a state restricted to a finite region usually scales with the volume of the region (if the boundary of the region is regular enough). The prefactor of the volume-like growth-rate, the *entropy density*, can be used for a variational characterisation of these finite temperature states. Ground states of certain models are often pure states on the whole lattice algebra, but of course, even then their restrictions on subsystems might be mixed. Nevertheless, the von Neumann entropy of the subsystems scales typically in a subvolume-like manner, i.e., the entropy density is zero. It has been conjectured for a long time that the entropy density of *all* pure translation-invariant states on fermionic lattices is zero. This is called the *zero-entropy-density* conjecture. Even if the entropy density of pure ground states is zero, it has been shown in recent years that the asymptotics itself might provide some information about the model. For one-dimensional models the (sublinear) entropy asymptotics of pure ground states was found to depend on the criticality or non-criticality of the model, and also a connection with the central charge of the corresponding conformal field theory has been derived in many analytical and numerical studies.

The entropy asymptotics of pure translation-invariant states on fermionic lattices is hence of great interest. In this thesis we further restrict our scope: we will investigate only quasifree states. Some of these arise as ground states of certain models, but they can also be studied without a reference to particular models. On the other hand, we will see that it suffices to take into account only these states in order to prove certain impossibility theorems, and then of course our conclusions hold in full generality. For instance, we prove that even though the entropy density of these states is zero, they give rise to rise to arbitrary fast subvolume-like entropy growth . Hence it is impossible to sharpen the zero-entropy-density conjecture for pure translational-invariant states. We also prove a lower bound for the entropy asymptotics of all pure translation-invariant quasifree states (except the trivial ones), and present numerical data that are consistent with the conformal field theoretical predictions.

The thesis is divided into five chapters. In the first chapter we give a short, but hopefully self-contained, introduction to the basic notions of fermion lattice systems, and we also introduce quasifree states. The second chapter is devoted to the role of the von Neumann entropy in lattice quantum statistical mechanics. Our own results are contained in the third and fourth chapters. In the third chapter a proof for the lower bound of the entropy asymptoics and our numerical results are presented, while in the fourth chapter we prove the sharpness of the zero-entropy-density conjecture. In the final fifth chapter we summarise our results and discuss some open questions. Since the formalism of the thesis uses in some degree the language of functional analysis and C^*-algebras, we have added two mathematical appendices at the end of the thesis, where we collect the basic definitions and theorems from these fields.

Chapter 1

States on the CAR -algebra

The aim of this chapter is to describe the C^*-algebra of fermionic creation and annihilation operators, called the *canonical anticommutation relations* algebra (CAR-algebra), and to introduce the concept of a *state* in the C^*-algebraic setting. We will also define a particular set of states, called quasifree states, which will be the main subject of the rest of the thesis. We end the chapter by showing how these states arise naturally as ground and finite temperature states of certain families of Hamiltonians.

Historically, the introduction of the canonical anticommutation relations was the result of the marriage of two developments of quantum physics taking place in the 1920's. The first was *Pauli's exclusion principle*. In 1925, to explain the spectra of alkali atoms, Pauli postulated that two or more electrons cannot be in the same quantum state [49]. A year later this principle was restated by Dirac and Heisenberg as the antisymmetry property of the composite wavefunction of electrons with respect to the interchange of electrons [17, 30]. The statistical physical implication of the exclusion principle was already studied in the same year (1926) by Fermi [26], and thereby his name was attached to particles with this property, which are called fermions now. The second development was the attempt to quantise field theories. In 1928, for the purpose of quantising the electron field, the fermionic creation and annihilation operators were introduced by Jordan and Wigner [35]. They realised that in order to map antisymmetric composite wavefunctions to antisymmetric composite wavefunctions (with higher or lower particle number) using these creation and annihilation operators, the latter have to satisfy the canonical anticommutation relations. They also proved that the CAR-algebra over a d-dimensional Hilbert space are equivalent with the algebra of $2^d \times 2^d$ matrices, hence in this case there is one (up to unitary equivalence) unique $*$-representation.[1] The lack of uniqueness for systems with infinite degrees of freedom, however, caused a lot of confusion which was not fully clarified until the early 1960's. In 1964 Haag and Kastler proposed a C^*-algebraic reformulation of quantum theories with infinite degrees of freedom [29], in which they stressed the importance of the C^*-algebra structure of the observables and the significance of the existence of inequivalent representations for the discussions of topics such as physical equivalence and superselection rules (for a monograph on this subject see [28]).

Quasifree states were formally, i.e., in a C^*-algebraic way, defined only in 1964 by Shale and Stinespring [55], but these states arose in a less formal way much earlier in quantum statistical mechanics, e.g. as ground and finite temperature states of lattice fermionic models with only free hopping terms, and as (Jordan-Wigner transformed) Gibbs states of certain quantum spin chain models as it was shown in the paper by Lieb, Schultz and Mattis [41] in 1961, their derivation was put on a rigorous basis by Araki and Matsui in 1980's [7, 3].

The structure of this chapter is the following. Before introducing the C^*-algebraic concepts that are used in the modern description of fermionic systems, we begin the chapter by presenting the basics of the traditional Fock space approach. The second section deals with the definition of the CAR-algebra and quasifree states on the CAR-algebra. In the third section we show how one can transfer translation-invariant states from a fermionic chain to a quantum spin chain. We end the chapter by discussing some quantum spin chain and fermionic lattice models with ground states and finite temperature states that are quasifree. We omit the proofs of the presented statements and theorems in this introductory chapter, they can be found in the monographs [13] and[1].

[1]The corresponding, but much harder, uniqness theorem for the Weyl-algebra with finite degrees of freedom, was proved by von Neumann three year later later [45].

1.1 The Fock space approach to fermionic systems

In this section we recapitulate very shortly the key concepts of one-particle quantum mechanics, and then discuss the case of n identical particles with fermionic statistics. After this we naturally arrive at the concept of the Fermi-Fock space, a space that describes all the different n-particle spaces, and to the concept of creation and annihilation operators, which act between these different n-particle spaces. We close the section by showing the limitations of this approach, the problems arising here will be cured in the next section.

1.1.1 The Hilbert space approach to quantum mechanics

In the traditional framework of quantum mechanics, the *states* of a physical system are identified with the *density matrices*, i.e., with the positive, linear operators of unit trace, acting on a complex, separable Hilbert space $\mathcal{H}$. [2] The *observables* are identified with the self-adjoint linear operators acting on $\mathcal{H}$. Let ρ be a density matrix. When the system is in the state corresponding to ρ, the *expectation value* of a bounded observable A is given by the formula:

$$\langle A \rangle_\rho := \mathrm{Tr}_{\mathcal{H}}(\rho A).$$

The *statistical mixture* with normalised weights λ_1 and λ_2 ($\lambda_1 + \lambda_2 = 1$; $\lambda_1, \lambda_2 \geq 0$) of two states corresponding to density matrices ρ_1 and ρ_2 is the state described by $\rho := c_1\rho_1 + c_2\rho_2$. There is a special set of density matrices that cannot be obtained as a statistical mixture of two *different* density matrices, these are the projections of unit trace. Because of this extremality property, states corresponding to projections of unit trace are called *pure*, while other states are called *mixed*. For any pure state there exists a normed vector $\psi \in \mathcal{H}$ ($\|\psi\| = 1$), which is unique up to a complex phase, such that the projection corresponding to the state is equal to P_ψ, which is defined by

$$P_\psi(\varphi) := \psi\langle\psi, \varphi\rangle,$$

[2]The term density operator would be more correct, since the word "matrix" usually refers to a basis. We shall, however, stick to this traditional nomenclature.

for any $\varphi \in \mathcal{H}$. Any density matrix can be written as a convex combination of finite or countably many commuting projections, i.e., for any density matrix ρ, there is an orthonormal basis $\{\phi_i\}_{i\in\mathbb{I}}$ of $\mathcal{H}$ such that

$$\rho = \sum_i \lambda_i P_{\phi_i}, \quad \lambda_i \geq 0, \quad \sum_i \lambda_i = 1.$$

Let ρ_a and ρ_b be two density matrices on the Hilbert space $\mathcal{H}$, and let the sequences $\{\lambda_i^a\}_{i\in\mathbb{N}^+}$ and $\{\lambda_i^b\}_{i\in\mathbb{N}^+}$ denote their eigenvalues arranged in decreasing order. We say that ρ_a is more mixed than ρ_b (or ρ_a majorises ρ_b) if

$$\sum_{i=1}^{n} \lambda_i^a \leq \sum_{i=1}^{n} \lambda_i^b$$

for all $n \in \mathbb{N}^+$.

1.1.2 The system of n indistinguishable fermions

The states of a system composed of a finite number of *distinguishable* particles correspond to the density matrices of the tensor product Hilbert space of the different one-particle Hilbert spaces, while the observables correspond to the self-adjoint operators of this tensor product Hilbert space. On the other hand, considering n number of *indistinguishable* particles, only certain density matrices and self-adjoint operators of the n-fold tensor product Hilbert space $\mathcal{H}^{\otimes n}$ correspond to *allowed* states and observables, namely, those that commute with a certain projection on $\mathcal{H}^{\otimes n}$ which is determined by the quantum statistics of the indistinguishable particles. In the case of *fermions*, this projection is defined through the rule

$$P_F^{(n)}\left(\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_n\right) := \frac{1}{\sqrt{n!}} \sum_{\pi\in S_n} \epsilon(\pi)\, \psi_{\pi(1)} \otimes \psi_{\pi(2)} \otimes \cdots \otimes \psi_{\pi(n)},$$

where the sum, as denoted, is carried over all π permutations of the N indices $1, 2, \ldots, N$, and $\epsilon(\pi)$ is ± 1 according to the parity of π.

It is useful to introduce the notation

$$\psi_1 \wedge \psi_2 \wedge \ldots \wedge \psi_n := P_F^{(n)}\left(\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_n\right),$$

which is called the antisymmetrization of the vector $\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_n$. The range of $P_F^{(n)}$ is a closed subspace of $\mathcal{H}^{\otimes n}$ which is denoted by $\wedge^n \mathcal{H}$. Vectors of the form $\psi_1 \wedge \psi_2 \wedge \cdots \wedge \psi_n$ span $\wedge^n \mathcal{H}$. Moreover, $\wedge^n \mathcal{H}$ is a Hilbert space with the the inner product inherited from the Hilbert space $\mathcal{H}^{\otimes n}$:

$$\langle \psi_1 \wedge \psi_2 \wedge \cdots \wedge \psi_n \, , \, \varphi_1 \wedge \varphi_2 \wedge \cdots \wedge \varphi_n \rangle = \det\left(\left[\langle \psi_i, \varphi_j \rangle\right]\right). \tag{1.1}$$

Let $(\wedge^n \mathcal{H})^C$ denote the complementary Hilbert space of $\wedge^n \mathcal{H}$ in the full tensor product Hilbert space $\mathcal{H}^{\otimes n}$. Then $\mathcal{H}^{\otimes n} = \wedge^n \mathcal{H} \otimes (\wedge^n \mathcal{H})^C$. Since an allowed observable A and an allowed density matrix ρ commute with $P_F^{(n)}$, they can be be written as $\rho_F \otimes \mathbb{1}_{(\wedge^n \mathcal{H})^C}$ and $\mathcal{A}_F \otimes \mathbb{1}_{(\wedge^n \mathcal{H})^C}$, respectively, where A_F is a self-adjoint operator and ρ_F is a self-adjoint, positive, linear operator of unit trace,i.e, a density matrix on $\wedge^n \mathcal{H}$. Hence the allowed density matrices and observables can be identified with the density matrices and observables on the Hilbert space $\wedge^n \mathcal{H}$. If the set $\{\phi_1, \phi_2, \ldots\}$ is an orthonormal basis of $\mathcal{H}$, then the set

$$\{\phi_{i_1} \wedge \ldots \wedge \phi_{i_n} \mid i_1 < \ldots < i_n\}$$

forms an orthonormal basis over $\wedge^n \mathcal{H}$.

1.1.3 The Fock space

It is often useful or necessary to consider systems composed of many identical fermions without restricting their precise number. The Fock-space construction deals with such situation by the introduction of a Hilbert space that contains all the n-particle Hilbert spaces as subspaces. More concretely, the Fermi-Fock space $\mathcal{F}(\mathcal{H})$ over the one-particle Hilbert space $\mathcal{H}$ is

$$\mathcal{F}(\mathcal{H}) := \bigoplus_{n \in \mathbb{N}} \wedge^n \mathcal{H},$$

where $\wedge^0 \mathcal{H}$ is the one-dimensional Hilbert space $\mathbb{C}$. This zeroth level describes the state without particles, and one calls the state corresponding to the vector

$$\Omega := 1 \oplus 0 \oplus 0 \cdots$$

the *Fock vacuum state*. By definition, the n-particle space $\wedge^n \mathcal{H}$ can naturally be viewed as a subspace of $\mathcal{F}(\mathcal{H})$, and hence elements of the form $\psi_1 \wedge \ldots \wedge \psi_n$ as elements of $\mathcal{F}(\mathcal{H})$. Let $\{\phi_i\}_{i\in\mathbb{I}}$ be an orthonormal basis of $\mathcal{H}$, where $\mathbb{I}$ is an ordered finite or countable index set (depending on the dimension of $\mathcal{H}$). For any finite subset of indices $\mathbb{J} \subset \mathbb{I}$, we define the following vector in $\mathcal{F}(\mathcal{H})$

$$\phi_{\mathbb{J}} := \bigwedge_{i\in\mathbb{J}} \phi_i,$$

where the wedge product is taken with respect to the ordering in $\mathbb{I}$, and $\phi_\emptyset = \Omega$. The set $\{\phi_{\mathbb{J}} \mid \mathbb{J} \subset \mathbb{I},\ |\mathbb{J}| < \infty\}$ forms an orthonormal basis of $\mathcal{F}(\mathcal{H})$.

1.1.4 Creation and annihilation operators

For every vector $\psi \in \mathcal{H}$, let us define the operator $a(\psi)$ on the Fock space $\mathcal{F}(\mathcal{H})$ by the formulas

$$a(\psi)\Omega := 0,\ \ a(\psi)\,(\varphi_1 \wedge \ldots \wedge \varphi_n) := \sum_{j=1}^{n} (-1)^j \langle \psi, \varphi_j \rangle \varphi_1 \wedge \ldots \wedge \varphi_{j-1} \wedge \varphi_{j+1} \ldots \wedge \varphi_n.$$

The operator $a(\psi)$ is bounded for any ψ, and its adjoint, $a^\dagger(\psi)$ acts on $\mathcal{F}(\mathcal{H})$ in the following way:

$$a^\dagger(\psi)\Omega = \psi, \quad a^\dagger(\psi)\,(\varphi_1 \wedge \ldots \wedge \varphi_n) = \psi \wedge \varphi_1 \wedge \ldots \wedge \varphi_n.$$

The operators $a^\dagger(\psi)$ and $a(\psi)$ are called creation and annihilation operators, respectively. They satisfy the so-called *canonical anticommutation relations*:

$$\begin{aligned} a(\psi)a^\dagger(\varphi) + a^\dagger(\varphi)a(\psi) &= \langle \psi, \varphi \rangle \mathbb{1}, \\ a(\psi)a(\varphi) + a(\varphi)a(\psi) &= 0. \end{aligned} \tag{1.2}$$

It follows from the definition of these operators, that for an ordered basis $\{\phi_i\}_{i\in\mathbb{I}}$, any vector in the basis set $\{\phi_{\mathbb{J}} \mid \mathbb{J} \subset \mathbb{I},\ |\mathbb{J}| < \infty\}$ of $\mathcal{F}(\mathcal{H})$ can be obtained from any other vector in this set by the action of a certain monomial of the operators $a(\phi_i)$ and $a^\dagger(\phi_i)$.

1.1.5 The Fock space of lattice fermions

Since the focus of the present thesis is lattice fermions, we will shortly summarise the Fock space approach for these particular systems, and introduce some definitions that we will use later.

First, we consider the case of fermions on a finite chain consisting of L number of sites. Let us label the sites by integers from 0 to $L-1$. The one-particle Hilbert space is $\ell^2(\mathbb{I}_L)$, where $\mathbb{I}_L = \{0, 1, \ldots, L-1\}$, i.e., the one-particle Hilbert space is the L-dimensional complex vector space of functions $f : \mathbb{I}_L \to \mathbb{C}$, endowed with the scalar product

$$\langle f, g\rangle := \sum_{i=0}^{L-1} f^*(i)g(i) \quad f, g \in \ell^2(\mathbb{I}_L).$$

The characteristic functions $\{\chi_i\}_{i\in\mathbb{I}_L}$ $(\chi_i(j) := \delta_{i,j})$ form an orthonormal basis of this one-particle Hilbert space, and the projection P_{χ_i} corresponds to the state describing a fermion localised on lattice point i. If $N \leq L$, then the set $\{\chi_{i_1} \wedge \ldots \wedge \chi_{i_N} \mid 1 \leq i_1 < \ldots < i_N \leq L\}$ is a basis of the N-fermion Hilbert space $\wedge^N \ell^2(\mathbb{I}_L)$, and its dimension is therefore $\binom{N}{L}$, while in the $N > L$ case $\wedge^N \mathcal{H} = 0$. Adding this up, the dimension of the Fock space $\mathcal{F}(\ell^2(\mathbb{I}_L))$ turns out to be 2^L.

For an infinite chain, the one-particle Hilbert space is $\ell^2(\mathbb{Z})$, while for an infinite d-dimensional lattice it is $\ell^2(\mathbb{Z}^d)$, and the set of characteristic functions $\{\chi_{\underline{k}}\}_{\underline{k}\in\mathbb{Z}^d}$ $(\chi_{\underline{k}}(\underline{m}) := \delta_{\underline{k},\underline{m}}$, for any $\underline{m} \in \mathbb{Z}^d)$ is an orthonormal basis. Hence $\{\phi_{\mathbb{J}} \mid \mathbb{J} \subset \mathbb{Z}^d,\ |\mathbb{J}| < \infty\}$ is an orthonormal basis of the Fock space $\mathcal{F}(\ell^2(\mathbb{Z}^d))$.[3] Of course, for any d these Fock spaces are equivalent, as all separable Hilbert spaces are equivalent, however, it is convenient to use these particular one-particle Hilbert spaces, since in this formalism the state corresponding to vector $\phi_{\mathbb{J}}$ $(\mathbb{J} \subset \mathbb{Z}^d, |\mathbb{J}| < \infty)$ can be interpreted as a state of fermions occupying the lattice sites in $\mathbb{J}$. Consequently, also the action of the operators V_i describing the translations on the lattice can be written in a very simple form:

$$\begin{aligned} V_i\Omega &= \Omega, \\ V_i\phi_{\mathbb{J}} &= \phi_{\mathbb{J}+\underline{e}_i}, \end{aligned}$$

[3] In the definition of ϕ_J we take the lexicographical ordering in $\mathbb{Z}^d$.

where $i \in \{1, 2, \dots d\}$ and $\underline{e}_1 = (1, 0, 0, \dots, 0)$, $\underline{e}_2 = (0, 1, 0, \dots, 0), \dots, \underline{e}_d = (0, 0, 0, \dots 1)$.

Since in the lattice case we have a distinguished set of one-particle vectors $\chi_{\underline{k}}$, it is useful to introduce a short notation for the creation and annihilation operators corresponding to them: $a^\dagger_{\underline{k}} := a^\dagger(\chi_{\underline{k}})$ and $a_{\underline{k}} := a(\chi_{\underline{k}})$. From the canonical anticommutation relations (1.2) we can derive that these operators satisfy the following relations for any $\underline{k}, \underline{l} \in \mathbb{Z}^d$.

$$\begin{aligned} a_{\underline{k}} a^\dagger_{\underline{l}} + a^\dagger_{\underline{l}} a_{\underline{k}} &= \delta_{\underline{k},\underline{l}} \mathbb{1}, \\ a_{\underline{k}} a_{\underline{l}} + a_{\underline{l}} a_{\underline{k}} &= 0. \end{aligned} \tag{1.3}$$

For any finite subset $\mathbb{J}$ of $\mathbb{Z}^d$ the *particle number operator* belonging to region $\mathbb{J}$ can be expressed in an easy way with the above defined operators: $\sum_{\underline{k} \in \mathbb{J}} a^\dagger_{\underline{k}} a_{\underline{k}}$.

1.1.6 Problems with the Fock space approach

In quantum statistical mechanics one usually wants to treat infinite lattices of fermions with a finite particle density, and often translation-invariant systems of such. The Fock space approach fails in this context, since the only translation-invariant state in $\mathcal{F}(\ell(\mathbb{Z}^d))$ is the projection corresponding to the vacuum vector Ω, moreover, the average particle number per site

$$n(\rho) = \lim_{L \to \infty} \frac{1}{(2L+1)^d} \mathrm{Tr} \left(\rho \sum_{\underline{k} \in \{-L, \dots, L\}^d} a^\dagger_{\underline{k}} a_{\underline{k}} \right),$$

will vanish for any density matrix ρ on $\mathcal{F}(\ell^2(\mathbb{Z}))$.

The modern way to circumvent this problem is to treat the abstract algebra of creation and annihilation operators as the basic ingredient of the theory of fermions, and not its particular Fock representation. It will turn out that the Fock representation is only one of the many inequivalent representations of this algebra, and using also other representations one can avoid the above mentioned problems. The next section is devoted to this C*-algebraic approach.

1.2 The C*-algebraic approach to fermionic systems

In this section we give a short introduction to the C*-algebraic formalism of lattice fermionic systems. First, we introduce the *canonical anticommutation relations algebra*, i.e. the CAR-algebra, which is isomorphic to the closure in operator norm of the algebra generated by the creation and annihilation operators on the Fermi-Fock space considered in the last section. Then we define the states in this approach as certain functionals on this algebra, which map an "expectation value" to each algebra element. For finite fermionic chains this definition of states is equivalent with the definition of states in the Fock space approach, but for infinite systems the C*-algebraic definition is much wider. We discuss a particular class of states, called quasifree states, at the end of the section, and we show that for infinite lattice systems the Fock-representation is only one of the many possible representations of the CAR-algebra.

1.2.1 The CAR-algebra

The CAR($\ell^2(\mathbb{Z}^d)$)-algebra corresponding to fermionic systems on a d-dimensional cubic lattice $\mathbb{Z}^d$ is the unital C*-algebra (with $\mathbb{1}$ being the unit) generated by operators $\{c_{\underline{k}}\}_{\underline{k}\in\mathbb{Z}^d}$, satisfying the canonical anticommutation relations [4]:

$$\begin{aligned} c_{\underline{k}}c_{\underline{l}} + c_{\underline{l}}c_{\underline{k}} &= 0, \\ c^*_{\underline{k}}c_{\underline{l}} + c_{\underline{l}}c^*_{\underline{k}} &= \delta_{\underline{k},\underline{l}}\mathbb{1}. \end{aligned} \tag{1.4}$$

For any d, the C*-algebras CAR($\ell^2(\mathbb{Z}^d)$) are isomorphic to each other, but it is useful to consider these different particular presentations for different dimensions, since now the action of the translation automorphism can be conveniently written down:

$$\tau_i(c_{\underline{k}}) = c_{\underline{k}+\underline{e}_i},$$

[4] In order to avoid confusion, we follow the standard way of denoting by c and c^* the abstract C*-algebra generators, and by a and $a^\dagger$ the particular Fock-representation of the creation and annihilation operators.

where $\{\underline{e}\}_{i\in\{1,\ldots,d\}}$ denotes the standard basis in $\mathbb{Z}^d$

$$\underline{e}_1 = (1,0,0,\ldots,0), \quad \underline{e}_2 = (0,1,0,\ldots,0), \quad \ldots \quad , \underline{e}_d = (0,0,0,\ldots 1). \qquad (1.5)$$

In the case of a one-dimensional fermionic lattice, the translation automorphism will simply denoted by τ.

For treating subsystems of the whole lattice, we will introduce for any finite subset $\mathbb{J}$ of $\mathbb{Z}^d$ the corresponding C*-algebra $\mathrm{CAR}(\ell^2(\mathbb{J}))$. It is the C*-subalgebra of $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ generated by the finite number of generators $\{c_{\underline{k}}\}_{\underline{k}\in\mathbb{J}}$. The dimension of this C*-algebra is $2^{2|\mathbb{J}|}$, as we will show in subsection 1.2.3. Any element that is contained in such a $\mathrm{CAR}(\ell^2(\mathbb{J}))$ subalgebra for some finite set $\mathbb{J} \subset \mathbb{Z}^d$ is called a *local element*, and these elements form a dense subset in $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$.

1.2.2 States in the C*-algebraic approach and the GNS theorem

In the C*-algebraic approach to quantum physics, a state of a physical system is described by the expectation values of elements of the C*-algebra corresponding to the system. More precisely, let $\mathcal{A}$ be a unital C*-algebra, a state is a normalised positive linear functional $\omega : \mathcal{A} \to \mathbb{C}$. If a state ω cannot be written as a convex combination of two other states, then it is called *pure*, else it is called *mixed*.

The relation of this definition to the density matrix approach is the following: if π is an irreducible representation of a C*-algebra $\mathcal{A}$ on a separable Hilbert space $\mathcal{H}$ and ρ is a density matrix on $\mathcal{H}$, then the function $\omega(A) = \mathrm{Tr}(\rho\pi(A))$ $(A \in \mathcal{A})$, is a state on $\mathcal{A}$. Not all mixed states on $\mathcal{A}$ can be written in this form, however, for pure states this form is general (moreover ρ is a projection in this case) according to the following theorem - a version of the Gelfand-Naimark-Segal (GNS) theorem (for the whole theorem see Appendix B):

Theorem. *For any pure state ω over the C*-algebra $\mathcal{A}$, there exists a Hilbert space $\mathcal{H}_\omega$, an irreducible representation π of $\mathcal{A}$ on $\mathcal{H}_\omega$ and a unit vector Ω_ω in $\mathcal{H}_\omega$, so that the following conditions hold:*

$$\omega(A) = \langle\Omega_\omega, \pi_\omega(A)\Omega_\omega\rangle,$$

for any $A \in \mathcal{A}$.

A state on the d-dimensional lattice fermion algebra $\mathrm{CAR}(\mathbb{Z}^d)$ is called translation-invariant if $\omega_Q \circ \tau_i = \omega_Q$ for all $i \in \{1, \dots d\}$. A translation-invariant state is called ergodic if it cannot be decomposed as a mixture of two other translation-invariant states.

1.2.3 Finite fermionic lattices

Before introducing a particular class of states on infinite fermionic lattices, let us consider the case of a finite fermionic chain of L sites. To see the structure of the C*-algebra $\mathrm{CAR}(\ell^2(\mathbb{I}_L))$ corresponding to this system, we will introduce a new set of generators instead of the set original defining set $\{c_k\}_{k\in\mathbb{I}_L}$. We begin by introducing for any non-negative integer n smaller than 2^L the notation $(b_{L-1}(n)b_{L-2}(n)\dots b_0(n))$ for the binary representation of n, i.e.

$$n = \sum_{i=0}^{L-1} b_i(n)2^i, \qquad b_i(n) \in \{0, 1\}.$$

Let us now introduce the following operators for any integers $k, l \in \{0, 1, \dots 2^L{-}1\}$:

$$\begin{aligned}\hat{E}_{k,l} \;:=\; & (2c_0^*c_0 - \mathbb{1})^{(b_0(k)+b_0(l))}A_0(b_0(k), b_0(l)) \times \\ & ((2c_0^*c_0 - \mathbb{1})(2c_1^*c_1 - \mathbb{1}))^{(b_1(k)+b_1(l))}\, A(b_1(k), b_1(l)) \times \cdots \\ & \prod_{m=0}^{L-1}(2c_m^*c_m - \mathbb{1})^{(b_{L-1}(k)+b_{L-1}(l))}A(b_{L-1}(k), b_{L-1}(l)),\end{aligned}$$

where for any $i \in \{0, 1, \dots L-1\}$ the operators $A_i(b, c)$ are defined as

$$A_i(0,0) := c_i^*c_i\,, \quad A_i(0,1) := c_i^*, \quad A_i(1,0) := c_i\,, \quad A_i(1,1) := c_i\,c_i^*.$$

The operators $\hat{E}_{k,l}$ are linearly independent and any monomial of c_k and c_l^* can be linearly expressed by these operators, i.e., they form a vector space basis of the algebra $\mathrm{CAR}(\ell^2(\mathbb{I}_L))$, which is thus 2^{2L} dimensional. Since $\hat{E}_{k,l}$ satisfy exactly the matrix unit relations

$$\hat{E}_{k,l}\hat{E}_{m,n} = \delta_{l,m}\hat{E}_{k,n},$$

the CAR($\ell^2(\mathbb{I}_L)$)-algebra is isomorphic to the C*-algebra of $2^L \times 2^L$ matrices $\mathcal{M}_{2^L}$ (see theorem B2 in Appendix B). From theorem B5 in Appendix B, we know that to any linear functional $f : \mathcal{M}_n \to \mathbb{C}$ on a finite matrix algebra, there exists a matrix D such that:

$$f(M) = \mathrm{Tr}\,(DM),$$

for all $M \in \mathcal{M}_n$. If we also require the functional to be positive and normalised, the matrix D has to be positive and of unit trace, i.e., it has to be a density matrix. Hence in the case of a finite fermionic chain the C*-algebraic definition of a state is equivalent with the traditional definition.

Similarly, for any finite $\mathbb{J} \in \mathbb{Z}^d$, the algebra CAR($\ell^2(\mathbb{J})$) is then isomorphic to the C*-algebra of $2^{|\mathbb{J}|} \times 2^{|\mathbb{J}|}$ matrices. Any state on this subalgebra corresponds to a density matrix, i.e. to a positive element of unit trace in CAR($\ell^2(\mathbb{J})$). The restriction of a state ω on CAR($\ell^2(\mathbb{Z})$) to this subalgebra will be denoted by $\omega_{\mathbb{J}}$, and the corresponding *restricted density matrix* by $\rho^{\omega}_{\mathbb{J}}$ (the superscript ω will sometimes be omitted, if there is no possibility of confusion). Let $\{\mathbb{J}_n\}_{n\in\mathbb{N}}$ be a family of growing finite subsets of $\mathbb{Z}^d$ with the property that for any $\underline{k} \in \mathbb{Z}^d$ there exists an $n(\underline{k})$ such that for any $m > n(\underline{k})$ the point $\underline{k}$ is contained in $\mathbb{J}_m$. Since local elements form a dense subset in CAR($\ell^2(\mathbb{J})$) the states ω_1 and ω_2 coincide if and only if $\rho^{\omega_1}_{\mathbb{J}_n} = \rho^{\omega_2}_{\mathbb{J}_n}$ for any $n \in \mathbb{N}$. Thus the restricted density matrices of a state ω determine the state uniquely.

1.2.4 Quasifree states on infinite fermionic lattices

In this thesis we will investigate a particular class of states on the CAR-algebra, called quasifree states, which we introduce in this section. Let Q be a bounded operator on $\ell^2(\mathbb{Z}^d)$ satisfying $0 \leq Q \leq \mathbb{1}$. A linear functional ω_Q on the CAR($\ell^2(\mathbb{Z}^d)$)-algebra that assigns to monomials of creation and annihilation operators the values

$$\omega_Q\left(c^*_{\underline{k}_1} \ldots c^*_{\underline{k}_n} c_{\underline{l}_m} \ldots c_{\underline{l}_1}\right) = \delta_{n,m}\det\left(\left[\langle \chi_{\underline{k}_i}, Q\chi_{\underline{l}_j}\rangle\right]^n_{i,j=1}\right), [5] \tag{1.6}$$

[5] This formula is sometimes called the Wick-expansion.

extends to a state. ω_Q is called the quasifree state corresponding to operator Q [6]. The operator Q is usually called the symbol of the state ω_Q. The quasifree state is pure if and only if Q is a projection.

In the case of d-dimensional lattice fermions, a quasi-free state ω_Q is *translation-invariant* if and only if its symbol in the $\{\chi_{\underline{k}}\}_{\underline{k}\in\mathbb{Z}^d}$ basis, $Q_{\underline{k},\underline{l}} := \langle \chi_{\underline{k}}, Q\chi_{\underline{l}}\rangle$ is a Toeplitz matrix, i.e., there exists a sequence $\{q_{\underline{k}}\}_{\underline{k}\in\mathbb{Z}^d}$ so that $Q_{\underline{k},\underline{l}} = q_{\underline{k}-\underline{l}}$. By the Fourier transform

$$\tilde{q}(\underline{\theta}) = \sum_{\underline{k}\in\mathbb{Z}^d} q_{\underline{k}} e^{i\underline{k}\cdot\underline{\theta}}, \quad \text{and its inverse} \quad q_{\underline{k}} = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} d\underline{\theta}\, \tilde{q}(\underline{\theta}) e^{-i\underline{k}\cdot\underline{\theta}},$$

with the d-dimensional torus $\mathbb{T}^d$ being parametrised by $[-\pi,\pi)^d$, the symbol of a translation-invariant quasifree state is unitary equivalent with the multiplication operator by $\tilde{q}$ on $\mathcal{L}^2(\mathbb{T}^d, d\underline{\theta})$. This function satisfies $0 \le \tilde{q} \le 1$ almost everywhere. A Toeplitz matrix Q is a projection, and hence the translation-invariant quasifree state ω_Q is pure, if and only if its the Fourier transform $\tilde{q}$ is a characteristic function $\Xi_{\mathbb{M}}$ of a measurable set $\mathbb{M} \subset \mathbb{T}^d$. In this case $\mathbb{M}$ is called the *Fermi sea* of the state, and the boundary of the interior points of $\mathbb{M}$ is called the *Fermi surface*. In the one dimensional case, the elements of a discrete Fermi surface are called the *Fermi points*.

By representing the C*-algebra CAR$(\ell^2(\mathbb{Z}^d))$ on the Fock space $\mathcal{F}(\ell^2(\mathbb{Z}^d))$ through the the rule $\pi(c_{\underline{k}}) := a_{\underline{k}}$, and defining for any $A \in$ CAR$(\ell^2(\mathbb{Z}^d))$ the expectation value $\omega_{Fock}(A) := \langle\Omega, \pi(A)\Omega\rangle$ we obtain exactly the quasifree state corresponding to the symbol 0.[7] Two pure quasi free states $\omega_{Q_{(1)}}$ and $\omega_{Q_{(2)}}$ lead to (unitary) equivalent irreducible GNS representations if and only if the operators $Q_{(1)} - Q_{(2)}$ are Hilbert-Schmidt operators (for the definition of Hilbert-Schmidt operators, see Appendix A). Since for any nonzero projection Q is of Toeplitz form, it cannot be a Hilbert-Schmidt operator. Hence for all pure *translation-invariant* quasifree state (other than the Fock state $Q = 0$) we must use a representation *inequivalent* to the Fock representation.

[6]Sometimes a broader defi nition is used for quasifree states, see [5], and in that context the states we term quasifree states are called gauge-invariant quasifree states. We will stick to our terminology of quasifree states throughout the whole thesis.

[7]ω_0 is called the Fock state, while $\omega_{\mathbb{1}}$ is called the anti-Fock state.

Let $\mathbb{J}$ be a finite subset of $\mathbb{Z}^d$, and let $P_{\mathbb{J}}$ be the projection from $\ell^2(\mathbb{Z}^d)$ to the subspace $\ell^2(\mathbb{J})$, which is linearly generated by the functions $\{\chi_{\underline{k}}\}_{\underline{k}\in\mathbb{J}}$, i.e.

$$P_{\mathbb{J}}\chi_{\underline{k}} = \begin{cases} \chi_{\underline{k}} & \text{if } \underline{k} \in \mathbb{J} \\ 0 & \text{if } \underline{k} \notin \mathbb{J} \end{cases} .$$

The operator $Q_{\mathbb{J}} := P_{\mathbb{J}} Q P_{\mathbb{J}}$ will be called the restriction of operator Q to the subspace $\ell^2(\mathbb{J})$. If we restrict a quasifree state ω_Q to the finite subregion $\mathbb{J}$, then the corresponding restricted density matrix will be of the form

$$\rho_{\mathbb{J}}^{\omega_Q} = \prod_{i=1}^{|\mathbb{J}|} \left(q_i c_{(i)} c_{(i)}^* + (1 - q_i) c_{(i)}^* c_{(i)} \right) ,$$

where $0 \le q_i \le 1$ are the eigenvalues of the positive operator $Q_{\mathbb{J}} \le \mathbb{1}$ belonging to the normalised orthogonal eigenvectors $v_i := \sum_{\underline{k}\in\mathbb{J}} \alpha_{\underline{k}}^{(i)} \chi_{\underline{k}}$ ($\alpha_{\underline{k}}^{(i)} \in \mathbb{C}$), and the operators $c_{(i)}$ are defined as:

$$c_{(i)} := \sum_{\underline{k}\in\mathbb{J}} \alpha_{\underline{k}}^{(i)} c_{\underline{k}} . \tag{1.7}$$

1.3 Transferring translation-invariant states from fermion chains to quantum spin chains

Translation-invariant quasifree states defined in the previous section play an important role in the study of fermionic models, but also in the context of quantum spin chain models. In this section we show how one can transfer a translation-invariant state defined on the fermion chain algebra $\mathrm{CAR}(\ell^2(\mathbb{Z}))$ to the quantum spin chain algebra.

1.3.1 The quantum spin chain algebra

The observable algebra of an infinite chain of $\frac{1}{2}$-spins is the unital C*-algebra generated by elements σ_a^k ($a = 1, 2, 3;\ k \in \mathbb{Z}$) satisfying the Pauli relations

$$\sigma_a^k \sigma_b^l = \sigma_b^l \sigma_a^k, \quad \text{when} \quad k \neq l,$$

$$\sigma_a^l \sigma_b^l = \mathrm{i}\varepsilon_{abc}\sigma_c^l + \delta_{ab}\mathbb{1}.$$

Alternatively, one can say that it is the C*-inductive limit:

$$\mathcal{S} := \bigotimes_{i=-\infty}^{+\infty} \mathcal{A}_i, \quad \mathcal{A}_i \cong M_2,$$

where M_2 denotes the algebra of 2×2 matrices. One can then identify the elements σ_a^k ($a = 1, 2, 3;\ k \in \mathbb{Z}$) with the Pauli matrices embedded into the kth M_2 factor of $\mathcal{S}$. The translation automorphism τ_S on $\mathcal{S}$ is defined by $\tau_S(\sigma_a^k) = \sigma_a^{k+1}$.

The C*-algebras $\mathcal{S}$ and CAR($\ell^2(\mathbb{Z})$) are isomorphic. However, there exists no isomorphism $\iota\colon \mathcal{S} \to \mathrm{CAR}(\ell^2(\mathbb{Z}))$ that satisfies the property $\iota \circ \tau_{\mathcal{S}} = \tau \circ \iota$.[8] This intertwining property is needed to derive the translation invariance of a state $\omega \circ \iota$ on $\mathcal{S}$ from that of ω on CAR($\ell^2(\mathbb{Z})$). However, we will be able to treat this problem by a generalisation of the Jordan-Wigner transformation.

1.3.2 The Jordan-Wigner isomorphism

Let us consider a finite fermionic chain and a finite spin chain both having L sites. The Jordan-Wigner transformation establishes an isomorphism between the finite spin chain algebra $\mathcal{S}_L \cong M_2^{\otimes L}$ (generated by the finite number of Pauli matrices $\{\sigma_a^k\}_{a\in\{1,2,3\},k\in\{0\ldots L-1\}}$) and the finite fermionic chain algebra CAR($\ell^2(\mathbb{I}_\mathbb{L})$) in following way:[9]

$$\begin{aligned}
\iota_{JW}^L(\sigma_1^k) &:= \prod_{m=0}^{k-1}(2c_m c_m^* - \mathbb{1})(c_k^* + c_k),\\
\iota_{JW}^L(\sigma_2^k) &:= \prod_{m=0}^{k-1}(2c_m c_m^* - \mathbb{1})i(c_k^* - c_k),\\
\iota_{JW}^L(\sigma_3^k) &:= 2c_k c_k^* - \mathbb{1}.
\end{aligned}$$

As we have mentioned, the Jordan-Wigner transformation cannot be generalised to be a translation-intertwining isomorphism between the infinite lattice

[8] This is clear if we note that $(\mathcal{S}, \tau_{\mathcal{S}})$ is asymptotically Abelian, while (CAR($\ell^2(\mathbb{Z})$), τ) is not.

[9] This is essentially the same transformation as the one defi ned in subsection 1.2.3.

algebras $\mathcal{S}$ and $\mathrm{CAR}(\ell^2(\mathbb{Z}))$.[10] This problem can be circumvented by the Araki construction [3], in the next subsection we will present a bit modified but equivalent formulation of this method.

1.3.3 The Araki-Jordan-Wigner isomorphism

The basic idea of transferring translation-invariant states from the fermionic chain to the quantum spin chain is to find a translation-intertwining isomorphism α not between the algebras $\mathcal{S}$ and $\mathrm{CAR}(\ell^2(\mathbb{Z}))$, since such isomorphism doesn't exists, but between two appropriate subalgebras $\mathcal{S}_+$ and $\mathrm{CAR}(\ell^2(\mathbb{Z}))_+$, which are invariant under the translation automorphisms $\tau_{\mathcal{S}}$ and τ, respectively. An ω translation-invariant state on $\mathrm{CAR}(\ell^2(\mathbb{Z}))$ will be restricted to $\mathrm{CAR}(\ell^2(\mathbb{Z}))_+$, and this restricted state ω^+ will then be transfered to a state $\omega^+_{\mathcal{S}} := \omega^+ \circ \alpha$ on $\mathcal{S}_+$, and finally we will extend this state to a $\tau_{\mathcal{S}}$-invariant state $\omega_{\mathcal{S}}$ on $\mathcal{S}$.

Firstly, let us introduce the parity automorphism π on $\mathrm{CAR}(\ell^2(\mathbb{Z}))$. It is defined by $\pi(c_k) = -c_k$. The elements of $\mathrm{CAR}(\ell^2(\mathbb{Z}))_+ := \{A \in \mathrm{CAR}(\ell^2(\mathbb{Z})) \mid \pi(A) = A\}$ are called even, while those of $\mathrm{CAR}(\ell^2(\mathbb{Z}))_- := \{A \in \mathrm{CAR}(\ell^2(\mathbb{Z})) \mid \pi(A) = -A\}$ are called odd. Alternatively, one can say that $\mathrm{CAR}(\ell^2(\mathbb{Z}))_+$ is the C*-subalgebra of $\mathrm{CAR}(\ell^2(\mathbb{Z}))$ generated by the elements $c_k c_l$ and $c_k^* c_l$ $(k, l \in \mathbb{Z})$. Any element $A \in \mathrm{CAR}(\ell^2(\mathbb{Z}))$ can uniquely be written in the form $A = A_+ + A_-$, where $A_+ \in \mathrm{CAR}(\ell^2(\mathbb{Z}))_+$, and $A_- \in \mathrm{CAR}(\ell^2(\mathbb{Z}))_-$. Thus, $\mathrm{CAR}(\ell^2(\mathbb{Z})) = \mathrm{CAR}(\ell^2(\mathbb{Z}))_+ + \mathrm{CAR}(\ell^2(\mathbb{Z}))_-$. The translation automorphism τ leaves the subalgebra $\mathrm{CAR}(\ell^2(\mathbb{Z}))_+$ invariant, and we will denote its restriction to this subalgebra by τ^+. A state ω on $\mathrm{CAR}(\ell^2(\mathbb{Z}))$ is called even if $\omega \circ \pi = \omega$.

Secondly, we do a similar decomposition of the quantum spin chain algebra. Let $\mathcal{S}_+$ be the C^*-subalgebra of $\mathcal{S}$ generated by σ_3^k and $\sigma_1^k \sigma_1^l$ $(k, l \in \mathbb{Z})$, and let us define the subspace $\mathcal{S}_- := \{\sigma_1^0 C_+ \mid C_+ \in \mathcal{S}_+\}$. Any element $C \in \mathcal{S}$ can uniquely written in the form $C = C_+ + C_-$, where $C_+ \in \mathcal{S}_+$ and $C_- \in \mathcal{S}_-$, hence $\mathcal{S} = \mathcal{S}_+ + \mathcal{S}_-$. The translation automorphism on the quantum spin chain $\tau_{\mathcal{S}}$ leaves the subalgebra $\mathcal{S}_+$ invariant, and its restriction to this subalgebra will be denoted by $\tau^+_{\mathcal{S}}$. $\mathcal{S}_+$ is isomorphic to $\mathrm{CAR}(\ell^2(\mathbb{Z}))_+$, an explicit isomorphism α is given by

[10] In an informal way, we could say that an element of the form "$\prod_{m=-\infty}^{k-1}(2c_m c_m^* - \mathbb{1})$" would be needed in the definition of a "two-sided infinite chain Jordan-Wigner transformation", which doesn't exists in $\mathrm{CAR}(\ell^2(\mathbb{Z}))$.

the Araki-Jordan-Wigner transformation:

$$\begin{aligned} \alpha(\sigma_3^k) &:= 2c_k^* c_k - \mathbb{1}, \\ \alpha(\sigma_1^k \sigma_1^l) &:= -\prod_{m=k}^{l-1} (2c_m^* c_m - \mathbb{1})(c_k^* + c_k)(c_l^* + c_l) \quad \text{when} \quad k < l. \end{aligned}$$

Moreover, α is an isomorphism that intertwines the translations $\tau_{\mathcal{S}}^+$ and τ^+, i.e. $\tau^+ \circ \alpha = \alpha \circ \tau_{\mathcal{S}}^+$. Now, let ω^+ be the restriction of a state ω on $\mathrm{CAR}(\ell^2(\mathbb{Z}))$ to $\mathrm{CAR}(\ell^2(\mathbb{Z}))_+$. If ω is a translation-invariant state, i.e. $\omega \circ \tau = \omega$, then the state $\omega_{\mathcal{S}}^+ := \omega_+ \circ \alpha$ on $\mathcal{S}_+$, is τ_+-invariant. The state $\omega_{\mathcal{S}}^+$ can be extended to a state $\omega_{\mathcal{S}}$ on $\mathcal{S}$ by $\omega_{\mathcal{S}}(C) = \omega_{\mathcal{S}}(C_+ + C_-) := \omega_{\mathcal{S}}^+(C_+)$, where $C_+ \in \mathcal{S}_+$, and $C_- \in \mathcal{S}_-$. This way a translation-invariant state ω on $\mathcal{S}$ is obtained. Moreover, if ω is even, which is satisfied for all translation-invariant states, then the restricted density matrices of ω and $\omega_{\mathcal{S}}$ are transformed into each other by the isomorphism α, and $\omega_{\mathcal{S}}$ is pure if and only if ω is pure. We will call $\omega_{\mathcal{S}}$ the state Araki-Jordan-Wigner transformed state of ω.

1.4 Gibbs states and ground states

In this section the concept of ground states and finite temperature Gibbs states are defined. We presented two models for which these latter states are known. The first of these models is the tight-binding fermion model with only hopping terms, the Gibbs states of these models are quasifree states, the second is the XX quantum spin chain model, the Gibbs states of which are Jordan-Wigner transformed quasifree states.

1.4.1 The definition of Gibbs states and ground states

A lattice fermion interaction is defined as a function Φ from the finite subsets $\mathbb{J}$ of $\mathbb{Z}^d$ into the hermitian elements of $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ such that $\Phi(\mathbb{J}) \in \mathrm{CAR}(\ell^2(\mathbb{J}))$. A Hamiltonian associated to the interaction Φ is a function that from the finite subsets of $\mathbb{Z}^d$ to the hermitian elements of $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ defined in the following way:

$$H(\mathbb{J}) = \sum_{\mathbb{J}' \subset \mathbb{J}} \Phi(\mathbb{J}').$$

We restrict our discussion to translation-invariant interactions, which satisfy the additional requirement

$$\tau_i(\Phi(\mathbb{J})) = \Phi(\mathbb{J} + \underline{e}_i) ,$$

for any $i \in \{1, \ldots, d\}$ and any finite $\mathbb{J} \subset \mathbb{Z}^d$.

A *local Gibbs state* at inverse temperature $\beta := \frac{1}{T}$ (working in units where $k = 1$) and chemical potential μ belonging to the local Hamiltonian $H(\mathbb{J})$ is defined as the following state on $\mathrm{CAR}(\ell^2(\mathbb{J}))$[11]

$$\omega_{\mathbb{J},\beta,\mu}(A) := \frac{\mathrm{Tr}\ \left(A \exp\left(-\beta\left(H(\mathbb{J}) - \mu N(\mathbb{J})\right)\right)\right)}{\mathrm{Tr}\ \exp\left(-\beta\left(H(\mathbb{J} - \mu N(\mathbb{J})\right)\right)} ,$$

where $N_{\mathbb{J}}$ denotes the particle number operator corresponding to the region $\mathbb{J}$:

$$N(\mathbb{J}) := \sum_{\underline{k} \in \mathbb{J}} c^*_{\underline{k}} c_{\underline{k}}$$

In the thermodynamic limit we will restrict ourselves to increasing families of cubes centred around the origin[12], and hence we will introduce the following notation: for any two integers K, L with $K \leq L$ let us define $[K, L]^d := \{\underline{k} = (k_1, \ldots, k_d) \mid \underline{k} \in \mathbb{Z}^d\ K \leq k_i \leq L\}$. Let H be a Hamiltonian corresponding to a translation-invariant interaction. If the limits

$$\omega_{\beta,\mu}(A) := \lim_{L\to\infty} \omega_{[-L,L]^d,\beta,\mu}(A)$$

exist for all local elements A, we can extend this functional to the whole algebra $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ by continuity so that $\omega_{\beta,\mu}$ becomes a state on this algebra. The resulting state is called the *limiting Gibbs state* at inverse temperature β and

[11] Tr means the "dimension normalised trace-function" on the fi nite C*-algebra $\mathrm{CAR}(\ell^2(\mathbb{J}))$, see Appendix B.

[12] One can of course use other (more strict) defi nitions. For example, in the monographs [13, 48] parallelepipeds are used, and perhaps the physically most satisfactory is the so-called *van Hove limit* (see [7]), where the limit is taken on even more general increasing subsets of $\mathbb{Z}^d$. These different limits may not coincide, but for the models we discuss in the next subsection they do, hence we choose this simplest defi nition.

chemical potential μ belonging to the Hamiltonian H. If the limits

$$\omega_\mu(A) := \lim_{\beta\to\infty} \omega_{\beta,\mu}(A)$$

exist for all $A \in \mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ and form a state, then the resulting state is called the ground state at chemical potential μ of the Hamiltonian H.

On the quantum spin chain algebra the concept of a Hamiltonian and of Gibbs and ground states can be defined analogously, except for the absence of the chemical potential term in this case.

In the next subsection we shall consider a class of models where these limits exist, and where the resulting Gibbs and ground states are quasifree. For a more complete treatment, e.g. for sufficient conditions for the existence of the Gibbs states and analysis of large classes of models see the monograph [13].

1.4.2 The ground and finite temperature Gibbs states of certain lattice fermion and quantum spin chain models

Our first set of examples are the tight-binding fermion models with finite range hopping terms. Let T denote an operator on $\ell^2(\mathbb{Z}^d)$ which is of a Toeplitz form in the basis $\{\chi_{\underline{k}}\}_{\underline{k}\in\mathbb{Z}^d}$ and has the following finite range property in this basis: there exists an integer n, so that $T_{\underline{k},\underline{k}+m\underline{e}_i} = 0$ for any $m \geq n$ and for any standard unit vector $\{\underline{e}_i\}_{i\in\{1,\dots,d\}}$. Let us define the interaction function Φ on the subsets containing two elements as

$$\Phi_T(\{\underline{k},\underline{l}\}) = T_{\underline{k},\underline{l}}c^*_{\underline{k}}c_{\underline{l}},$$

and as 0 for all other finite subsets of $\mathbb{Z}^d$. The corresponding Hamiltonians are then

$$H(\mathbb{J}) := \sum_{\underline{k},\underline{l}\in\mathbb{J}} T_{\underline{k},\underline{l}}c^*_{\underline{k}}c_{\underline{l}} \ .$$

The limiting Gibbs state $\omega_{\beta,\mu}$ for this set of Hamiltonians is the quasifree state belonging to the symbol $Q(\beta,\mu)$, which has a Fourier transform of the form

$$\tilde{q}_{\beta,\mu}(\underline{\theta}) = \frac{1}{1+\exp\left(\beta\tilde{t}(\underline{\theta})-\mu\right)} ,$$

where $\tilde{t}(\underline{\theta})$ is the Fourier transform of the Toeplitz operator T:

$$\tilde{t}(\underline{\theta}) := \sum_{\underline{k}\in\mathbb{Z}^d} T_{\underline{k},\underline{0}} e^{i\underline{k}\cdot\underline{\theta}} .$$

The ground states of these models at chemical potential μ are the pure quasifree states belonging to the symbol with the following Fourier transform:

$$\tilde{q}_{\mu}^{(gs)}(\underline{\theta}) = \frac{1}{2}\left(1 - \frac{\tilde{t}(\underline{\theta})-\mu}{|\tilde{t}(\underline{\theta})-\mu|}\right) .$$

That is, $\tilde{q}_{gs,\mu}$ is the characteristic function of the set of $\underline{\theta}$s where the expression $\tilde{t}(\underline{\theta})-\mu$ is negative, and the Fermi surface is located at the points where the equation $\tilde{t}(\underline{\theta})=\mu$ is satisfied.

Our next example is the XX quantum spin chain model in a transverse magnetic field. In this case we have two real parameters J and h, and the interaction function belonging to sets of one element is defined as

$$\Phi^{XX}_{J,h}(\{k\}) := -h\sigma_3^k,$$

the interaction function belonging to sets of two elements is defined as

$$\Phi^{XX}_{J,h}(\{k,l\}) := -(\delta_{k,l+1}+\delta_{k+1,l})J(\sigma_1^k\sigma_1^l+\sigma_2^k\sigma_2^l),$$

and Φ is 0 for all other finite subsets of $\mathbb{Z}$. The corresponding local Hamiltonians on an interval centred around the origin is

$$H^{XX}_{J,h}([-L,L]) = -\sum_{k=-L}^{L-1} J(\sigma_1^k\sigma_1^{k+1}+\sigma_2^k\sigma_2^{k+1}) - h\sum_{k=-L}^{L}\sigma_3^k.$$

The Gibbs state at inverse temperature β belonging to this set of local Hamiltonians is the Jordan-Wigner transformed state of a quasifree state on CAR($\ell^2(\mathbb{Z})$). This quasifree state corresponds to the Fourier transformed symbol of

$$\tilde{q}_\beta^{XX}(\theta) = \frac{1}{1 + \exp\left(-\beta(J\cos(\theta) + h)\right)} ,$$

while the ground state is described by the following characteristic function

$$\tilde{q}_{gs}^{XX}(\theta) = \frac{1}{2}\left(1 + \frac{J\cos(\theta) + h}{|J\cos(\theta) + h|}\right) .$$

Chapter 2

The von Neumann entropy of restricted density matrices on lattice models

A state on the CAR($\ell^2(\mathbb{Z}^d)$)-algebra is uniquely determined by its restricted density matrices corresponding to subsystems of growing hypercubes centred around the origin. The von Neumann entropy of a density matrix ρ provides a good characterisation of the mixedness of ρ, thus knowing how the von Neumann entropy depends on the size of the corresponding cubes, we should be able to gain some information about the entire state. It turns out that this is indeed the case. In this chapter first we will give a brief introduction to the variational characterization of local and limiting Gibbs states based on the von Neumann entropy and its density. Then we show in which way this quantity (in some cases) measures the size of the subspace to which we can truncate a restricted density matrix without loosing too much information about the state of the subsystem. Many numerical methods like the density matrix renormalization group (DMRG) [51] rely on this compressibility property of the restricted density matrices.

Usually, the von Neumann entropy is introduced as a quantum version of the Shannon entropy. We will also follow this path in our discussion. However, historically von Neumann defined this quantity named after him already in 1927

[46], much earlier than the Shannon entropy was introduced [56].[1] Since the importance of this quantity was not obvious in the early days of "few-body quantum mechanics", there was not much activity concerning the von Neumann entropy for several decades. At the end of the 1960's, when the rigorous formulations of quantum statistical mechanics were laid by Ruelle, Araki and others, and the role of the von Neumann entropy in this field was recognised, an extensive study of this quantity began (see e.g. [60]). At the end of the 1980's and beginning of the 1990's it was also realised that the von Neumann entropy plays an important role in quantum information theory. Considering a tensor product Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, the von Neumann entropy of the restriction of a pure state on $\mathcal{H}$ to the subalgebra acting on one of the tensor factors (e.g. on $\mathcal{H}_1$) is a good measure of entanglement and it quantifies well "how much" this state can be used for quantum information processing [9]. We will not consider this topic in the present thesis, for a monograph on this subject, see [47]. In 2003 a new function of this quantity was found again in the theory of quantum phase transitions. The growth of the von Neumann entropy of restricted density matrices of ground states of fermionic and quantum spin chains with the subsystem size was related to the quantum criticality or non-criticality of the corresponding models [59, 39]. We will discuss these studies in the next chapter.

In this chapter we will concentrate only on how the von Neumann entropy of restricted density matrices characterise different translation-invariant states. The first section is devoted to its role in finite temperature statistical physics, while in the second section we present how it characterises the essential subspaces of certain restricted density matrices.

2.1 The von Neumann entropy and Gibbs states

In the first part of this section the definition of the von Neumann entropy is introduced, in the second subsection it is shown how this quantity can be used to give a variational condition for Gibbs states.

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[1] It was in fact von Neumann who advised the term "entropy" to Shannon saying:"You should call it entropy (...) nobody knows what entropy really is, so in a debate you will always have the advantage" [57].

2.1.1 The definition of the von Neumann entropy

Let $\mu : \mathbb{A} \to [0,1]$ be a probability measure on a finite set $\mathbb{A} = \{a_1, a_2, \ldots, a_d\}$ of d elements. A measure of the unsharpness of this probability distribution is the *Shannon entropy*, which is defined as[2]

$$S(\mu) := -\sum_{i=1}^{d} \mu(a_i) \log \mu(a_i).$$

There are many beautiful theorems that show the usefulness of this measure, we will just mention one of them. Suppose that a source produces L-long messages from the alphabet $\mathbb{A} = \{a_1, \ldots, a_d\}$, such that a letter a_i appears with probability $\mu(a_i)$. The number of possible messages is d^L. However, it turns out that for large L a typical sequence will be in a much smaller subspace of $\sim \exp(LS(\mu))$ number of elements, moreover, these typical sequences all have approximately the same probability $\sim \exp(-LS(\mu))$. More precisely, we can state the following theorem (a weak version of the Shannon-McMillan theorem [44]):[3]

Theorem. *Let μ be a probability measure on the finite set $\mathbb{A}$. For any $\epsilon > 0$ there exists an integer $L(\epsilon)$ such that for all $L \geq L(\epsilon)$ the $(1-\epsilon)$-entropy-typical subset $T^L_\epsilon \subset \mathbb{A}^{\times L}$:*

$$T^L_\epsilon := \{\, \underline{a} = (a_{i_1}, a_{i_2}, \ldots, a_{i_L}) \in \mathbb{A}^{\times L} \mid \mu^{\times L}(\, \underline{a}\,) \in (e^{-L(S(\mu)-\epsilon)}, e^{-L(S(\mu)+\epsilon)})\}$$

satisfies

$$\mu^{\times L}(T^L_\epsilon) \geq 1 - \epsilon\,,$$

and

$$|T^L_\epsilon| \in (e^{+L(S(\mu)-\epsilon)}, e^{+L(S(\mu)+\epsilon)})\,.$$

Since the set of eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_d\}$ of a d-dimensional density matrix ρ form a probability measure, one can also define the analogue of the Shannon

[2]Throughout the thesis "log" will denote the natural logarithm. However, it should be mentioned that in the information theoretical setting sometimes the base 2 logarithm is used in the defi nition of the Shannon and von Neumann entropies, relating to the the bit (and qubit) as the fundamental information unit.

[3]In this theorem $\mathbb{A}^{\times L}$ means the L-times Descartes product of the set $\mathbb{A}$, and $\mu^{\times L}$ the (L-times) product measure of μ on it.

entropy on them, called the *von Neumann entropy* of ρ:

$$S(\rho) := -\mathrm{Tr}\,\rho\log\rho = -\sum_{i=1}^{d}\lambda_i\log\lambda_i.$$

The von Neumann is in some sense a measure of the mixedness of the state belonging to ρ. When ρ is a projector the von Neumann entropy of ρ is 0, while for the density matrix $\frac{1}{d}\mathbb{1}$, which we regard as the most mixed state, the von Neumann entropy reaches its maximum value $\log d$, and if ρ_a is "more mixed" than ρ_b,[4] then $S(\rho_a) \geq S(\rho_b)$.

In this thesis we will be mainly interested in the von Neumann entropy of restricted density matrices of translation-invariant states. In subsection 2.2.1 we will discuss a theorem showing that for certain types of states the von Neumann entropy will characterise the dimension of an "essential subspace" where the density matrix is basically supported, in the same way as the Shannon entropy characterises the size of the set of typical sequences of random words. Before entering into these details, we present the more traditional role of the von Neumann entropy in quantum statistical mechanics in the next subsection.

2.1.2 The variational characterisation of Gibbs states

The von Neumann entropy appears naturally in quantum statistical mechanics, since it allows a variational characterisation of local Gibbs states and in some cases of limiting Gibbs states as well. The variational characterisation of local Gibbs states is straightforward, as we have the following theorem [13, 48]:

Theorem. *Let* $H(\mathbb{J})$ *be a local Hamiltonian, i.e. a selfadjoint element in* $\mathrm{CAR}(\ell^2(\mathbb{J}))$*. Let us define the following functional on the set of density matrices of* $\mathrm{CAR}(\ell^2(\mathbb{J}))$*:*

$$F_{\beta,\mu}(\rho) := \mathrm{Tr}\,(\rho\,(H(\mathbb{J}) - \mu N(\mathbb{J}))) - \beta^{-1}S(\rho).$$

This functional is called the local free energy functional at inverse temperature

[4] In the sense of the defi nition presented in subsection 1.1.1, or more precisely, by the analogous fi nite dimensional defi nition.

β and chemical potential μ corresponding to the local Hamiltonian $H(\mathbb{J})$. The unique density matrix that minimises the functional $F_{\beta,\mu}$ is the density matrix corresponding to the Gibbs state at inverse temperature β and chemical potential μ belonging to the local Hamiltonian $H(\mathbb{J})$.

For a similar characterisation of some limiting Gibbs states we need the notion of free energy density. Fortunately, the entropy and particle number densities exist for all translation-invariant states on $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ [7]:

Theorem. *Let ω be a translation-invariant state on $CAR(\ell^2(\mathbb{Z}^d))$. The limits*

$$\begin{aligned} s(\omega) &:= \lim_{L\to\infty} \frac{S\left(\rho^{\omega}_{[0,L-1]^d}\right)}{L^d}, \\ n(\omega) &:= \lim_{L\to\infty} \frac{\mathrm{Tr}\left(\rho^{\omega}_{[0,L-1]^d} N([0,L-1]^d)\right)}{L^d} \end{aligned}$$

exist and the quantities $s(\omega)$ and $n(\omega)$ are called the entropy and particle densities of the state ω, respectively.[5]

However, we do not have such a general theorem for the existence of the energy density for all kinds of translation-invariant interactions. Suppose we are given a Hamiltonian H corresponding to some translation-invariant interaction function. Let us define the following quantity for any density matrix ρ in $\mathrm{CAR}(\ell^2([K,L]^d))$

$$E_{[K,L]^d}(\rho) := \mathrm{Tr}\,\left(\rho H([K,L]^d)\right)\,,$$

which is called the local energy functional associated with the local Hamiltonian $H([K,L]^d)$. Suppose that for any translation-invariant state ω on $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ the

[5]Note, that we can use this "one-sided" defi nition due to translation-invariance, since the above limits equal the "two-sided" limits

$$\begin{aligned} s(\omega) &:= \lim_{L\to\infty} \frac{S\left(\rho^{\omega}_{[-L,L]^d}\right)}{(2L+1)^d}, \\ n(\omega) &:= \lim_{L\to\infty} \frac{\mathrm{Tr}\left(\rho^{\omega}_{[-L,L]^d} N([-L,L]^d)\right)}{(2L+1)^d}. \end{aligned}$$

limit

$$e(\omega) = \lim_{L\to\infty} \frac{E_{[0,L-1]^d}\left(\rho^{\omega}_{[0,L-1]^d}\right)}{L^d}$$

exists, which is called energy density functional of the Hamiltonian H. We can then define the *free energy density of* ω at inverse temperature β and chemical potential μ as:

$$f_{\beta,\mu}(\omega) = e(\omega) - \mu n(\omega) - \beta^{-1} s(\omega).$$

The translation-invariant states that minimise this functional, are called the *free-energy-density variational states*. For a large class of suitably tempered interactions satisfying some technical constraints (that are met for instance by the famous Hubbard model) it has been proved [7] that the free-energy-density variational states corresponding to these interactions are unique and equal to the corresponding limiting Gibbs states. This variational characterisation of Gibbs states may look of only academic interest, since we have little knowledge of the state space structure of CAR($\ell^2(\mathbb{Z}^d)$), and usually we can't find the free-energy-density variational state. However, this variational principle is also used in approximations. For example, for quasifree states we have a formula for the entropy density (see subsection 2.2.2) and the particle density [1] and for many interactions also the energy density can be calculated, and hence the quasifree state of the lowest free energy density can often be found. The state obtained in this way is then used in approximating the ground state (e.g. certain ground state expectation values). This method is called the (gauge- and translation-invariant) Hartree-Fock approximation.

2.2 The essential subspace of restricted density matrices and the zero-entropy-density conjecture

In this section a theorem and some conjectures about how the von Neumann entropy characterises the size of the essential subspaces of restricted density matrices of translation-invariant states are presented. We also discuss the so-called zero-entropy-density conjecture, and show in the second subsection that this conjecture holds for pure translation-invariant quasifree states.

2.2.1 Entropy growth and the essential subspace of restricted density matrices of ergodic states

Recently numerical studies have given birth to the physicist folklore that the restricted density matrices $\rho_{[0,L-1]^d}$ of translation-invariant states are essentially concentrated on a subspace of dimension of $\sim \exp(S(\rho_{[0,L-1]^d}))$. This has not only been observed in many numerical studies [43, 40, 50, 54], but is also used in numerical studies e.g. in DMRG studies.[6] In the rigorous setting, however, up to now there is only a proof for such a statement for *ergodic* states on quantum spin chains with non-vanishing entropy densities (which can also be used directly for the analogous inverse-Jordan-Wigner transformed fermionic states). This statement is the far reaching quantum generalisation of the classical Shannon-McMillan theorem (see [31, 10, 11] for different versions of the following theorem):

Theorem. *Let ω be an ergodic state on the quantum spin chain algebra $\mathcal{S}$, with restricted density matrices $\rho_L := \rho^{\omega}_{[0,L-1]}$, and entropy density s. For any $\epsilon > 0$ there exists an integer $L(\epsilon)$ such that for all $L \geq L(\epsilon)$ there exists an "$(1-\epsilon)$-essential-subspace projection" $P_{L,\epsilon}$ in the subalgebra $\mathcal{S}_L$ with the properties*

$$
\begin{aligned}
Tr\,(\rho_L P_{L,\epsilon}) &> 1-\epsilon, \\
Tr\,(P_{L,\epsilon}) &< 2^{L(s+\epsilon)}.
\end{aligned}
$$

Moreover, for all projections $P \in \mathcal{S}([0, L-1])$ with $Tr\,(P) < 2^{L(s-\epsilon)}$ we have $Tr\,(\rho_L P) < \epsilon$.
Letting ϵ go to zero, the above statements imply, that there exists a sequence of projections $P_L \in \mathcal{S}_L$ so that:

$$
\lim_{L\to\infty} \mathrm{Tr}(\rho_L P_L) = 1 \quad \textit{and} \quad \lim_{L\to\infty} \frac{\log(\mathrm{Tr}(P_L))}{L} = s,
$$

[6] In DMRG theory the von Neumann entropy is actually used to determine the needed subspace above the truncation-limit.[40]

and this statement is sharp in the sense that there does not exists a sequence of projections $P'_L \in \mathcal{S}_L$ so that:

$$\lim_{L\to\infty} \mathrm{Tr}(\rho_L P'_L) = 1 \quad \textit{and} \quad \lim_{L\to\infty} \frac{\log\left(\mathrm{Tr}(P'_L)\right)}{L} < s.$$

Hence for ergodic states with non-zero entropy density s, the restricted density matrices are supported asymptotically on subspaces with exponentially growing dimension, with a growth exponent of s since for large subsystems $L \cdot s \sim S(L)$ (when $s > 0$), the physicist folklore is supported in this case. However, in the case when $s = 0$, this theorem for ergodic states tells us only that the support grows slower than an exponential function and up to now there is no stronger rigorous statement. In physics the $s = 0$ case usually corresponds to the ground state of a Hamiltonian, which is in many cases a translation-invariant pure state. In the mathematical physics community it has been conjectured for a long time, that the entropy density should be zero for all translation-invariant states on the algebras $\mathrm{CAR}(\mathbb{Z})$. Every known example of translation-invariant pure state has zero entropy density, moreover, the pure states arising as ground states of local Hamiltonians showed at most a $S(\rho_{[0,L-1]^d}) \sim L^{d-1}\log L$ growth. This might suggest that there could be an even stricter restriction on the growth of the $S(\rho_{[0,L-1]^d})$ than that it is subvolume-like. This is, however, not the case. We will show in chapter 4 that the zero-entropy-density conjecture is sharp in the sense that for any function F_L growing slower than L^d, i.e. $\lim_{L\to\infty} F_L/L^d = 0$, there is a pure translation-invariant ω^F state on $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ for which $S(\rho^{\omega^F}_{[0,L-1]^d})$ is greater than F_L for large enough L.

In the next subsection we give a formula for the entropy density of quasifree state, which illustrates that for these states the zero-entropy-density conjecture is satisfied.

2.2.2 The entropy density of quasifree states

From subsection 1.2.4 we know that the restricted density matrix $\rho^{\omega_Q}_{\mathbb{J}}$ of a quasifree state ω_Q has the following form:

$$\rho_{\mathbb{J}}^{\omega_Q} = \prod_{i=1}^{|\mathbb{J}|} \left(q_i c_{(i)} c^*_{(i)} + (1-q_i) c^*_{(i)} c_{(i)} \right) ,$$

where $0 \le q_i \le 1$ are the eigenvalues of $Q_{\mathbb{J}}$, and the operators $c_{(i)}$ are defined in Eq. (1.7). By this definition, for any i, j the operators $(q_i c_{(i)} c^*_{(i)} + (1-q_i) c^*_{(i)} c_{(i)})$ and $(q_j c_{(j)} c^*_{(j)} + (1-q_j) c^*_{(j)} c_{(j)})$ commute, and the spectra of the operator $(q_i c_{(i)} c^*_{(i)} + (1-q_i) c^*_{(i)} c_{(i)})$ is $\{q_i, 1-q_i\}$, thus the $2^{|\mathbb{J}|}$ number of eigenvalues of $\rho_{\mathbb{J}}^{\omega_Q}$ are

$$E\left(\{n_i\}_{i\in\{1,\dots,|\mathbb{J}|\}}\right) = \prod_{i=1}^{|\mathbb{J}|} f_{n_i}(q_i),$$

where n_i can be 0 or 1 for any $i \in \{1, \dots, |\mathbb{J}|\}$, and $f_0(x) := x$ and $f_1(x) := 1 - x$. Hence the von Nemunann entropy of $\rho_{\mathbb{J}}^{\omega_Q}$ is:

$$S\left(\rho_{\mathbb{J}}^{\omega_Q}\right) = -\sum_{n_1=0}^{1} \cdots \sum_{n_{|\mathbb{J}|}=0}^{1} E\left(\{n_i\}_{i\in\{1,\dots,|\mathbb{J}|\}}\right) \log E\left(\{n_i\}_{i\in\{1,\dots,|\mathbb{J}|\}}\right) ,$$

or equivalently,

$$S\left(\rho_{\mathbb{J}}^{\omega_Q}\right) = -\mathrm{Tr}\ \left(Q_{\mathbb{J}} \log Q_{\mathbb{J}} + (\mathbb{1} - Q_{\mathbb{J}}) \log(\mathbb{1} - Q_{\mathbb{J}})\right) . \tag{2.1}$$

For the one-dimensional case, the entropy density can simply be calculated from Szegő's theorem, which states the following [1]:

Theorem. *Let T be such an operator on $\ell^2(\mathbb{Z})$ that its matrix in the $\{\chi_k\}_{k\in\mathbb{Z}}$ basis is a Toeplitz matrix, i.e., there exists an integrable function $\tilde{t}$ on the one-dimensional torus $\mathbb{T}$ parametrised by $[-\pi, \pi)$ so that*

$$T_{k,l} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta\ \tilde{t}(\theta) e^{-i(k-l)\theta} ,$$

where $T_{k,l} = \langle \chi_k, T\chi_L \rangle$, and let $\lambda_i(L)$ $(i \in \{1, \dots, L\})$ denote the the eigenvalues of the restricted operator $T_{[0,L-1]}$. For any continuous complex function f defined on *the (essential) range of $\tilde{\iota}$ the following holds*

$$\lim_{L\to\infty} \frac{\sum_{i=1}^{L} f(\lambda_i(L))}{L} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta f(\tilde{\iota}(\theta)).$$

By this theorem, the entropy density of a translation-invariant quasifree state ω_Q is:

$$\begin{aligned} s(\omega_Q) &= \lim_{L\to\infty} \frac{S\left(\rho_{[0,L-1]}^{\omega_Q}\right)}{L} \\ &= \lim_{L\to\infty} \frac{-\mathrm{Tr}\,\left(Q_{[0,L-1]} \log Q_{[0,L-1]} + (\mathbb{1} - Q_{[0,L-1]}) \log (\mathbb{1} - Q_{[0,L-1]})\right)}{L} \\ &= -\frac{1}{2\pi} \int_{\mathbb{T}} d\theta \, (\tilde{q}(\theta) \log \tilde{q}(\theta) + (1 - \tilde{q}(\theta)) \log(1 - \tilde{q}(\theta)))\,, \end{aligned}$$

where $\tilde{q}$ denotes the Fourier transform of the symbol Q.

The derivation of the d-dimensional case is more involved, the details can be found in [20], but the result is analogous: the entropy density of a translation-invariant quasifree state ω on CAR($\ell^2(\mathbb{Z}^d)$) is

$$s(\omega_Q) = -\frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} d\underline{\theta} \left(\tilde{q}(\underline{\theta}) \log \tilde{q}(\underline{\theta}) + (1 - \tilde{q}(\underline{\theta})) \log(1 - \tilde{q}(\underline{\theta}))\right), \qquad (2.2)$$

where $\tilde{q}(\underline{\theta})$ is the Fourier transform of the symbol of the state. For pure translation-invariant states, as we mentioned in subsection 1.2.4, $\tilde{q}$ is 0 or 1 almost everywhere, according to Eq.(2.2) this means, that their entropy density vanishes. Thus the zero-entropy-density conjecture holds for these pure states. Surprisingly enough, the zero-entropy-density conjecture cannot be improved even for this special class of states, as we will see in chapter 4.

Chapter 3

Lower bound for the entropy asymptotics of pure quasifree states

In this chapter we derive a lower bound for the entropy asymptotics of all nontrivial pure translation-invariant quasifree states on $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$. We prove that for these states the von Neumann entropy of a cubic subsystem with edge length L cannot grow slower than $cL^{d-1}\log L$ (for some positive constant c, which depends on the state). We also present numerical results for the one-dimensional case. Our results support the conjecture that when the Fermi sea of the pure one-dimensional quasifree state is composed of a finite n number of intervals, i.e., there are $2n$ number of Fermi points, the entropy grows asymptotically as $\frac{n}{3}\log L+\mathrm{const}$, which is consistent with the conformal field theoretical prediction.

The study of the von Neumann entropy asymptotics of pure translation-invariant states on fermionic and spin lattices was initiated in the mathematical and mathematical physics literature by the zero-entropy-density conjecture, which we discussed in the previous chapter (for relatively older papers, from the early 1990's, discussing entropy growth of pure states, see [22, 23]). In the physicist community the studies on these asymptotics began (at quite a high intensity) after the two papers [59, 39] by Vidal and his coworkers from 2003 and 2004, and the investigations usually concentrate on the pure ground states of certain Hamiltonians. We will summarise the numerical findings of the aforementioned two papers in this paragraph. Suppose we have a lattice

Hamiltonian corresponding to a finite ranged translation-invariant interaction function in which the local operators are taken into account with prefactors called coupling strengths, which will be the "parameters" of the Hamiltonian. If the expectation value of some observable in the limiting ground state depends non-analytically on this set of parameters, then we say that the system undergoes a *quantum phase transition*. In most cases that have been studied in the physics literature, at a quantum phase transition point some spin-spin or electron-electron correlations in the ground state decay algebraically with the distance (and the ground state is called critical), while at non-critical points the two-point correlations decay exponentially [53]. Vidal and coworkers studied the entropy asymptotics both for critical and non-critical pure ground states of quantum spin chain models. They found that in the studied critical cases the von Neumann entropy growth with the subsystem size is logarithmic, and the prefactor of the logarithmic growth is one-third of the central charge of the corresponding conformal field theory, while for non-critical ground states the entropy growth is bounded by a constant. There have also been many analytical studies supporting these findings [15, 33, 34, 36, 37]. The conformal field theoretical background of this behaviour has actually been derived much earlier [32] in a surprisingly different context, namely in the field of black hole thermodynamics. Owning to the recent interest in this subject this, conformal field theoretical derivation has been generalised and made more precise in the recent years [38, 14].

In the higher dimensional case there is no such direct connection between quantum criticality and entropy asymptotics. One of the first multidimensional models that were investigated numerically and analytically in this context were the different versions of the tight-binding fermion models with only hopping terms (the models discussed in section 1.4). The ground states of these models are quasifree states, and with certain restrictions on the Fermi sea structure a $L^{d-1}\log L$ type of entropy asymptotics was found [61, 27, 8]. In this chapter we will prove *without any restriction* on the Fermi sea structure (except for non-triviality) that this is a general lower bound, however, there exist quasifree states with much faster entropy asymptotics. For other (both for critical and non-critical) models studied in the physics literature, only a L^{d-1} type of asymptotics, a so-called "area law", was found [52, 8, 58]. Hence the connection between entropy asymptotics and quantum criticality is only limited to one-dimensional systems.

This chapter is divided into three sections. The first two sections constitute the part where we prove the mentioned lower bound for the von Neumann entropy asymptotics of any (non-trivial) pure translation-invariant quasifree state on CAR($\ell^2(\mathbb{Z}^d)$). We divided this part into two sections. The reason for this is that the proof in the one-dimensional case is relatively easy, but quite instructive, so the first section is devoted to this. The much harder proof for the multidimensional case is included in section 2. In the third section we present our numerical results for a set of special pure translation-invariant one-dimensional quasifree states. Our numerical results are in a complete agreement with the conformal field theoretic predictions, which we will also discuss. Our proofs for the lower bound appeared in the papers [24, 25], while the results of the numerical simulation were published partly in Ref. [19].

3.1 Lower bound in the one dimensional case

In this section we first present a lower estimate for the formula (2.1), which was introduced in [21], and which is only quadratic in the symbol Q and therefore easy to handle. Then, using this estimate, we prove in the second subsection that the entropy asymptotics for any (nontrivial) pure translation-invariant quasifree state on CAR($\ell^2(\mathbb{Z})$) is at least logarithmic.

3.1.1 A quadratic lower estimate

Let ω_Q be a pure translation-invariant quasifree state on the CAR($\ell^2(\mathbb{Z})$)-algebra. This means that Q is a projection on $\ell^2(\mathbb{Z})$, and there exists a measurable set $M \subset \mathbb{T}$ (we parametrise the one-dimensional torus $\mathbb{T}$ by $[-\pi, \pi)$, as usual) so that

$$Q_{k,l} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \; \Xi_M e^{-i(k-l)\theta},$$

where Ξ_M is the characteristic function of M. Let us introduce the notations: $S_L := S(\rho^{\omega_Q}_{[0,L-1]})$ and $Q_L := Q_{[0,L-1]}$. According to Eq. (2.1), S_L can be expressed as:

$$S_L = -\mathrm{Tr}\ (Q_L \log Q_L + (\mathbb{1} - Q_L)\log(\mathbb{1} - Q_L))\ .$$

In order to simplify further calculations we work with the following quadratic lower bound of S_L (introduced in [21]):

$$S_L \geq B_L := \mathrm{Tr}\ Q_L(\mathbb{1} - Q_L). \tag{3.1}$$

That B_L is indeed a lower bound of S_L can be simply proved by the aid of the inequality $x(1-x) \leq -x \ln x - (1-x)\ln(1-x)$, which holds for $0 \leq x \leq 1$.

Connected to this lower bound we will later need the following formulas:

$$B_L = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)}\Lambda_M(\theta), \tag{3.2}$$

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta\, \Lambda_M(\theta)\frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)}, \geq \frac{4L^2}{\pi^3}\int_{0}^{\pi/L} d\theta\, \Lambda_M(\theta), \tag{3.3}$$

$$\int_{0}^{\delta} d\theta\, \frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)} \geq c_1 L, \tag{3.4}$$

$$\int_{0}^{\delta} d\theta\, \theta\, \frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)} \geq c_2 \log L, \tag{3.5}$$

where c_1, c_2 are two positive numbers that depend on $0 < \delta < \pi/2$, and Λ_M is the function:

$$\Lambda_M(\theta) = |(M + \theta) \setminus M|, \tag{3.6}$$

here $|\cdot|$ denotes the Haar-Lebesgue measure, and $M + \theta$ denotes the image of M under a rotation by θ on $\mathbb{T}$. The derivation of the last three inequatilities (3.3)-(3.5) are straightforward (the reader is referred to [21]), while the tricky derivation of Eq. (3.2), presented also in [21], can be summarised (using that $Q_{k,l}$ is a Toeplitz matrix belonging to the characteristic function Ξ_K) in the following set of manipulations:

$$\begin{aligned}
\mathrm{Tr}\, Q_L(\mathbb{1} - Q_L) &= \sum_{k=0}^{L-1} Q_{k,k} - \sum_{k,l=0}^{L-1} |Q_{k,l}|^2 = LQ_{0,0} - L \sum_{k=-(L-1)}^{L-1} \left(1 - \frac{|k|}{L}\right) |Q_{k,0}|^2 \\
&= \frac{L}{2\pi} \int_{-\pi}^{\pi} d\theta_1\, \Xi_M(\theta_1) - \frac{L}{4\pi^2} \int_{-\pi}^{\pi} d\theta_1 \int_{-\pi}^{\pi} d\theta_2\, \Xi_M(\theta_1)\, \Xi_M(\theta_2) \sum_{k=-(L-1)}^{L-1} \frac{L-|k|}{L} e^{ik(\theta_1-\theta_2)} \\
&= \frac{L}{2\pi} \int_{-\pi}^{\pi} d\theta_1\, \Xi_M(\theta_1) - \frac{L}{4\pi^2} \int_{-\pi}^{\pi} d\theta_1 \int_{-\pi}^{\pi} d\theta_3\, \Xi_M(\theta_1)\, \Xi_M(\theta_1 - \theta_3) \frac{\sin^2(L\theta_3/2)}{L\,\sin^2(\theta_3/2)} \\
&= \frac{L}{4\pi^2} \int_{-\pi}^{\pi} d\theta_1 \int_{-\pi}^{\pi} d\theta_3\, \Xi_M(\theta_1)\, [1 - \Xi_M(\theta_1 - \theta_3)]\, \frac{\sin^2(L\theta_3/2)}{L\,\sin^2(\theta_3/2)} \\
&= \frac{1}{4\pi^2} \int_{-\pi}^{\pi} d\theta_3 \frac{\sin^2(L\theta_3/2)}{\sin^2(\theta_3/2)} \int_{-\pi}^{\pi} d\theta_1\, \Xi_M(\theta_1)\, [1 - \Xi_M(\theta_1 - \theta_3)] \\
&= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta_3 \frac{\sin^2(L\theta_3/2)}{\sin^2(\theta_3/2)} |M \setminus (M + \theta_3)|.
\end{aligned}$$

3.1.2 Lower bound for the entropy asymptotics

In the trivial cases, $|M| = 0$ or $|M| = |\mathbb{T}| = 1$, the entropy asymptotics function S_L is identically zero and, as we have mentioned in the introduction of this chapter, there are pure states with a finite, but bounded entropy asymptotics, and there are also pure states with logarithmic and faster than logarithmic entropy growth. However, interestingly, until now no pure translation-invariant state on the fermion or spin chain algebras have been found with a non-bounded sub-logarithmic growth, but up to now there is no proof for their non-existence. We will now prove that at least among the pure translation-invariant quasifree states there exists no such state.

Theorem. *Let ω_Q be a pure translation-invariant state on $CAR(\mathbb{Z})$ and $Q \notin \{0, \mathbb{1}\}$. Then there exists a positive constant c such that $S_L \geq c \log L$, where $S_L = S(\rho^{\omega_Q}_{[0,L-1]})$.*

Proof: Let the Fourier transform of $q(k) = Q_{k,0}$ be the characteristic function

Ξ_M of (the Fermi sea) $M \subset [-\pi, \pi)$. It is known from Lebesgue's density theorem that for any measurable set M, $|M| = |M_d|$ holds, where M_d denotes the set of the density points of M:

$$M_d = \left\{ x \in M \,\middle|\, \lim_{\delta \to 0} \frac{|(x-\delta, x+\delta) \cap M|}{2\delta} = 1 \right\}.$$

It can be inferred from this theorem that for any M of positive measure, there is such a point $x \in M$ that

$$\forall \epsilon > 0 : \ \exists \delta > 0 \ \text{ so that for every interval } I \text{ that satisfies } x \in I, \text{ and } |I| < \delta, \quad |M \cap I| > (1-\epsilon)|I|. \tag{3.7}$$

Disregarding the trivial cases (that is, the cases when $Q \in \{0, \mathbb{1}\}$), the measure of the complement $M^c := \mathbb{T} \setminus M$ is also positive. This means that M^c also has a point that satisfies (3.7). We denote this point by y. For a given ϵ, we can choose a common δ to x and y. Let I be an interval shorter than this δ: $|I| < \delta$, and $x \in I$. There is an integer n such that $y \in (I + n|I|)$. The set $(I + n|I|)$ can be assured to be disjoint from I by choosing a sufficiently small δ. The following inequalities hold for I:

$$|M \cap I| > (1-\epsilon)|I|, \qquad |M^c \cap (I + n|I|)| > (1-\epsilon)|I|. \tag{3.8}$$

The estimate on Λ_M (defined in Eq.(3.6)) below, though seemingly weak, is the core of the proof:

$$\begin{aligned}
\Lambda_M(|I|) &= |(M + |I|) \setminus M| \\
&\geq \left| \left(\bigcup_{k=1}^{n-1} (I + k|I|) \cap (M + |I|) \right) \setminus M \right| \\
&= \sum_{k=1}^{n-1} \Big| ((I + k|I|) \cap (M + |I|)) \setminus ((I + (k)|I|) \cap M) \Big| \\
&\geq \sum_{k=1}^{n-1} \Big(\big| ((I + k|I|) \cap (M + |I|)) \big| - \big| (I + k|I|) \cap M \big| \Big)
\end{aligned}$$

$$= \sum_{k=1}^{n-1} \left|((I + k|I|) \cap (M + |I|))\right| - \sum_{k=1}^{n-1} \left|(I + (k+1)|I|) \cap (M + |I|)\right|$$
$$= \left|I \cap M\right| - \left|(I + n|I|) \cap M\right|.$$

Having a look at (3.8), we obtain that for arbitrary positive ϵ,

$$\Lambda_M(|I|) \geq (1 - 2\epsilon)|I|$$

if $|I|$ is sufficiently small. Hence if we choose a fix $\epsilon < 1/2$ and define $\kappa := 1 - 2\epsilon > 0$, then there exists a $\delta > 0$ so that $\Lambda_M(\theta) \geq \kappa\theta$ for $0 \leq \theta \leq \delta$. Now, if we restrict the integration region to $[0, \delta]$ in the quadratic lower bound (3.2) for the entropy, and we use the just derived inequality for $\Lambda_M(\theta)$ together with (3.5), we can estimate the entropy asymptotics function as

$$S_L \geq B_L = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \Lambda_M(\theta) \frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)} \geq \frac{1}{2\pi} \int_{0}^{\delta} d\theta \Lambda_M(\theta) \frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)}$$
$$\geq \frac{1}{2\pi} \int_{0}^{\delta} d\theta\, \kappa\theta \frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)} \geq c \log L,$$

thus we arrived at the proposition stated in the theorem.

3.2 Lower bound in the d-dimensional case

We have seen in the previous section that all nontrivial pure translation-invariant quasifree states on CAR($\ell^2(\mathbb{Z})$) have at least a logarithmic entropy growth. Although the generalisation for arbitrary spatial dimension d is undoubtedly plausible (the conjectured result being a $L^{d-1} \log L$ lower bound), and it seems to be straightforward at first sight, the actual reasoning of the proof is much more involved and more care and other methods are to be used. This is due to the complicated spatial structure the Fermi seas might have in higher dimensions - compared with the one-dimensional case.

Let ω_Q be a pure translational-invariant quasifree state on CAR($\ell^2(\mathbb{Z}^d)$), and let the Fourier transform of $q(\underline{k}) = Q_{\underline{k},\underline{0}}$ be the characteristic function $\Xi_{\mathbb{M}}$ of the measurable set $\mathbb{M} \subset \mathbb{T}^d$, and let us again introduce the notation $S_L := S(\rho^{\omega_Q}_{[0,L-1]^d})$. The analogue of the one dimensional quadratic lower bound can again be used [61]:

$$S_L \geq \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} d\theta_1 \ldots \int_{-\pi}^{\pi} d\theta_d \, \Lambda_{\mathbb{M}}(\theta_1, \ldots \theta_d) \prod_{i=1}^{d} k_L(\theta_i). \tag{3.9}$$

The definitions of k_L and $\Lambda_{\mathbb{M}}$ are the following:

$$k_L(\theta) = \frac{\sin^2 L\theta/2}{\sin^2 \theta/2}, \quad \text{and} \quad \Lambda_{\mathbb{M}}(\underline{\theta}) = |\mathbb{M} \setminus \mathbb{M} + \underline{\theta}|,$$

where $|\cdot|$ again denotes the Lebesgue measure, and for any $\underline{\theta} = (\theta_1, \theta_2, \ldots \theta_d)$ $\mathbb{R}^d$-vector $\mathbb{M} + \underline{\theta}$ is the image of $\mathbb{M}$ under a translation of the points of the torus $\mathbb{T}^d = \times_{i=1}^d S^1$ defined by rotating the first S^1-factor by θ_1, the second S^1-factor by θ_2, and so on.

Theorem. *The entropy growth function $S_L := S(\rho^{\omega_Q}_{[0,L-1]^d})$ of the pure translation-invariant quasifree state ω_Q (with $Q \notin \{0, \mathbb{1}\}$) is bounded from below by $cL^{d-1}\log L$ for some $c > 0$ (which depends on Q).*

Proof:

We will use again the notation that $\Xi_{\mathbb{M}}$ is the Fourier transform of $q(\underline{k}) = Q_{\underline{k},\underline{0}}$. To be more transparent, the proof it is divided into four steps. In the first two steps some general properties of $\Lambda_{\mathbb{M}}$ are derived. Then putting these properties together, we obtain a lower bound for $\Lambda_{\mathbb{M}}$ in the third part, and by the aid of this, the proof can be easily completed in the fourth step.

1. Continuity and subadditivity of $\Lambda_{\mathbb{M}}$

The continuity of $\Lambda_{\mathbb{M}}$ can be proven from Stone's theorem (theorem A7 in Appendix A). According to this theorem the representation of the translations in $\mathcal{L}^2(\mathbb{T}^d)$ given by $(U_{\underline{\theta}}\,\psi)(\underline{\alpha}) := \psi(\underline{\theta} + \underline{\alpha})$ is continuous in the strong topology, hence in the weak topology as well (see theorem A6 in Appendix A). The difference $\Lambda_{\mathbb{M}}(\underline{\theta}_1) - \Lambda_{\mathbb{M}}(\underline{\theta}_2)$ can be written as:

$$\begin{aligned}
\Lambda_{\mathbb{M}}(\underline{\theta}_1) - \Lambda_{\mathbb{M}}(\underline{\theta}_2) &= \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} d\underline{\theta}\, \Xi_{\mathbb{M}}(\underline{\theta})(1 - \Xi_{\mathbb{M}}(\underline{\theta} + \underline{\theta}_1)) \\
&- \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} d\underline{\theta}\, \Xi_{\mathbb{M}}(\underline{\theta})(1 - \Xi_{\mathbb{M}}(\underline{\theta} + \underline{\theta}_2)) \\
&= \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} d\underline{\theta}\, \Xi_{\mathbb{M}}(\underline{\theta})(\Xi_{\mathbb{M}}(\underline{\theta} + \underline{\theta}_2) - \Xi_{\mathbb{M}}(\underline{\theta} + \underline{\theta}_1)) \\
&= \langle \Xi_{\mathbb{M}}, (U_{\underline{\theta}_2} - U_{\underline{\theta}_1})\Xi_{\mathbb{M}}\rangle.
\end{aligned}$$

Weak continuity of $U_{\underline{\theta}}$ implies that this expression goes to zero as $\underline{\theta}_1$ goes to $\underline{\theta}_2$, thus $\Lambda_{\mathbf{M}}$ is continuous.

Next, for any two translations $\underline{\theta}_1$ and $\underline{\theta}_2$ the following holds:

$$\mathbb{M} \setminus (\mathbb{M} + \underline{\theta}_1 + \underline{\theta}_2) \subset \left[\mathbb{M} \setminus (\mathbb{M} + \underline{\theta}_1)\right] \cup \left[(\mathbb{M} + \underline{\theta}_1) \setminus (\mathbb{M} + \underline{\theta}_1 + \underline{\theta}_2)\right].$$

By monotony and translational invariance of the Haar-Lebesgue measure on $\mathbb{T}^d$, we obtain the subadditivity property:

$$\Lambda_{\mathbb{M}}(\underline{\theta}_1 + \underline{\theta}_2) \le \Lambda_{\mathbb{M}}(\underline{\theta}_1) + \Lambda_{\mathbb{M}}(\underline{\theta}_2).$$

2. Irrelevant and relevant directions of $\Lambda_{\mathbb{M}}$

The subspace $\{a\underline{\theta} \mid a \in \mathbb{R}\}$ generated by a vector $\underline{\theta} \in \mathbb{R}^d$ is called an *irrelevant direction* (with respect to $\mathbb{M}$) if $\Lambda_{\mathbb{M}}(a\underline{\theta}) = 0$ for all $a \in \mathbb{R}$ (see Fig.3.2 on the next page), otherwise it is called a *relevant direction*. Subadditivity of $\Lambda_{\mathbb{M}}$ implies that vectors generating irrelevant directions form a vector space:

$$\Lambda_{\mathbb{M}}(a\underline{\theta}_1 + b\underline{\theta}_2) \le \Lambda_{\mathbb{M}}(a\underline{\theta}_1) + \Lambda_{\mathbb{M}}(b\underline{\theta}_2) = 0.$$

However, if $\underline{\theta}_1$ and $\underline{\theta}_2$ generate relevant directions, then a linear combination of $\underline{\theta}_1$ and $\underline{\theta}_2$ can generate either a relevant or an irrelevant direction.

It is easy to show that there exists at least one relevant direction of $\Lambda_{\mathbb{M}}$ if $\mathbb{M}$ is nontrivial (i.e., if $0 < |\mathbb{M}| < |\mathbb{T}^d|$). If all directions were irrelevant, then

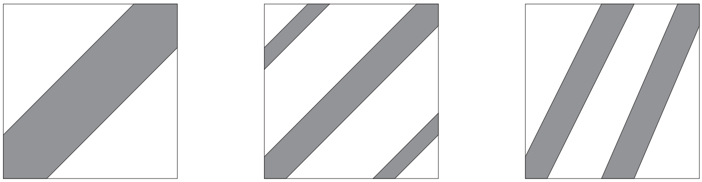

Figure 3.1: Three $\mathbb{M} \subset \mathbb{T}^2$ Fermi seas with irrelevant directions. (The two-dimensional torus $\mathbb{T}^2$ is represented as the square with opposites sides identifi ed.)

by definition, $\mathbb{M}$ would remain invariant (up to a zero measure set) under any translation. In this case one could define a translation-invariant measure μ on every Haar-Lebesgue measurable set $\mathbb{L}$ by the formula $\mu(\mathbb{L}) := |\mathbb{M} \cap \mathbb{L}|$. According to Haar's theorem, any translation-invariant measure on the torus is equal to the Haar-Lebesgue measure times a constant, i.e., $\mu(\mathbb{M}) = k|\mathbb{M}|$. If $k = 0$ then $|\mathbb{M}| = |\mathbb{M} \cap \mathbb{M}| = \mu(\mathbb{M}) = 0$, if $k > 0$, then $|\mathbb{T}^d| = \mu(\mathbb{T}^d)/k = |\mathbb{M} \cap \mathbb{T}^d|/k = |\mathbb{M} \cap \mathbb{M}|/k = \mu(\mathbb{M})/k = |\mathbb{M}|$.

Let $\underline{e}_i$ denote the ith standard unit vector of $\mathbb{R}^d$, $\underline{e}_1 = (1, 0, 0, \ldots 0)$, $\underline{e}_2 = (0, 1, 0, \ldots 0)$, etc. Vectors of the form $a\underline{e}_i$ act on the torus $\mathbb{T}^d = \times_{i=1}^d S^1$ by rotating only the ith S^1 factor and leaving the other S^1 factors invariant. We call the one-parameter subspaces of the form $\{a\underline{e}_i : a \in \mathbb{R}\}$ *principal directions*. It follows from the previous discussion that all principal directions cannot be irrelevant (if $\mathbb{M}$ is nontrivial). By a permutation of the S^1 factors, we can achieve that the first m ($m > 0$) standard unit vectors each generate a relevant direction, while the last $d - m$ generate irrelevant directions.

3. Lower bound for $\Lambda_{\mathbb{M}}$

First we show that for every fixed relevant direction there exists a linear lower bound for $\Lambda_{\mathbb{M}}$. Let $\underline{\theta}$ be a vector for which $\Lambda_{\mathbb{M}}(\underline{\theta}) > 0$. Continuity of $\Lambda_{\mathbb{M}}$ implies that there is an $\epsilon > 0$ and a $c > 0$ such that $\Lambda_{\mathbb{M}}(b\underline{\theta}) > c$ for any $1 - \epsilon \leq b \leq 1$. Let us denote by $\lfloor x \rfloor$ the "lower integer part" of x ($x \geq \lfloor x \rfloor$). Now, $1 - \epsilon \leq \lfloor 1/a \rfloor a \leq 1$ holds if $0 < a \leq \epsilon$. Using the subadditivity of $\Lambda_{\mathbb{M}}$, we obtain $c < \Lambda_{\mathbb{M}}(\lfloor 1/a \rfloor a\underline{\theta}) \leq \lfloor 1/a \rfloor \Lambda_{\mathbb{M}}(a\underline{\theta}) \leq \Lambda_{\mathbb{M}}(a\underline{\theta})/a$. Summarising, for any $\underline{\theta}$

that generates a relevant direction, there exist a $c > 0$ and an $\epsilon > 0$ so that

$$\Lambda_{\mathbb{M}}(a\underline{\theta}) > ca \quad \text{for } 0 < a < \epsilon.$$

However, this is not enough for an estimate of the integrand in (3.9), which is our goal. Next we have to show that there exists a sufficiently large set of relevant directions. As we have mentioned in the previous part of the proof, we can assume that the first m standard basis vectors $\{\underline{e}_i\}_{i=1}^m$ each generate a relevant direction. This does not mean that a linear combination of them also generates a relevant direction, but we can circumvent this problem by finding an m-dimensional subregion in which the positive linear combinations (positive cone) of vectors have this property.

If there is a (nonzero) vector $\underline{\theta}_{\{s_i\}_{i=1}^m}$ generating an irrelevant direction for all cones $\{\sum_{i=1}^m p_i(s_i\underline{e}_i) \mid p_i \geq 0\}$ determined by the choice of signs $\{s_i\}_{i=1}^m$ ($_i \in \{-1, 1\}$), then these irrelevant vectors $\underline{\theta}_{\{s_i\}_{i=1}^m}$ will linearly generate the whole $\mathbb{R}^m$ vector space spanned by the first m standard basis vectors $\underline{e}_i$, which contradicts the assumptions that $\{\underline{e}_i\}_{i=1}^m$ generate relevant directions. Therefore there is a choice of signs $\{s_i\}_{i=1}^m$ such that any vector in the compact set $V := \{(s_1p_1, s_2p_2, \ldots, s_mp_m, 0, \ldots, 0) \mid p_i \geq 0,\ \sum_i p_i^2 = 1\}$ generates a relevant direction.

For any relevant direction we have a linear lower bound for $\Lambda_{\mathbb{M}}$ if the translation is sufficiently small. Unfortunately, the prefactor and the validity region of the linear lower bound depend on the direction, so for a global lower bound of $\Lambda_{\mathbb{M}}$ we have to get rid of this direction dependence. For this purpose, let us consider the following function defined on V:

$$s(\underline{\vartheta}) := \sup\left\{ c \in \mathbb{R}^+ \mid \exists\epsilon > 0 \text{ so that } \Lambda_{\mathbb{M}}(a\underline{\vartheta}) \geq ca \text{ for any } 0 \leq a \leq \epsilon\right\}.$$

We show that if $s_- = \inf_{\underline{\vartheta}\in V} s(\underline{\vartheta}) = 0$, then there would exist an irrelevant generator in V in contradiction to its definition, therefore s_- is positive. Since V is compact, if $s_- = 0$ then there is a sequence $\{\underline{\vartheta}(n)\}_{n\in\mathbb{N}^+} \subset V$, which is convergent, and $\lim_{n\to\infty} s(\underline{\vartheta}(n)) = 0$. Let the limit of $\underline{\vartheta}(n)$ be $\underline{\vartheta}$. By subadditivity of $\Lambda_{\mathbb{M}}$ and the definition of the function s, for any positive integer k there is an index n_k so that

$\Lambda_{\mathbb{M}}(a\underline{\vartheta}(n_k)) < a/k$ for any a. By continuity of $\Lambda_{\mathbb{M}}$,

$$\Lambda_{\mathbb{M}}(a\underline{\vartheta}) = \lim_{k\to\infty} \Lambda_{\mathbb{M}}(a\underline{\vartheta}(n_k)) \leq \lim_{k\to\infty} \frac{a}{k} = 0.$$

Let $0 < \sigma < s_-$. It is important that σ is strictly smaller than s_-. We define a function on V (whose σ-dependence is suppressed because σ is fixed from now on):

$$\epsilon(\underline{\vartheta}) := \sup\left\{ \epsilon \mid \Lambda_{\mathbb{M}}(a\underline{\vartheta}) \geq \sigma a \text{ if } a \leq \epsilon \right\}.$$

We show that $\epsilon_- := \inf_{\underline{\vartheta}\in V} \epsilon(\underline{\vartheta}) > 0$. The argument is similar to the one we have just finished. Suppose the contrary. V is compact, so we have a convergent sequence $\{\underline{\vartheta}(n)\}_{n\in\mathbb{N}^+}$, with limit $\underline{\vartheta}$, such that $\lim_{n\to\infty} \epsilon(\underline{\vartheta}(n)) = 0$. Note that our choice $\sigma < s_-$ guarantees that ϵ is strictly positive on V. Continuity of $\Lambda_{\mathbb{M}}$ implies that $\Lambda_{\mathbb{M}}(\epsilon(\underline{\vartheta})\,\underline{\vartheta}) = \sigma\epsilon(\underline{\vartheta})$. Consequently,

$$\begin{aligned} \lim_{n\to\infty} \Lambda_{\mathbb{M}}\left(\left\lfloor \tfrac{a}{\epsilon(\underline{\vartheta}(n))} \right\rfloor \epsilon(\underline{\vartheta}(n))\,\underline{\vartheta}(n)\right) &\leq \lim_{n\to\infty} \left\lfloor \tfrac{a}{\epsilon(\underline{\vartheta}(n))} \right\rfloor \Lambda_{\mathbb{M}}\left(\epsilon(\underline{\vartheta}(n))\,\underline{\vartheta}(n)\right) \\ &= \lim_{n\to\infty} \left\lfloor \tfrac{a}{\epsilon(\underline{\vartheta}(n))} \right\rfloor \epsilon(\underline{\vartheta}(n))\sigma = \sigma a \end{aligned} \tag{3.10}$$

for any a. But $\lim_{n\to\infty}\lfloor a/\epsilon(\underline{\vartheta}(n))\rfloor\epsilon(\underline{\vartheta}(n))\,\underline{\vartheta}(n) = a\underline{\vartheta}$, and $\Lambda_{\mathbb{M}}(a\underline{\vartheta}) > \sigma a$ for some a (the latter inequality is strict, this is the point where our choice $\sigma < s_-$ comes into play again), which contradicts (3.10).

At last we arrived at the advertised lower bound for $\Lambda_{\mathbb{M}}$:

$$\Lambda_{\mathbb{M}}(\underline{\vartheta}) \geq \sigma \,\|\underline{\vartheta}\| \quad \text{if } \frac{\underline{\vartheta}}{\|\underline{\vartheta}\|} \in V, \text{ and } \|\underline{\vartheta}\| < \epsilon_-. \tag{3.11}$$

4. A lower bound for the entropy asymptotics

We can write the lower bound (3.9) as

$$
\begin{aligned}
S_L &\geq \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} d\theta_1 \ldots \int_{-\pi}^{\pi} d\theta_m \prod_{i=1}^{m} k_L(\theta_i) \Lambda_{\mathbb{M}}(P_R \underline{\theta}) \left(\int_{-\pi}^{\pi} d\theta_{m+1} \ldots \int_{-\pi}^{\pi} d\theta_d \prod_{i=d-m}^{d} k_L(\theta_i) \right) \\
&\geq \frac{L^{d-m}}{(2\pi)^m} \left| \int_0^{s_1 \epsilon_- / \sqrt{m}} d\theta_1 \ldots \int_0^{s_m \epsilon_- / \sqrt{m}} d\theta_m \, \sigma \, \| P_R \underline{\theta} \| \right| \\
&\geq \frac{L^{d-m}}{(2\pi)^m} \sigma \int_0^{\epsilon_- / \sqrt{m}} d\theta_1 \ldots \int_0^{\epsilon_- / \sqrt{m}} d\theta_m \, \theta_1 \prod_{i=1}^{m} k_L(\theta_i) \\
&\geq c L^{d-1} \log L.
\end{aligned}
$$

In the first inequality we simply used the fact that the irrelevant translations alter $\mathbb{M}$ only by a zero measure set, so in the argument of $\Lambda_{\mathbb{M}}$ the last $d-m$ components can be set to zero (P_R is the standard projection from $\mathbb{R}^d = \mathbb{R}^m \times \mathbb{R}^{d-m}$ to the subspace $\mathbb{R}^m$ generated by the first m standard unit vectors), and the integrations over the irrelevant principal directions can be pulled out. Next, these integrals were performed, and the integration region was shrunk into a hypercube where the lower bound (3.11) can be applied. Then we replaced the Euclidean norm of $P_R \underline{\theta}$ with its first component. Finally, using the inequalities (3.4) and (3.5) the proof is completed (with some constant $c > 0$).

3.3 Numerical results

In this section some numerical results for the entropy asymptotics of pure translation-invariant quasifree states on one-dimensional fermion systems are presented. Calculating the von Neumann entropy asymptotics of states on quantum spin or fermionic chains is usually a very hard numerical problem, even if the restricted density matrices of the subsystems (subchains) are known. It is so because one has to diagonalise a $2^L \times 2^L$ dimensional density matrix to obtain

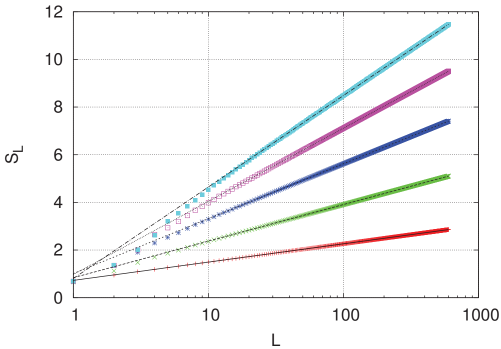

Figure 3.2: Numerically calculated von Neumann entropy of restricted density matrices of different pure translational-invariant quasifree states as a function of the subsystem size L (in a logarithmic scale). The red points belong to the case of 2 Fermi points situated at $\{-\pi/2, \pi/2\} \in [-\pi, \pi)$, the green points to the case of 4 Fermi points at $\{-\pi/, 0, \pi/4, \pi/2\}$, the blue points to the case of 6 Fermi points at $\{-3\pi/4, -\pi/4, 0, \pi/4, \pi/2, 3\pi/4\}$, the purple points to the case of 8 Fermi points at $\{-3\pi/4, -\pi/2, -\pi/4, 0, \pi/4, \pi/2, 3\pi/4, 7\pi/8\}$, and finally the cyan coloured points belong to the case of 10 Fermi points situated at $\{-7\pi/8, -3\pi/4, -\pi/2, -\pi/4, 0, \pi/8, \pi/4, \pi/2, 3\pi/4, 7\pi/8\}$. Straight lines were fitted on the numerically calculated entropies of subsystems as a function of $\log L$, i.e., of the form $S_L = a \log L + b$. The obtained fit parameters have the following values (the subscript indicates the number of Fermi points): $a_2 = 0.333333952$, $b_2 = 0.726063128$; $a_4 = 0.666694765$, $b_4 = 0.837985960$; $a_6 = 1.000055552$, $b_6 = 1.012651221$; $a_8 = 1.333474220$, $b_8 = 0.972334872$; $a_{10} = 1.666963228$, $b_{10} = 0.806282809$.

the entropy belonging to a subchain of length L. Hence only the entropy of small subsystems can be calculated.[1] In the quasifree case, however, we are faced with an exponentially easier numerical problem, since the entropy of a density matrix belonging to a subchain of length L can be obtained by finding the eigenvalues of only an $L \times L$ matrix (the $Q_{[0,L-1]}$ matrix), due to Eq. (2.1).

We will consider the special case of one-dimensional pure translation-invariant quasifree states ω_Q for which the the Fourier transform of $q(k) = Q_{k,0}$ is (almost

[1] It is even very hard to store with a given precision a general state of e.g. 50 spins (or a state of fermions on a lattice of 50 sites).

everywhere) equal to the characteristic function of a set $M \subset \mathbb{T}$ which is the union of finitely many disjoint closed intervals. In the physicist terminology (described in subsection 1.2.4) one would say that the Fermi sea is composed of a finite number of intervals, or that there is a finite number of Fermi points. If M is such a set belonging to the symbol Q, then its complement M^c belongs to the symbol $\mathbb{1} - Q$. From Eq. (2.1) we can infer that the entropy asymptotics of the state ω_Q is equal to the asymptotics of $\omega_{(\mathbb{1}-Q)}$. This means in this case that only the locations of the Fermi points are important.

The states described in the previous paragraph arise for instance as ground states of tight binding models with only finite ranged hopping terms. This was discussed in subsection 1.4.2. In the conformal field theoretical language, the central charge for such a tight binding fermion model is equal to one-half times the number of "fermionic soft modes" (the zero crossings of the spectral function $f(\theta) := (\tilde{t}(\theta) - \mu)$ defined in subsection 1.4.2) [37], i.e., one-half times the number of Fermi points. Let $2n$ denote the number of Fermi points. The conformal field theoretical derivation [14, 38], would then suggest a $\frac{n}{3} \log L + const$ entropy asymptotics. Our numerical results[2] shown in Fig.3.3 are in complete agreement with the conformal field theoretical predictions.

Based on these numerical results (and the conformal field theoretic predictions) one can state the following conjecture for these one-dimensional pure quasifree states:

Conjecture. *Let ω_Q be such a pure translation-invariant quasifree state on $CAR(\ell^2(\mathbb{Z}))$ for which the Fourier transform of the function $q(k) = Q_{k,0}$ is (almost everywhere) equal to the characteristic function of n disjoint closed intervals. Then*

$$\lim_{L\to\infty} \frac{S\left(\rho^{\omega_Q}_{[0,L-1]}\right)}{\log L} = \frac{n}{3},$$

[2]These numerical observations were partially made when we investigated in [19] an extension of the XX model (introduced in [2]). During the completion of this article also analytical works appeared [36, 37] where the same results were obtained, but only for symmetrically placed Fermi points on the interval $(-\pi, \pi)$.

and that the follwoing limits exists:

$$\lim_{L\to\infty}\left(S\left(\rho^{\omega_Q}_{[0,L-1]}\right)-\frac{n}{3}\log L\right).$$

Chapter 4

Sharpness of the zero-entropy-density conjecture

As mentioned in previous chapters, it is a natural and long-standing conjecture in mathematical quantum statistical physics that the entropy density for all translation-invariant pure states on $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ vanishes. However, until now mathematicians and physicists have not succeeded in finding a proof (or a counter example) for this conjecture. The pure states appearing in the physics literature had at most a $L^{d-1}\log L$ entropy growth [59, 61, 27]. Based on these observations one could think that even a stronger restriction applies to general translation-invariant pure states than the conjectured subvolume-like asymptotics. In [21] Fannes, Haegeman, and Mosonyi tried to push the entropy asymptotics of such states to the limits, and were able to find for any $\alpha \in (0, 1)$ a one-dimensional pure translation-invariant quasifree state for which the entropy growth S_L is faster than L^α. They conjectured that there are pure translation-invariant states with even faster entropy asymptotics, e.g. $L/\log L$, and that the zero-entropy-conjecture cannot be sharpened in the sense that arbitrary fast sublinear entropy asymptotics might be reached.[1] We will prove exactly this type of sharpness of the zero-entropy-conjecture in this chapter. For any sub-L^d function F_L,[2] we will find a

[1]However, they believed that their quadratic lower estimate (3.1) for the entropy asymptotics of quasifree states might not be efficient enough for fi nding such states. But in fact in proving their conjecture this quadratic estimate will be sufficient.

[2]That is for any F_L satisfying $\lim_{L\to\infty} F_L/L^d = 0$.

pure translation-invariant quasifree state on CAR($\ell^2(\mathbb{Z}^d)$) with a faster entropy asymptotics than F_L. The theorems presented in this chapter were published in our papers [24, 25].

4.1 Proof for the sharpness of the zero-entropy-density conjecture

We will first prove the sharpness of the zero-entropy-density conjecture for the one-dimensional case. The extension to the multidimensional is trivial.

The pure translation-invariant quasifree states leading to the L^α-type entropy asymptotics considered in the paper by Fannes et al [21] had Fermi seas with a "thick Cantor set"-like structure. Our starting point for choosing the Fermi seas will be the numerical observation presented in the previous chapter. As we showed numerically, for Fermi seas consisting of finite number of intervals on $[-\pi, \pi)$, the entropy asymptotics increases with the number of intervals which the Fermis seas are composed. Hence our idea was to consider Fermi seas consisting of an *infinite* number of intervals (with decreasing length).

Theorem. *For any function $f\colon \mathbb{N} \to \mathbb{R}^+$ which is sublinear ($\lim_{L\to\infty} f_L/L = 0$), there exists a pure translation-invariant quasifree state for which S_L is bounded from below by f_L, that is, $S_L \geq f_L$ for every sufficiently large L.*

Proof: Our proof will be based again on the quadratic lower bound (3.1), and the inequality (3.3). Using this inequality, we reduce the problem to showing the existence of a set $M \subset [-\pi, \pi)$ for which the right hand side of (3.3) grows not slower than the given f_L as L goes to infinity.

The construction of the Fermi sea M is based on two non-negative sequences: a sequence of integers $(n_i)_{i\in\mathbb{N}}$ and another one of real numbers $(\ell_i)_{i\in\mathbb{N}}$, where $\ell_i \geq 2\ell_{i+1}$. Let M be the union of infinitely many disjoint intervals, the endpoints of which are determined by these two sequences as below:

$$\begin{aligned} M = \bigcup_{i\in\mathbb{N}} \bigcup_{k=1}^{n_i} I_i^k, \quad I_i^k = [a_i^k, b_i^k], \quad b_i^k - a_i^k = \ell_i; \\ a_0^1 = 0; \quad a_i^1 = b_{i-1}^{n_{i-1}} + \ell_{i-1}, \quad \text{if } i > 0; \\ a_i^k = b_i^{k-1} + \ell_i, \quad \text{if } k > 1. \end{aligned} \tag{4.1}$$

The $(\ell_i)_{i\in\mathbb{N}}$ and $(n_i)_{i\in\mathbb{N}}$ are chosen so that the set M constructed above is bounded, and for convenience, we suppose additionally that $n_i\ell_i$ is monotonically decreasing, and:

$$\sum_{i=0}^{\infty} n_i\ell_i < \frac{\pi}{2}.$$

Thus $M \subset [0, \pi)$. With construction (4.1), Λ_M takes the form

$$\Lambda_M(\theta) = \sum_{i=0}^{\infty} \sum_{k=1}^{n_i} \left|(I_i^k + \theta) \setminus M\right| \geq \sum_{i=i_\theta}^{\infty} \sum_{k=1}^{n_i} \left|(I_i^k + \theta) \setminus K\right|,$$

where i_θ is the smallest index for which $2n_i\ell_i < \theta$ for all $i \geq i_\theta$. Each translated interval $(I_i^k + \theta)$ with $i \geq i_\theta$ is situated in a region where the original intervals in the construction of M and the gaps between them are not longer than $\ell_i/2$ (or where M has no point at all). For this reason $|(I_i^k + \theta) \setminus M| \geq \ell_i/3$ for every term in the last summation. Therefore we obtain

$$\Lambda_M(\theta) \geq \frac{1}{3} \sum_{i=i_\theta}^{\infty} n_i\ell_i.$$

Now, let f_L be an arbitrary sublinear function, i.e. $\lim_{L\to\infty} f_L/L = 0$. Obviously, there exists a monotonically increasing continuously differentiable function $g\colon [0, \pi] \to \mathbb{R}^+$ with the properties:

$$g(0) = 0, \qquad \frac{4}{\pi^2} g\left(\frac{\pi}{L}\right) \geq \frac{f_L}{L}.$$

Let us define the function h as $h(x) = \frac{d}{dx}(xg(x))$. h is continuous, and $h(0) = 0$. We suppose that h is strictly monotonically increasing in the neighbourhood of zero. If not, we choose a continuous, strictly monotonically increasing $\hat{h}$ such that

$\hat{h} \geq h$, and $\hat{h}(0) = 0$.[3] This $\hat{h}$ can be derived from a $\hat{g}$ for which $\hat{g} \geq g$, and then the argument can be continued with $\hat{h}$ instead of h.

The next step is to specify $(n_i)_{i\in\mathbb{L}}$ and $(\ell_i)_{i\in\mathbb{L}}$ so that

$$\Lambda_M(\theta) \geq h(\theta) \geq \frac{1}{3}\sum_{i=i_\theta}^{\infty} n_i\ell_i \tag{4.2}$$

should hold for sufficiently small θ.

Let s_i be the solution of the following recursive equation, starting from a given s_0 $(0 < s_0 < \pi)$:

$$h\left(6(s_i - s_{i+1})\right) = s_{i+1}. \tag{4.3}$$

It is clear from the required properties of h that there is a solution that satisfies the equalities $0 \leq s_{i+1} \leq s_i$ for every i. Since $(s_i)_{i\in\mathbb{N}}$ is bounded from below and monotonically decreasing, it has a limit at infinity. Suppose that this limit differs from zero, say it is $s_\infty > 0$. Taking an arbitrary small $\epsilon > 0$, there is an i for which $\epsilon > 6(s_i - s_{i+1})$, and we find that $h(\epsilon) \geq h(6(s_i - s_{i+1})) = s_{i+1} \geq s_\infty$ for any ϵ, so $h(0) \geq s_\infty$ in contradiction with $h(0) = 0$. Thus $\lim_{i\to\infty} s_i = 0$.

Now we are ready to specify the values of ℓ_i and n_i by the equation

$$s_i = \frac{1}{3}\sum_{j=i}^{\infty} n_j\ell_j \tag{4.4}$$

Considering that $(s_i)_{i\in\mathbb{N}}$ is a monotonically decreasing sequence tending to zero, these equalities can be satisfied by some series $(n_i)_{i\in\mathbb{N}}$ and $(\ell_i)_{i\in\mathbb{N}}$. Starting with a particular ℓ_i, we can always determine the next term by choosing some $\ell_{i+1} \leq \ell_i/2$. The only restriction on the choice of ℓ_i is that $s_i - s_{i+1}$ should be an integral multiple of ℓ_i. This requirement can undoubtedly be met, and then $s_i - s_{i+1} = \frac{1}{3}n_i\ell_i$ yields the value of n_i. The inclusion $M \subset [0, \pi)$ can be assured by choosing sufficiently small s_0.

Recall that $(n_i\ell_i)_{i\in\mathbb{N}}$ has been required to be monotonic. We can easily convince ourselves that $(n_i\ell_i)_{i\in\mathbb{N}}$ constructed from $(s_i)_{i\in\mathbb{N}}$ has this property. Indeed, it follows immediately from the strict monotonicity of h: $h(2n_i\ell_i) = h(6(s_i - s_{i+1})) = s_{i+1} \leq$

[3] A possible choice is $\hat{h}(x) := \max\{h(y) \mid y \in [0, x]\} + x$.

$s_i = h(6(s_{i-1} - s_i)) = h(2n_{i-1}\ell_{i-1})$.

Monotonicity of $(s_i)_{i\in\mathbb{N}}$ and its behaviour at infinity entail that for any θ below a certain bound, there is an index i for which $6(s_i - s_{i+1}) \leq \theta \leq 6(s_{i-1} - s_i)$. Notice that this index is nothing but i_θ. Thus putting together (4.3), and (4.4), we arrive at the desired estimate (4.2). Consequently, for sufficiently large L, in the region of the integration in (3.3), $\Lambda_M(\theta) \geq h(\theta)$ holds. Performing the integration in (3.3) completes the proof:

$$S_L \geq B_L \geq \frac{4L^2}{\pi^3}\int_0^{\frac{\pi}{L}} \Lambda_M(\theta)d\theta \geq \frac{4L^2}{\pi^3}\int_0^{\frac{\pi}{L}} h(\theta)d\theta =$$

$$\frac{4L^2}{\pi^3}\int_0^{\frac{\pi}{L}} \frac{d}{d\theta}(\theta g(\theta))d\theta = \frac{4L}{\pi^2}g\left(\frac{\pi}{L}\right) \geq f_L.$$

As we mentioned at the beginning of this section, the higher dimensional version of this sharpness result is a simple consequence of the one-dimensional proof.

Theorem. *Let $F : \mathbb{N} \to \mathbb{R}^+$ be a function that satisfies $\lim_{L\to\infty} F_L/L^d = 0$. There exists a pure quasi-free state such that $S_L \geq F_L$ for sufficiently large L.*

Proof: Let us define the function $f_L := F_L/L^{d-1}$. This satisfies $\lim_{L\to\infty} f_L/L = 0$. In the previous proof we showed that for every such f_L there exists an $M \in [-\pi, \pi)$ satisfying the following inequality for sufficiently large L:

$$\frac{4L^2}{\pi^3}\int_0^{\frac{\pi}{L}} \Lambda_M(\theta)d\theta \geq f_L \tag{4.5}$$

Let us define the following (Fermi sea or) measurable subset of $[-\pi, \pi)^d$: $\mathbb{M} = \times_{i=1}^{d-1}[-\pi, \pi)\times M$, and let the inverse Fourier transform of the characteristic function $\Xi_{\mathbb{M}}$ define the Toeplitz operator Q on $\ell^2(\mathbb{Z}^d)$. Then the quadratic lower bound for the quasifree state ω_Q simplifies to

$$
\begin{aligned}
S_L &\geq \frac{1}{(2\pi)^d}\left(\int_{-\pi}^{\pi} d\theta' \,\frac{\sin^2(L\theta'/2)}{\sin^2(\theta'/2)}\right)^{d-1} \int_{-\pi}^{\pi} d\theta \,\frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)})\, \Lambda_M(\theta) \\
&= \frac{L^{d-1}}{2\pi}\int_{-\pi}^{\pi} d\theta \,\frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)}\, \Lambda_M(\theta).
\end{aligned}
$$

Restricting the integration region and using (3.3) and (4.5), we obtain for sufficiently large L the final inequality:

$$
\begin{aligned}
S_L &\geq \frac{L^{d-1}}{2\pi}\int_{0}^{\pi/L} d\theta \,\frac{\sin^2(L\theta/2)}{\sin^2(\theta/2)}\, \Lambda_M(\theta) \\
&\geq L^{d-1}\frac{4L^2}{\pi^3}\int_{0}^{\pi/L} d\theta \,\Lambda_M(\theta) \geq \frac{4L^d}{\pi^2} g\left(\frac{\pi}{L}\right) \geq L^{d-1} f_L = F_L.
\end{aligned}
$$

Chapter 5

Conclusion and Outlook

The aim of the present thesis was to study the von Neumann entropy asymptotics of translation-invariant quasifree states of fermions on d-dimensional lattices. It is known that the entropy density for such states is zero. However, the long-standing question whether the entropy-asymptotics of *all* pure translation-invariant state is subvolume-like, that is, whether they have a vanishing entropy density, is still unanswered. We showed that if the above mentioned zero-entropy-density conjecture is true, then it cannot be sharpened in the sense that for any sub-L^d function F_L there exists a pure translation-invariant quasifree state with a faster entropy asymptotics than F_L. Another natural question that arises in this context is whether there exists for any monotonically increasing sub-L^d function G_L a pure translation-invariant state on $\mathrm{CAR}(\ell^2(\mathbb{Z}^d))$ with an entropy asymptotics S_L such that $\lim_{L\to\infty} \frac{S_L}{G_L} = c$, where $c > 0$ (or even more strictly, $c = 1$). We showed that at least in the case of pure translation-invariant quasifree states the answer is negative. We proved that for pure quasifree states the entropy growth is either identically 0, or at least as fast as $c\,L^{d-1}\log L$. Moreover, the numerical data presented in the third chapter for one-dimensional pure quasifree states with a finite $2n$ number of Fermi points suggest a $(\frac{n}{3}\log L + const)$-type of asymptotics, in agreement with the conformal field theoretical calculations. Based on these results and other results presented in the literature, one might conjecture that the entropy asymptotics of the ground state of a d-dimensional lattice Hamiltonian corresponding to translation-invariant local interactions respects a kind of area law, i.e., asymptotically it is aL^{d-1} ($a \geq 0$) or it violates this law by a logarithmic factor at most ($cL^{d-1}\log L$). This conjecture and the zero-entropy-density conjecture are two important unsolved problems in this field.

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Appendix A

Hilbert spaces and bounded operators on Hilbert spaces

In this appendix we collect some basic definitions and theorems about Hilbert spaces and about bounded operators on Hilbert spaces in order to make this thesis more self-contained. For a monograph on this subject, see [12].

A.1 Hilbert spaces

A Euclidean space $\mathcal{E}$ is a vector space endowed with a scalar product i.e., with a function $\langle\cdot,\cdot\rangle_{\mathcal{E}} : \mathcal{E}\times\mathcal{E} \to \mathcal{E}$ satisfying the following properties

(i) Sesquilinearity:[1]
$\langle a_1\psi_1+a_2\psi_2\, ,\, b_1\varphi_1+b_2\varphi_2\rangle_{\mathcal{E}} = \overline{a}_1 b_1 \langle\psi_1,\varphi_1\rangle_{\mathcal{E}}+\overline{a}_1 b_2 \langle\psi_1,\varphi_2\rangle_{\mathcal{E}}+\overline{a}_2 b_1 \langle\psi_2,\varphi_1\rangle_{\mathcal{E}}+ \overline{a}_2 b_2 \langle\psi_2,\varphi_2\rangle_{\mathcal{E}}$, holds for all $\psi_1,\psi_2,\varphi_1,\varphi_2 \in \mathcal{E}$, and for all $a_1,a_2,b_1,b_2 \in \mathbb{C}$.

(ii) Positivity:
$\langle\psi,\psi\rangle_{\mathcal{E}} \geq 0$, holds for all $\psi \in \mathcal{E}$, and $\langle\psi,\psi\rangle_{\mathcal{E}} = 0$ if and only if $\psi = 0$.

Using the above axioms we obtain that the inequality

$$0 \leq \langle\psi + z\varphi, \psi + z\varphi\rangle_{\mathcal{E}} = \langle\psi,\psi\rangle_{\mathcal{E}} + z\,\langle\psi,\varphi\rangle_{\mathcal{E}} + \overline{z}\,\langle\varphi,\psi\rangle_{\mathcal{E}} + |z|^2\,\langle\varphi,\varphi\rangle_{\mathcal{E}}$$

[1]In the mathematical literature, sesquilinearity is usually defi ned the other way around: $\langle a_1\psi_1 + a_2\psi_2\, ,\, b_1\varphi_1 + b_2\varphi_2\rangle_{\mathcal{E}} = a_1\overline{b}_1\,\langle\psi_1,\varphi_1\rangle_{\mathcal{E}} + a_1\overline{b}_2\,\langle\psi_1,\varphi_2\rangle_{\mathcal{E}} + a_2\overline{b}_1\,\langle\psi_2,\varphi_1\rangle_{\mathcal{E}} + a_2\overline{b}_2\,\langle\psi_2,\varphi_2\rangle_{\mathcal{E}}$, but in this thesis we follow the physicist convention.

is true for any two vectors $\psi, \varphi \in \mathcal{E}$ and complex number z. The necessary and sufficient conditions for this quadratic expression in z to be nonnegative are

$$\langle\psi,\varphi\rangle_{\mathcal{E}} = \overline{\langle\varphi,\psi\rangle}_{\mathcal{E}} \tag{A.1}$$
$$|\langle\psi,\varphi\rangle_{\mathcal{E}}| \leq \langle\psi,\psi\rangle_{\mathcal{E}}\,\langle\varphi,\varphi\rangle_{\mathcal{E}}, \tag{A.2}$$

which hold thus for all $\varphi, \psi \in \mathcal{E}$. Eq. (A.1) is the so-called *Hermiticity property* of the scalar product, while (A.2) is called the *Cauchy-Schwarz inequality*. Now we can define a norm on $\mathcal{E}$:

$$||\psi||_{\mathcal{E}} := \sqrt{\langle\psi,\psi\rangle_{\mathcal{E}}}$$

Using the axioms of the scalar product and the Cauchy-Schwarz inequality, one can easily show that the properties

(i) $||\psi||_{\mathcal{E}} \geq 0$, and $||\psi||_{\mathcal{E}} = 0$ if and only if $\psi = 0$,

(ii) $||z\psi||_{\mathcal{E}} = |z|\,||\psi||_{\mathcal{E}}$,

(iii) $||\psi + \varphi||_{\mathcal{E}} \leq ||\psi||_{\mathcal{E}} + ||\varphi||_{\mathcal{E}}$,

are satisfied for all $\psi, \varphi \in \mathcal{H}$ and $z \in \mathbb{C}$.

A Euclidean space which is complete under the norm, that is, for which all Cauchy sequences have a limit in the norm, is called a *Hilbert space*.[2] Let $\mathcal{H}$ be a Hilbert space, a set of vectors $\{\phi_i\}_{i\in\mathbb{I}}$ in $\mathcal{H}$ satisfying the properties

(i) $\langle\phi_i,\phi_j\rangle_{\mathcal{H}} = \delta_{i,j}$ for all $i, j \in \mathbb{I}$,

(ii) the set $\{\sum_{j\in\mathbb{J}} a_j\phi_j \mid a_j \in \mathbb{C}, \mathbb{J} \subset \mathbb{I}, |\mathbb{J}| < \infty\}$ is dense in $\mathcal{H}$ (in the topology induced by the norm $||\cdot||_{\mathcal{H}}$),

is called an *orthonormal basis* of $\mathcal{H}$.

[2] A sequence of vectors $\{\psi_i\}_{i\in\mathbb{N}^+}$ has a limit in the norm $||\cdot||_{\mathcal{E}}$, if there exists a vector ψ such that $\lim_{i\to\infty} ||\psi_i - \psi||_{\mathcal{E}} = 0$. A sequence of vectors $\{\psi_i\}_{i\in\mathbb{N}^+}$ is said to be a *Cauchy sequence* under the norm $||\cdot||_{\mathcal{E}}$, if for every $\epsilon > 0$ there exists an integer $i(\epsilon)$ such that for any $n, m \geq i(\epsilon)$: $||\psi_n - \psi_m||_{\mathcal{E}} \leq \epsilon$.

Theorem A 1. *Let $\mathcal{H}$ be a Hilbert space. There exists an orthonormal basis in $\mathcal{H}$, every orthonormal basis in $\mathcal{H}$ has the same cardinality, any vector $\psi \in \mathcal{H}$ can be expanded in any orthonormal basis $\{\phi_i\}_{i\in\mathbb{I}}$, i.e.*

$$\psi = \sum_{i\in\mathbb{I}} z_i\phi_i, \quad \text{where} \quad z_i = \langle\phi_i, \psi\rangle,$$

and $\|\psi\|_{\mathcal{H}} = \sqrt{\sum_{i\in\mathbb{I}} |z_i|^2}$.[3]

The cardinality of an orthonormal basis in a Hilbert space $\mathcal{H}$ is called the dimension of $\mathcal{H}$. A Hilbert space $\mathcal{H}$ is *separable* if its dimension is finite or countably infinite.

The N-dimensional complex vector space $\mathbb{C}^N$ with the canonical scalar product

$$\langle(a_1, a_2, \ldots, a_N), (b_1, b_2, \ldots, b_N)\rangle_{\mathbb{C}^n} := \sum_{i=1}^{N} \overline{a}_i\, b_i, \quad \forall a_i, b_i \in \mathbb{C}, \tag{A.3}$$

is an N-dimensional Hilbert space. The linear space of square-summable functions on $\mathbb{Z}^d$

$$\ell^2(\mathbb{Z}^d) := \left\{ \xi : \mathbb{Z}^d \to \mathbb{C} \;\middle|\; \sum_{\underline{k}\in\mathbb{Z}^d} |\xi(\underline{k})|^2 < \infty \right\},$$

equipped with the scalar product

$$\langle\, \{\xi_{\underline{k}}\}_{\underline{k}\in\mathbb{Z}^d} \,,\, \{\zeta_{\underline{k}}\}_{\underline{k}\in\mathbb{Z}^d} \,\rangle_{\ell^2(\mathbb{Z}^d)} := \sum_{\underline{k}\in\mathbb{Z}^d} \overline{\xi}_{\underline{k}}\, \zeta_{\underline{k}} \tag{A.4}$$

forms also a Hilbert space. The set of characteristic functions of one-point sets of $\mathbb{Z}^d$, i.e. the set $\{\chi_{\underline{k}}\}_{\underline{k}\in\mathbb{Z}^d}$ (where $\chi_{\underline{k}}(\underline{m}) := \delta_{\underline{k},\underline{m}}$), is an orthonormal basis of $\ell^2(\mathbb{Z}^d)$. Similarly, let us consider the vector space of (Lebesgue-equivalence classes of) square-integrable functions on the d-dimensional torus $\mathbb{T}^d$, parametrised by

[3] More precisely, it can be proved for any Hilbert space $\mathcal{H}$ that only for a countable subset of indices does $z_i = \langle\phi_i, \psi\rangle$ not vanish. Let us denote this subset by $\mathbb{K}$. For any bijection $b : \mathbb{N}^+ \to \mathbb{K}$, let us defi ne $\psi_n^b := \sum_{l=1}^{n} z_{b(l)}\phi_{b(l)}$, then for any bijection b the sequence ψ_n^b converges to ψ in the norm $\|\cdot\|_{\mathcal{H}}$.

$[-\pi,\pi)^d$:

$$\mathcal{L}^2(\mathbb{T}^d) := \left\{ f : \mathbb{T}^d \to \mathbb{C} \;\middle|\; \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} d\theta_1 \ldots \int_{-\pi}^{\pi} d\theta_d \, |f(\theta_1, \theta_2, \ldots, \theta_d)|^2 < \infty \right\},$$

where f is identified with its equivalence class modulo the relation of equality almost everywhere.[4] This vector space endowed with the scalar product

$$\langle f, g \rangle_{\mathcal{L}^2(\mathbb{T}^d)} := \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} d\theta_1 \ldots \int_{-\pi}^{\pi} d\theta_d \, \overline{f}(\theta_1, \theta_2, \ldots, \theta_d)\, g(\theta_1, \theta_2, \ldots, \theta_d)$$

is also a separable Hilbert space. For every $\underline{k} \in \mathbb{Z}^d$ let us consider the square-integrable functions $f_{\underline{k}}(\underline{\theta}) := e^{i\underline{k}\cdot\underline{\theta}}$, where $\underline{\theta} = (\theta_1, \theta_2, \ldots, \theta_d) \in [-\pi, \pi)^d$, the set of these functions $\{f_{\underline{k}}\}_{\underline{k}\in\mathbb{Z}^d}$ forms an orthonormal basis of $\mathcal{L}(\mathbb{T}^d)$.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces, a vector space isomorphism $U : \mathcal{H}_1 \to \mathcal{H}_2$ satisfying the property

$$\langle U\psi, U\varphi \rangle_{\mathcal{H}_2} = \langle \psi, \varphi \rangle_{\mathcal{H}_1}, \quad \forall \psi, \varphi \in \mathcal{H}_1,$$

is called a *unitary map*. Two Hilbert spaces are isomorphic if there exists a unitary map between them. The unique linear map $\mathcal{F}_d : \ell^2(\mathbb{Z}^d) \to \mathcal{L}^2(\mathbb{T}^d)$ defined by the property

$$\mathcal{F}_d(\chi_{\underline{k}}) := f_{\underline{k}}$$

is a unitary map called the *Fourier transformation*. Hence $\ell^2(\mathbb{Z}^d)$ and $\mathcal{L}^2(\mathbb{T}^d)$ are isomorphic Hilbert spaces. Since any isometric bijection between two orthonormal bases can be extended uniquely to a unitary map, we have the following theorem:

Theorem A 2. *Any N dimensional Hilbert space is isomorphic to $\mathbb{C}^N$ (endowed with the scalar product* (A.3)*), and any infinite dimensional separable Hilbert space is isomorphic to $\ell^2(\mathbb{Z})$ (with the scalar product* (A.4)*).*

---

[4]Here $\int_{-\pi}^{\pi} d\theta_i/(2\pi)$ denotes the integration with respect to the Haar-Lebesgue measure on the ith $\mathbb{T}$-factor of $\mathbb{T}^d$.

We end this subsection by the Riesz representation theorem:

Theorem A 3. *Let $\mathcal{H}$ be a Hilbert space, and let $g : \mathcal{H} \to \mathbb{C}$ be a continuous*[5] *linear function. Then there exists a unique vector φ_g such that*

$$g(\psi) = \langle \varphi_g, \psi \rangle_{\mathcal{H}},$$

for all $\psi \in \mathcal{H}$, moreover,

$$\left\|\varphi_g\right\|_{\mathcal{H}} = \sup_{\psi \in \mathcal{H} \setminus \{0\}} \frac{|g(\psi)|}{\|\psi\|_{\mathcal{H}}}.$$

A.2 Bounded operators on Hilbert spaces

In this subsection a Hilbert space will always mean a separable Hilbert space. Let $\mathcal{H}$ be a Hilbert space, a linear mapping $A : \mathcal{H} \to \mathcal{H}$ is called *bounded* if the quantity

$$\|A\|_{\mathcal{B}(\mathcal{H})} := \sup_{\psi \in \mathcal{H} \setminus \{0\}} \frac{\|A\psi\|_{\mathcal{H}}}{\|\psi\|_{\mathcal{H}}} \tag{A.5}$$

is bounded. A linear mapping $A : \mathcal{H} \to \mathcal{H}$ is continuous (with respect to the Hilbert space norm $\|\cdot\|_{\mathcal{H}}$) if and only if A is bounded. The set of bounded linear operators (mappings) on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$, and for every $c_1, c_2 \in \mathbb{C}$ and $A, B \in \mathcal{B}(\mathcal{H})$ both $c_1 A + c_2 B$ and $AB := A \circ B$ are bounded. The bounded linear operator $\mathbb{1}_{\mathcal{H}}$, defined by the property

$$\mathbb{1}_{\mathcal{H}}\psi := \psi \quad \forall \psi \in \mathcal{H},$$

is called the *unit operator* on $\mathcal{H}$. The function $\|\cdot\|_{\mathcal{B}(\mathcal{H})} : \mathcal{B}(\mathcal{H}) \to \mathbb{R}$, defined by Eq. (A.5), satisfies the properties

(i) $\|A\|_{\mathcal{B}(\mathcal{H})} \geq 0$, and $\|A\|_{\mathcal{B}(\mathcal{H})} = 0$ if and only if $A = 0$,

(ii) $\|c\,A\|_{\mathcal{B}(\mathcal{H})} = |c|\,\|A\|_{\mathcal{B}(\mathcal{H})}$,

(iii) $\|A + B\|_{\mathcal{B}(\mathcal{H})} \leq \|A\|_{\mathcal{B}(\mathcal{H})} + \|B\|_{\mathcal{B}(\mathcal{H})}$,

[5]Continuous with respect to the topologies defi ned by the norms $|\cdot|$ on $\mathbb{C}$, and $\|\cdot\|_H$ on $\mathcal{H}$.

for all $A, B \in \mathcal{B}(\mathcal{H})$ and $c \in \mathbb{C}$, and $\|\cdot\|_{\mathcal{B}(\mathcal{H})}$ is called the *operator norm* on $\mathcal{B}(\mathcal{H})$. $\mathcal{B}(\mathcal{H})$ is closed under this norm, and for all $A, B \in \mathcal{B}(\mathcal{H})$

$$\|AB\|_{\mathcal{B}(\mathcal{H})} \leq \|A\|_{\mathcal{B}(\mathcal{H})} \|B\|_{\mathcal{B}(\mathcal{H})} .$$

Theorem A 4. *For any bounded linear operator A on $\mathcal{H}$, there exists a bounded linear operator $A^\dagger$ on $\mathcal{H}$ such that*

$$\langle \varphi, A\psi \rangle_{\mathcal{H}} = \langle A^\dagger \varphi, \psi \rangle_{\mathcal{H}},$$

for all $\varphi, \psi \in \mathcal{H}$. $A^\dagger$ is called the adjoint or Hermitian conjugate of A.

The *Hermitian conjugation* (as a $\mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ mapping) satisfies the following properties:

(i) $(A^\dagger)^\dagger = A$,

(ii) $(aA + bB)^\dagger = \overline{a}A^\dagger + \overline{b}B^\dagger$,

(iii) $(AB)^\dagger = B^\dagger A^\dagger$,

(iv) $\left\|A^\dagger A\right\|_{\mathcal{B}(\mathcal{H})} = \|A\|^2_{\mathcal{B}(\mathcal{H})}$,

for all $A, B \in \mathcal{B}(\mathcal{H})$ and all $a, b \in \mathbb{C}$.

An operator $U : \mathcal{H} \to \mathcal{H}$ is unitary if and only if $U \in \mathcal{B}(\mathcal{H})$ and $U^\dagger U = UU^\dagger = \mathbb{1}_{\mathcal{H}}$. If $U : \mathcal{H}_1 \to \mathcal{H}_2$ is a unitary operator, then the map defined for all $A \in \mathcal{B}(\mathcal{H}_1)$ as $\alpha_U(A) := UAU^{-1}$ is a linear bijection between $\mathcal{B}(\mathcal{H}_1)$ and $\mathcal{B}(\mathcal{H}_2)$, and satisfies the following properties

(i) $\alpha_U(AB) = \alpha_U(A)\alpha_U(B)$,

(ii) $\alpha_U(A^\dagger) = (\alpha_U(A))^\dagger$

(iii) $\|\alpha_U(A)\|_{\mathcal{B}(\mathcal{H}_2)} = \|A\|_{\mathcal{B}(\mathcal{H}_1)}$

for all $A, B \in \mathcal{B}(\mathcal{H}_1)$.

In particular, considering the Fourier transform $\mathcal{F}_d$ between $\ell^2(\mathbb{Z}^d)$ and $\mathcal{L}^2(\mathbb{T}^d)$, the function $\alpha_{\mathcal{F}_d}$ maps $\mathcal{B}(\ell^2(\mathbb{Z}^d))$ to $\mathcal{B}(\mathcal{L}^2(\mathbb{T}^d))$. An operator $T \in \mathcal{B}(\ell^2(\mathbb{Z}^d))$ is called a Toeplitz operator, if there exists a sequence $\{\varphi^T(\underline{k})\}_{\underline{k}\in\mathbb{Z}^d} \in \ell^2(\mathbb{Z}^d)$ such that

$$T_{\underline{k},\underline{l}} := \varphi^T(\underline{k}-\underline{l}),$$

for all $\underline{k},\underline{l} \in \mathbb{Z}^d$, where $T_{\underline{k},\underline{l}} := \langle \chi_{\underline{k}}, T\chi_{\underline{l}}\rangle_{\ell^2(\mathbb{Z}^d)}$. An operator $F \in \mathcal{B}(\mathcal{L}^2(\mathbb{T}^d))$ is called a multiplication operator, if there exists a function $g^F \in \mathcal{L}^2(\mathbb{T}^d)$ such that

$$F\, f(\underline{\theta}) = g^F(\underline{\theta}) f(\underline{\theta})$$

holds for all $f \in \mathcal{L}^2(\mathbb{T}^d)$ (and the equality is meant, as usual, for almost every $\underline{\theta} \in \mathbb{T}^d$). The function $\alpha_{\mathcal{F}_d}$ maps the Toeplitz operators on $\ell^2(\mathbb{Z}^d)$ onto the multiplication operators on $\mathcal{L}^2(\mathbb{T}^d)$ in the following way:

$$\alpha_{\mathcal{F}_d}(T) = F \quad \text{if and only if } \mathcal{F}_d(\varphi^T) = g^F. \tag{A.6}$$

Next we introduce the following three terms for elements of $\mathcal{B}(\mathcal{H})$ with some special properties: $S \in \mathcal{B}(\mathcal{H})$ is called *self-adjoint* if it satisfies $S = S^\dagger$, a self-adjoint operator $P \in \mathcal{B}(\mathcal{H})$ satisfying also $P = P^2$ is called a *projection*, an operator $A \in \mathcal{B}(\mathcal{H})$ for which $(\psi, A\psi) \geq 0$ holds for any $\psi \in \mathcal{H}$ is called a *positive operator*.

Any positive operator is self-adjoint, and for any $B \in \mathcal{B}(\mathcal{H})$, $B^\dagger B$ is positive. For any positive operator $A \in \mathcal{B}(\mathcal{H})$, there exists a unique positive operator $\mathrm{Sq}(A) \in \mathcal{B}(\mathcal{H})$ such that $A = (\mathrm{Sq}(A))^2$. $\mathrm{Sq}(A)$ is called the the *square root* of A, and we will use the notation $A^{1/2}$:=$\mathrm{Sq}(A)$. For any $A \in \mathcal{B}(\mathcal{H})$ we define the *absolute value* of A, as the positive operator $|A| := (A^\dagger A)^{1/2}$.

Let $\{\phi\}_{i\in\mathbb{I}}$ be an orthonormal basis of $\mathcal{H}$, for a bounded operator A on $\mathcal{H}$ the value of the series

$$\sum_{i\in\mathbb{I}} \langle \phi_i,\, |A|\, \phi_i\rangle_{\mathcal{H}} \tag{A.7}$$

is independent of the orthonormal basis, but can be infinite. If the series (A.7) is finite, then the series

$$\mathrm{Tr}\,(A) := \sum_{i\in\mathbb{I}} \langle \phi_i, A\phi_i\rangle_{\mathcal{H}} \tag{A.8}$$

is also finite, absolute convergent, and independent of the orthonormal basis. Such an A , for which the series (A.7) is finite, is said to be *trace class* operator, and the quantity (A.8) is called the *trace* of A. The set of trace class operators is denoted by $\mathcal{T}(\mathcal{H})$, and it is a linear subspace of $\mathcal{B}(\mathcal{H})$. Moreover, for any $A \in \mathcal{T}(\mathcal{H})$ and $B \in \mathcal{B}(\mathcal{H})$ the operators AB and BA are also trace class operators, i.e., $\mathcal{T}(\mathcal{H})$ is a (two-sided) ideal in $\mathcal{B}(\mathcal{H})$. The trace (as a mapping) is a linear functional on $\mathcal{T}(\mathcal{H})$ and satisfies the following properties as well:

(i) $\mathrm{Tr}\,(A^\dagger A) \geq 0, \quad \forall A \in \mathcal{T}(\mathcal{H}),$

(ii) $\mathrm{Tr}\,(AB) = \mathrm{Tr}\,(BA), \quad \forall A \in \mathcal{T}(\mathcal{H}),\ \forall B \in \mathcal{B}(\mathcal{H}).$

For any projection $P \in \mathcal{T}(\mathcal{H})$ with $\mathrm{Tr}\,(P) = 1$, there exists a unit vector $\psi_P \in \mathcal{H}$, which is unique up to a complex phase, such that:

$$P\psi = \varphi_P \langle \varphi_P, \psi \rangle_{\mathcal{H}}, \quad \forall \psi \in \mathcal{H}.$$

If for an $A \in \mathcal{B}(\mathcal{H})$ and a $\psi \in \mathcal{H}$

$$A\psi = \lambda\,\psi,$$

holds for some $\lambda \in \mathbb{C}$, then ψ is called an *eigenvector* of A belonging to the *eigenvalue* λ. Let $\{\lambda_i^T\}_{i\in\mathbb{I}}$ denote the eigenvalues of a self-adjoint trace class operator T on $\mathcal{H}$. The eigenvalues of T are then real, and for any non-zero eigenvalue λ_i^T, the eigenvectors belonging to λ_i^T form a finite-dimensional sub-Hilbert space of $\mathcal{H}$, which is called the *eigensubspace* of T belonging to the eigenvalue λ_i^T. Let d_i be the dimension of this eigensubspace, and let $\{\phi_k^{(i)}\}_{k\in\{1,\ldots,d_i\}}$ be an orthonormal basis of this eigensubspace. Then the eigenvalue λ_i^T is called a d_i-fold degenerate eigenvalue of T, and we can define the projection P_i belonging to this subspace by

$$P_i\,\psi := \sum_{k=1}^{d_i} \phi_k^{(i)} \langle \phi_k^{(i)}, \psi \rangle_{\mathcal{H}}\,, \quad \forall \psi \in \mathcal{H},$$

where P_i is independent of the choice of the orthonormal basis $\{\phi_k^{(i)}\}_{k\in\{1,\ldots,d_i\}}$. Moreover, the following equality, as a convergence in the operator norm, holds:

$$T = \sum_{i\in\mathbb{I}} \lambda_i P_i. \tag{A.9}$$

The series (A.9) is called the *discrete spectral decomposition* of the self-adjoint trace class operator T.

The Hilbert-Schmidt operators form a subset of $\mathcal{B}(\mathcal{H})$, which is slighlty broader than $\mathcal{T}(\mathcal{H})$. These operators play an important role in the classification of pure quasifree states generating inequivalent irreducible representations. Let $\{\phi\}_{i\in\mathbb{I}}$ be an orthonormal basis in $\mathcal{H}$ and $A \in \mathcal{B}(\mathcal{H})$, if

$$\sum_{i\in I} ||A\phi_i||_{\mathcal{H}} < \infty \tag{A.10}$$

holds, then A is called a *Hilbert-Schmidt operator*, and in this case the value of the left hand side of (A.10) is independent of the choice of the orthonormal basis, and the square root of this quantity is called the *Hilbert-Schmidt norm*.

Theorem A 5. *The set of all Hilbert-Schmidt operators $O_{HS}(\mathcal{H})$ in $\mathcal{B}(\mathcal{H})$ form self-adjoint (two-sided) ideal in $\mathcal{B}(\mathcal{H})$ which is complete under the Hilbert-Schmidt norm. Moreover, the product of two Hilbert-Schmidt operators is a trace class operator, and the subspace of Hilbert-Schmidt operators itself is a Hilbert space with the scalar product defined as:*

$$\langle A, B\rangle_{O_{HS}(\mathcal{H})} := Tr\,(A^\dagger B) \qquad \forall\ A, B \in O_{HS}(\mathcal{H}).$$

Now we turn to discuss different topologies on $\mathcal{B}(\mathcal{H})$. We have already got acquainted with the operator norm topology on $\mathcal{B}(\mathcal{H})$, the open sets in this topology are generated from the finite intersections and arbitrary unions of the sets (defined for all $A \in \mathcal{B}(\mathcal{H})$ and all $\epsilon \in \mathbb{R}^+$)

$$\mathcal{V}_n(A, \epsilon) := \{B \in \mathcal{B}(\mathcal{H}) \mid ||B - A||_{\mathcal{B}(\mathcal{H})} < \epsilon\},$$

and a sequence $\{\mathcal{A}_n\}_{n\in\mathbb{N}^+}$ converges to A in the operator norm topology if

$$\lim_{n\to\infty} \|A_n - A\|_{\mathcal{B}(\mathcal{H})} = 0.$$

In the theory of operator algebras and in quantum physics other topologies play important roles, too. In this thesis we have only mentioned two other topologies: the *strong* and the *weak topology*. The open sets of the strong topology are generated from the finite intersections and arbitrary unions of the sets (defined for all $A \in \mathcal{B}(\mathcal{H})$ and all $\psi \in \mathcal{H}$)

$$\mathcal{V}_s(A,\psi) := \{B \in \mathcal{B}(\mathcal{H}) \mid \|(B-A)\psi\|_{\mathcal{H}} < 1\}.$$

Hence a sequence $\{\mathcal{A}_n\}_{n\in\mathbb{N}^+}$ converges to A in the strong topology if

$$\lim_{n\to\infty} \|(A_n - A)\psi\|_{\mathcal{H}} = 0$$

holds for all $\psi \in \mathcal{H}$.

The open sets of the weak topology are generated from the finite intersections and arbitrary unions of the sets (defined for all $A \in \mathcal{B}(\mathcal{H})$ and all $\psi, \varphi \in \mathcal{H}$)

$$\mathcal{V}_w(A,\psi,\varphi) := \{B \in \mathcal{B}(\mathcal{H}) \mid |\langle \varphi, (B-A)\psi\rangle_{\mathcal{H}}| < 1\}.$$

Hence a sequence $\{\mathcal{A}_n\}_{n\in\mathbb{N}^+}$ converges to A in the weak topology if

$$\lim_{n\to\infty} \langle \varphi, A_n\psi\rangle_{\mathcal{H}} = \langle \varphi, A\psi\rangle_{\mathcal{H}}$$

holds for all $\psi, \varphi \in \mathcal{H}$.

These topologies are not equivalent. Let $\{\phi\}_{i\in\mathbb{N}^+}$ be an orthonormal basis of the infinite dimensional separable Hilbert space $\mathcal{H}$, and let us define for any $n \in \mathbb{N}$ the operator S_n as

$$S_n\phi_i := \begin{cases} 0 & \text{if } i \leq n \\ \phi_{i-n} & \text{if } i > n \end{cases}.$$

The sequence $\{S_n\}_{n\in\mathbb{N}}$ converges to 0 in the weak and in the strong topologies, but it does not converge in the operator norm topology. Now, let us consider the sequence of the Hermitian conjugates of S_n, which act on the basis elements as:

$$S_n^\dagger \phi_i = \phi_{i+n}.$$

The sequence $\{S_n^\dagger\}_{n\in\mathbb{N}}$ converges in the weak topology to 0, but it doesn't converge in the operator norm topology and in the strong topology.

The following important, although easy, theorem relates the three mentioned topologies on $\mathcal{B}(\mathcal{H})$ to each other.

Theorem A 6. *If a subset $O_1 \subset \mathcal{B}(\mathcal{H})$ is open in the weak operator topology, then it is open in the strong and the norm topology as well. If a subset $O_2 \subset \mathcal{B}(\mathcal{H})$ is open in the strong topology, then it is also open in the norm topology.*

Hence if a sequence of operators converges in the operator norm topology, it converges also in the strong and weak topologies; if a sequence converges in the strong topology, then it converges also in the weak topology.

More generally, let S be a set with a fixed topology. If a function $F : S \to \mathcal{B}(\mathcal{H})$ is continuous with respect to the operator norm topology on $\mathcal{B}(\mathcal{H})$, then it is continuous with respect to the strong and weak topologies on $\mathcal{B}(\mathcal{H})$. If a function $G : S \to \mathcal{B}(\mathcal{H})$ is continuous with respect to the strong topology, then it is continuous also in the weak topology.[6]

An important function, which is *not* continuous in the norm topology, is the function $U : \mathbb{T}^d \to \mathcal{B}(\mathcal{L}^2(\mathbb{T}^d))$ describing the group of translations, defined as:

$$\left(U(\underline{\theta})\psi\right)(\underline{\alpha}) := \psi(\underline{\theta} + \underline{\alpha}), \qquad \underline{\theta}, \underline{\alpha} \in \mathbb{T}^d, \ \forall \psi \in \mathcal{L}^2(\mathbb{T}^d). \tag{A.11}$$

Although this function is not continuous in the operator norm topology, we have the following theorem (called Stone's theorem)

Theorem A 7. *The group of translations $U : \mathbb{T}^d \to \mathcal{B}(\mathcal{L}^2(\mathbb{T}^d))$, defined by Eq.* (A.11) *is continuous in the strong topology.*

[6] Also the following holds: if a function $f : \mathcal{B}(\mathcal{H}) \to S$ is continuous with respect to the weak topology on $\mathcal{B}(\mathcal{H})$, then it is continuous in the strong and norm topologies; if a function $g : \mathcal{B}(\mathcal{H}) \to S$ is continuous with respect to the strong topology, it is continuous in the norm topology also.

Appendix B

Abstract C*-algebras

In this appendix we give a short introduction to the theory of C*-algebras and their representations. For useful monographs on this subject, see [4, 12, 16]

B.1 Definitions and basic examples

A $*$-*algebra* is an algebra $\mathcal{A}$ with an involution, i.e. with a map $* : \mathcal{A} \to \mathcal{A}$ satisfying the following properties:

(i) $(A^*)^* = A$,

(ii) $(z_1 A + z_2 B)^* = \bar{z}_1 A^* + \bar{z}_2 B^*$,

(iii) $(AB)^* = B^* A^*$,

for all $A, B \in \mathcal{A}$ and all $z_1, z_2 \in \mathbb{C}$. A C^*-*algebra* is a $*$-algebra $\mathcal{A}$ endowed with a norm $\|\cdot\|_{\mathcal{A}} : \mathcal{A} \to \mathcal{A}$ such that

(i) $\mathcal{A}$ is complete with respect to the norm $\|\cdot\|_{\mathcal{A}}$,

(ii) $\|AB\|_{\mathcal{A}} \leq \|A\|_{\mathcal{A}} \|B\|_{\mathcal{A}} \quad \forall A, B \in \mathcal{A}$,

(iii) $\|A^* A\|_{\mathcal{A}} = \|A\|^2_{\mathcal{A}} \quad \forall A \in \mathcal{A}$.

Let $\mathcal{A}$ be a C*-algebra. Any subalgebra of $\mathcal{A}$ which is invariant under the $*$-operation and closed in the operator norm is again a C*-algebra (with the restricted structures), and such a subalgebra is called a C*-subalgebra of $\mathcal{A}$. An $\mathcal{I}$ subalgebra of $\mathcal{A}$ is called a two-sided *ideal* of $\mathcal{A}$ if for any $A \in \mathcal{A}$ and any $I \in \mathcal{I}$ it holds that $AI, IA \in \mathcal{I}$. A C*-algebra that does not contain any two-sided ideal which is closed under the norm is called *simple*. A *C*-algebra* is *unital* if there exists an element $\mathbb{1}$ so that $\mathbb{1}A = A\mathbb{1} = A$ for all $A \in \mathcal{A}$, in this case $\mathbb{1}$ is called the *unit* of $\mathcal{A}$, and one can easily prove the uniqness of such an element. If the C*-algebra $\mathcal{A}$ is not unital, then one can *adjoin a unit* to it by extending $\mathcal{A}$ in a natural way. The new extended C*-algebra $\widetilde{\mathcal{A}}$ is $\mathbb{C} \oplus \mathcal{A}$ as a vector space. Introducing the notation: $z\mathbb{1} + A := z \oplus A$ (and $\mathbb{C}\mathbb{1} + \mathcal{A} := \widetilde{\mathcal{A}}$), the $*$-operation, the algebra product, and the norm is defined in the following way on $\widetilde{\mathcal{A}}$:

$$\begin{aligned}
(z\mathbb{1} + A)^* &:= \bar{z}\mathbb{1} + A^*, && \forall A \in \mathcal{A},\ \forall z \in \mathbb{C}, \\
(z_1\mathbb{1} + A)(z_2\mathbb{1} + B) &:= z_1 z_2 \mathbb{1} + z_1 B + z_2 A + AB, && \forall A, B \in \mathcal{A},\ \forall z_1, z_2 \in \mathbb{C}, \\
\|(z\mathbb{1} + A)\|_{\widetilde{\mathcal{A}}} &:= \sup_{B \in \mathcal{A}/\{0\}} \frac{\|zB + AB\|_{\mathcal{A}}}{\|B\|_{\mathcal{A}}}, && \forall A \in \mathcal{A},\ \forall z \in \mathbb{C}.
\end{aligned}$$

By these definitions $\widetilde{\mathcal{A}}$ becomes a unital C*-algebra. In the rest of the appendix by a C*-algebra we will always mean a unital C*-algebra.

Next we introduce the following terminology for elements of a C*-algebra with certain special properties: $A \in \mathcal{A}$ is called *self-adjoint* if $A^* = A$, an element $B \in \mathcal{A}$ is called *positive* if there exists a $C \in \mathcal{A}$ such that $B = C^*C$, an element P is called a *projection* if $P = P^* = P^2$, finally, $U \in \mathcal{A}$ is a *unitary* element if $UU^* = U^*U = \mathbb{1}$.

A *morphism*[1] $\alpha : \mathcal{A} \to \mathcal{B}$ between two C*-algebras is a linear map such that

$$\begin{aligned}
\alpha(AB) &= \alpha(A)\,\alpha(B), \\
\alpha(A^*) &= \alpha(A)^*
\end{aligned}$$

holds for all $A, B \in \mathcal{A}$. If a morphism is injective, it is a *monomorphism*, if it is surjective, it is an *epimorphism*, if it is bijective, it is an *isomorphism*. A morphism between the same two C*-algebras is called an *endomorphism* , while an isomorphism between the same two C*-algebras is termed *automorphism*.

[1] Sometimes the term $*$-morphism is also used.

Theorem B 1. *Let α be a morphism, and β a monomorphism between the C*-algebras $\mathcal{A}$ and $\mathcal{B}$, then*

$$\begin{aligned} \|A\|_{\mathcal{A}} &\geq \|\alpha(A)\|_{\mathcal{B}} \quad \forall A \in \mathcal{A}, \\ \|A\|_{\mathcal{A}} &= \|\beta(A)\|_{\mathcal{B}} \quad \forall A \in \mathcal{A}. \end{aligned}$$

The linear operators on the Hilbert space C^N, that is the $N \times N$ matrices with their natural algebra structure, the Hermitian conjugation as the $*$-operation, and the operator norm $\|\cdot\|_{\mathcal{B}(\mathbb{C}^n)}$ form a C*-algebra. We denote this C*-algebra by $\mathcal{M}_N$.

Theorem B 2. *Any (abstract) C*-algebra that is linearly generated by an N^2 number of linearly independent elements $\{\hat{E}_{k,l}\}_{k,l=\{1,2,\ldots,N\}}$ satisfying the relations*

$$\hat{E}_{k,l}\hat{E}_{m,n} = \delta_{l,m}\hat{E}_{k,n}\ , \quad \hat{E}^*_{k,l} = \hat{E}_{l,k} \tag{B.1}$$

is isomorphic to $\mathcal{M}_N$.

In $\mathcal{M}_N$, a particular set of operators satisfying (B.1) are the matrix units $E_{k,l}$ $(k, l \in \{1, \ldots N\})$:

$$E_{1,1} = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ \vdots & & & & \\ 0 & 0 & 0 & \ldots & 0 \end{pmatrix}, \quad E_{1,2} = \begin{pmatrix} 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ \vdots & & & & \\ 0 & 0 & 0 & \ldots & 0 \end{pmatrix}, \quad \ldots$$

$$E_{2,1} = \begin{pmatrix} 0 & 0 & 0 & \ldots & 0 \\ 1 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ \vdots & & & & \\ 0 & 0 & 0 & \ldots & 0 \end{pmatrix}, \quad E_{2,2} = \begin{pmatrix} 0 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ \vdots & & & & \\ 0 & 0 & 0 & \ldots & 0 \end{pmatrix}, \quad \ldots$$

$$\vdots \qquad\qquad\qquad \vdots$$

Furthermore, a finite direct sum of finite matrix algebras $\oplus_i \mathcal{M}_{N_i}$ forms a C*-algebra (with the natural algebra structure, the Hermitian conjugation as a $*$-

operation, and the operator norm derived from the natural embedding $\oplus_i \mathcal{M}_{N_i} \subset \mathcal{M}_{(\sum_i N_i)}$). We have the following classification theorem for finite dimensional C*-algebras:

Theorem B 3. *Any finite dimensional C*-algebra is isomorphic to some direct sum of full matrix algebras, i.e. to*

$$\bigoplus_{i=1}^{k} \mathcal{M}_{N_i}$$

for some finite sequence of positive integers $(N_1, N_2, \dots N_k)$. *Any simple finite dimensional C*-algebra is isomorphic to* $\mathcal{M}_N$ *for some positive integer* N.

Turning to infinite dimensional C*-algebras, the set of bounded operators acting on a Hilbert space $\mathcal{B}(\mathcal{H})$ with its natural algebra structure, the Hermitian conjugation as a $*$-operation, and the operator norm $||\cdot||_{\mathcal{B}(\mathcal{H})}$ forms a C*-algebra.[2] If a C*-algebra $\mathcal{A}$ has a countable number of elements that form a dense set in $\mathcal{A}$ (with respect to the norm $||\cdot||_{\mathcal{A}}$), then $\mathcal{A}$ is called a *separable* C*-algebra. The following generalisation of theorem B3 to infinite dimensional C*-algebras connects the abstract theory of C*-algebras with the theory of bounded operators on Hilbert spaces.

Theorem B 4. *Any C*-algebra* $\mathcal{A}$ *is isomorphic with a C*-subalgebra of* $\mathcal{B}(\mathcal{H})$ *for some Hilbert space* $\mathcal{H}$. *If* $\mathcal{A}$ *is separable, then it is isomorphic to a C*-subalgebra of bounded operators on a separable Hilbert space.*

Hence any abstract C*-algebra can be identified with a subspace of bounded linear operators on a Hilbert space $\mathcal{H}$. Of course, there might be non-trivial subspaces in $\mathcal{H}$ that are invariant under the action of the entire C*-algebra in question. In the quantum physical setting this would mean that the Hilbert space would contain many unphysical degrees of freedom, but with a set of "superselection rules" one could in principle distinguish the unphysical states from the physical ones. Hence at first sight working with abstract C*-algebras seems unnecessary . However, in the next section we shall see that this is not exactly the case.

[2] We do not require the separability of $\mathcal{H}$ here.

B.2 Linear functionals and representations of C*-algebras

We begin this section by introducing the vocabulary of the representation theory of C*-algebras. A *representation* of a C*-algebra $\mathcal{A}$ is a unit-preserving $*$-morphism $\Pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$.[3] A representation Π is called *irreducible* if there is no nontrivial subspace of $\mathcal{H}$ that is invarant under the action of all the operators in $\Pi(\mathcal{A}) \subset \mathcal{B}(\mathcal{H})$, or equivalently, the commutant of $\Pi(\mathcal{A})$ is $\mathbb{C}\mathbb{1}$.[4] A vector $\psi \in \mathcal{H}$ is called a *cyclic* vector under a representation Π if the set $\{\Pi(A)\psi \mid A \in \mathcal{A}\}$ is dense in $\mathcal{H}$. A representation Π is called *faithful* if it is a monomorphism. The representations $\Pi_1 : \mathcal{A} \to \mathcal{B}(\mathcal{H}_1)$ and $\Pi_2 : \mathcal{A} \to \mathcal{B}(\mathcal{H}_2)$ are (unitary) equivalent, if there exists a unitary operator $U : \mathcal{H}_1 \to \mathcal{H}_2$, such that $\Pi_1(A) = U^{-1}\Pi_2(A)U$ holds for all $A \in \mathcal{A}$.

We ended the last chapter by stating that any C*-algebra $\mathcal{A}$ is isomorphic with a subspace of bounded linear operators on a Hilbert space $\mathcal{H}$, i.e., there exists a faithful representation $\Pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$. Hence at first sight one would wonder why it is useful in quantum physics to introduce the concept of abstract C*-algebras, instead of working alone with bounded operators on Hilbert spaces. It is exactly in the theory of representations and linear functionals (a closely related field), where we can see the real merits of the C*-algebraic approach. We continue with the vocabulary of the theory of functionals. A *linear functional* is simply a linear function from a C*-algebra to the set of complex numbers. A linear functional $\omega : \mathcal{A} \to \mathbb{C}$ is called *positive* if $\omega(A^*A) \geq 0$ for all $A \in \mathcal{A}$, and if this positive linear functional is normed as $\omega(\mathbb{1}) = 1$, it is called a *state*. The *mixture* of two states ω_1 and ω_2 with normalised weights λ_1 and λ_2 ($\lambda_1 + \lambda_2 = 1$; $\lambda_1, \lambda_2 > 0$) is the state defined as $\lambda_1\omega_1 + \lambda_2\omega_2$. A state $\omega : \mathcal{A} \to \mathbb{C}$ is called *pure* if it is not a mixture of two different states, otherwise ω is called *mixed*.

At the beginning let us restrict our discussion to functionals and representations of C*-algebras of bounded operators on finite and infinite dimensional Hilbert spaces. We have already seen a positive functional on $\mathcal{M}_N$, namely, the *trace*. The trace of the unit operator of $\mathcal{M}_N$ is $Tr(\mathbb{1}) = N$, so the term "the unit-

[3] Sometimes also the term $*$-representation is used for such a morphism.
[4] The commutant of a subalgera $\mathcal{A}$ in $\mathcal{B}(\mathcal{H})$ is the set $\{B \in \mathcal{B}(\mathcal{H}) \mid AB = BA,\ \forall A \in \mathcal{A}\}$.

normed trace" is commonly used for the functional tr $:= \frac{1}{N}\mathrm{Tr}$, which is a state since $\mathrm{tr}(\mathbb{1}) = 1$.[5] By the trace functional we can endow $\mathcal{M}_N$ with the Hilbert-Schmidt scalar product $\langle AB \rangle_{HS} = \mathrm{Tr}\,(A^* B)$. With this scalar product $\mathcal{M}_N$ is a Hilbert space. Let ω be an arbitrary functional on $\mathcal{M}_N$. From the Riesz representation theorem (theorem A3) we can infer that there exists a unique element D such that $\omega(A) = \mathrm{Tr}\,(D^* A)$, and it is easy to prove that if ω is a positive linear functional, then the corresponding operator D must be a positive operator. One can also prove that a state ω is pure if and only if the corresponding D is a projection of unit trace. We can thus conclude this paragraph with the following theorem:

Theorem B 5. *For any linear functional $\omega : \mathcal{M}_N \to \mathbb{C}$, there exists a unique element $D \in \mathcal{M}_N$ such that*

$$\omega(A) = Tr\,(DA), \quad \forall\, A \in \mathcal{A}.$$

If ω is positive, then D is a positive operator; if ω is a state, then $Tr\,(D) = 1$; and if ω is a pure state, then D is a projection.

Hence for any pure state ω_P, there exists a unitvector $\underline{v} \in C^N$ such that:

$$\omega_P(A) := \langle \underline{v}, A\underline{v} \rangle_{C^N}, \quad \forall\, \mathcal{A} \in \mathcal{A}. \tag{B.2}$$

Let us now investigate the states on the C*-algebra of bounded operators on an infinite dimensional separable Hilbert space $\mathcal{H}$, i.e. on $\mathcal{B}(\mathcal{H})$. $\mathcal{B}(\mathcal{H})$ is similarly to $\mathcal{M}_N$ a simple C*-algebra. Let $D \in \mathcal{B}(\mathcal{H})$ be a trace class operator of unit trace, and let us define the functional ω_D as:[6]

$$\omega_D(A) := \mathrm{Tr}\,(DA), \quad \forall A \in \mathcal{B}(\mathcal{H}).$$

ω_D is a state on $\mathcal{B}(\mathcal{H})$, and ω_D is pure if D is a projection of unite trace. However, not all states on $\mathcal{B}(\mathcal{H})$ arise in this way! The representation theoretical reason for this difference is the following:

[5]Sometimes, to avoid confusion, we call Tr the "dimension-normed trace".

[6]Remember that for any $D \in \mathcal{T}(\mathcal{H})$ and $A \in \mathcal{B}(\mathcal{H})$: $DA \in \mathcal{T}(\mathcal{H})$.

Theorem B 6. *Let $\mathcal{H}$ be a separable Hilbert space. If $\mathcal{H}$ is finite dimensional, then any irreducible representation is unitary equivalent to the identity mapping $\iota : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ (i.e. $\iota : \mathcal{M}_N \to \mathcal{M}_N$). However, if $\mathcal{H}$ is infinite-dimensional, then there exist irreducible representations $\Pi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ that are not unitary equivalent to the identity mapping $\iota : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$.*[7]

The proper generalisation of Eq. (B.2) to the infinite dimensional case is that for any pure state ω_P on $\mathcal{B}(\mathcal{H})$, there exists an irreducible representation $\Pi_{\omega_P} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ and a unitvector $\psi_{\omega_P} \in \mathcal{H}$ such that

$$\omega_P(A) = \langle \psi_{\omega_P}, \Pi_{\omega_P}(A)\psi_{\omega_P}\rangle_{\mathcal{H}}\,, \quad \forall\, A \in \mathcal{B}(\mathcal{H}).$$

We mention here, that similarly to the C*-algebra $\mathcal{B}(\mathcal{H})$, the CAR($\ell^2(\mathbb{Z}^d)$)-algebra is also a simple C*-algebra, but with many inequivalent irreducible representations. Hence we have to consider the different irreducible representations, too, inorder to obtain its pure states.

Before we generalise theorem B5 to the infinite dimensional case, we shall state it in another way. Let ω be a state on $\mathcal{M}_N$, and let D_ω be the corresponding positive operator of unit trace such that

$$\omega(A) := \mathrm{Tr}\,(DA), \quad \forall\, A \in \mathcal{M}_N.$$

Since D_ω is a positive operator on $\mathbb{C}^N$, there exists a finite sequence $\{\lambda_i\}_{i\in\{1,2,\ldots,n(\omega)\}}$ ($n(\omega) \leq N$) of positive real numbers and a sequence of pairwise orthogonal $\mathbb{C}^N$ unitvectors $\{\,\underline{v}_i\,\}_{i\in\{1,2,\ldots,n(\omega)\}}$ such that

$$C_\omega = \sum_{i=1}^{n(\omega)} \lambda_i P_i,$$

where P_i denotes the projection onto the subspace generated by $\underline{v}_i$. Now, let us

[7] This is not in contrast with the uniquness theorem of von Neumann, since in the C*-algebraic approach, the primary observable C*-algebra of quantum-mechanics is the Weyl algebra and not $\mathcal{B}(\mathcal{H})$ [28]. The irreducible representations of this C*-algebra is unique(!), and $\mathcal{B}(\mathcal{H})$ arises as the weak closure of the represented Weyl-algebra.

consider the representation $\Pi^{[n(\omega)]} : \mathcal{M}_N \to \oplus_{i=1}^{n} \mathcal{M}_N$ defined as

$$\Pi^{[n(\omega)]}(A) := A \oplus A \oplus \cdots \oplus A, \quad \forall A \in \mathcal{M}_N.$$

Furthermore, let us consider the following vector in $\oplus_{i=1}^{n} \mathbb{C}^N$:

$$\underline{V}_\omega := (\lambda_1 \underline{v}_1) \oplus (\lambda_2 \underline{v}_2) \oplus \cdots \oplus (\lambda_n \underline{v}_n).$$

Using the above notations one can easily show that

$$\omega(A) = \langle \underline{V}_\omega, \Pi^{[n(\omega)]}(A) \underline{V}_\omega \rangle_{\oplus_{i=1}^{n} \mathbb{C}^N}, \quad \forall A \in \mathcal{M}_N,$$

and $\underline{V}_\omega$ is cyclic under the representation $\Pi^{n(\omega)}$.

Now, the analogue of theorem B5 to $\mathcal{B}(\mathcal{H})$, CAR$(\ell^2(\mathbb{Z}^d))$ and all other (unital) C*-algebras, called the Gelfand-Naimark-Segal (GNS) theorem, can be stated in the following way:

Theorem B 7. *Let ω be a state on a (unital) C*-algebra $\mathcal{A}$. There exists a representation $\Pi_\omega : \mathcal{A} \to \mathcal{H}_\omega$, a unit vector $\psi_\omega \in \mathcal{H}_\omega$ such that*

$$\omega(A) = \langle \psi_\omega, \Pi_\omega(A) \psi_\omega \rangle_{\mathcal{H}_\omega} \quad \forall A \in \mathcal{A},$$

and ψ_ω is cyclic under Π_ω. The triple $(\mathcal{H}_\omega, \Pi_\omega, \psi_\omega)$ is unique up to a unitary transformation in the following sense. If $(\mathcal{H}'_\omega, \Pi'_\omega, \psi'_\omega)$ is a similar triple, i.e.,

$$\omega(A) = \langle \psi'_\omega, \Pi'_\omega(A) \psi'_\omega \rangle_{\mathcal{H}'_\omega} \quad \forall A \in \mathcal{A},$$

then there exists a unitary map $U : \mathcal{H}_\omega \to \mathcal{H}'_\omega$ such that

$$\Pi'_\omega(A) = U \Pi_\omega(A) U^{-1}, \quad \forall A \in \mathcal{A},$$
$$U\psi_\omega = \psi'_\omega.$$

Π_ω is irreducible if and only if ω is pure.

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