SOME ASPECTS OF OPERATOR ALGEBRAS IN QUANTUM PHYSICS

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Abstract. Motivated by the sharp contrast between classical and quantum physics as probability theories, in these lecture notes I introduce the basic notions of operator algebras that are relevant for the algebraic approach to quantum physics. Aspects of the representation theory of C*-algebras will be motivated and illustrated in physical terms. Particular emphasis will be given to explicit examples from the theory of quantum phase transitions, where concepts coming from strands as diverse as quantum information theory, algebraic quantum physics and statistical mechanics agreeably converge, providing a more complete picture of the physical phenomena involved.

1. Introduction

This notes represent the written version of lectures I gave in mini-courses at Universidade de Brasília (April 3-6, 2013), Universidad Central de Venezuela (May 23-27, 2016) and at the Villa de Leyva Summer School “Geometric, Topological and Algebraic Methods for Quantum Field Theory” (July 15-27, 2013). They were mainly intended as an introduction to some aspects of operator algebras, emphasizing the prominent role they play in quantum physics. As the audience consisted of students of both physics and mathematics at different stages of their studies, my choice was to focus on the most basic structures and examples, in the hope that a good grasp of these would motivate them to go deeper into the subject. Now, something that to a physicist may appear as completely familiar (as, say, an experimental set-up with polarizers, or the distinction between a classical and a quantum field) to a mathematician may not. The same could be said of the proof that the spectrum of any element in a C*-algebra is never empty: It is a standard result in analysis, but may look quite awkward to many physics students. Therefore, the emphasis of these lecture notes will be on explaining why certain mathematical structures may be useful for the study of quantum theory. This will be illustrated by means of several examples that include a discussion of bipartite entanglement.
algebraic and geometric aspects of quantum phase transitions in spin chains, quasifree states in fermionic systems and applications to quantum field theory.

Our starting point will be based on the sharp distinction between classical probability and the probability theory inherent to quantum mechanics. This will provide a physical motivation to the various mathematical concepts we will be dealing with. After introducing the basic concepts about $C^*$-algebras, we will show how an algebraic approach to entanglement can lead to a resolution of certain discrepancies appearing when we deal with systems of identical particles. Then we will focus on the study of certain specific models (quantum Ising and XY models) that turn out to be ideal in order to illustrate how entanglement, geometry and the theory of CAR algebras\footnote{A special type of $C^*$-algebras used to model fermionic systems} are interrelated.

1.1. Quantum correlations: Bell-type inequalities. Our first objective will be to understand what are the main structural differences between classical and quantum physics, when regarded as probability theories. This will, by the way, provide a physical motivation for some of the mathematical notions we will consider in the next sections. Let us recall that classical physics is usually modeled on a configuration (or phase) space, with a dynamics governed by, e.g., Hamilton’s principle. On the other hand, quantum mechanics is modeled on a Hilbert space. So the first issue we want to explore is: Why do we have to use Quantum Mechanics to describe the microscopic world? Indeed, simple experiments with light polarizers make it clear that there is no way we can describe certain phenomena using classical physics or, better said, classical probability. Let us then explore some elementary polarization phenomena, following the presentation in [1].

First let us recall that light is just made of electromagnetic waves, their behavior being governed by Maxwell’s equations:

\[
\begin{align*}
\nabla \cdot E &= \rho / \epsilon_0, \\
\nabla \cdot B &= 0, \\
\n\nabla \times E &= -\frac{\partial B}{\partial t}, \\
\n\nabla \times B &= \epsilon_0 \mu_0 \frac{\partial E}{\partial t} + \mu_0 j,
\end{align*}
\] (1.1)

where $E$ (resp. $B$) stands for the electric (resp. magnetic) field, $\rho$ for the charge density and $j$ for the current density.

**Exercise 1.1.** Show that Maxwell’s equations (1.1) in vacuum ($\rho = 0$, $j = 0$) lead to plane-wave solutions for the electromagnetic field propagating at a speed $c = 1/\sqrt{\epsilon_0 \mu_0}$ and such that $E$ and $B$ are always perpendicular to each other and to the propagation direction. What is the relation between the intensity of the wave (defined as $I = \|E\|^2$) and the energy content of the fields?

In simple terms, a polarizer is a filter that only allows the transmission of light waves which have a specific polarization angle. If we let unpolarized light go through an ideal polarizer, the intensity $I_1$ of the transmitted wave will be found to be half the intensity $I_0$ of the incident wave: $I_1 = 1/2 I_0$ (Malus’ law). After passing through the polarizer, the light is said to be linearly polarized. Let us now suppose that we have a beam of linearly polarized light and we let it go through a second polarizer, such that its polarization axis has been rotated by an angle $\varphi$ with respect to the axis of the first polarizer. Then, experiment tells us that the intensity of the transmitted light will be $I_2 = \cos^2 \varphi I_1$. This is all fine if we are working with classical electromagnetic waves, which are described by Maxwell’s equations. In
A figure S (Calcium atom) emits a pair of photons, each of which may be detected by detectors located in the extremes (DA, DB). There is a polarizer between the Ca atom and each of the detectors.

In this case we just need to consider the projection of the field onto the direction singled out by the polarization axis. But we know that light is actually made of photons and, if their number is small, we are led to regard the $\cos^2\varphi$ term as a kind of “expectation value”.

In a very influential paper [2], Einstein, Podolski and Rosen presented a criticism of quantum theory in what is now known as the EPR paradox. This led to the development of alternative, so-called “hidden variable” theories that aimed at explaining physical phenomena using classical probability models. It was only until Bell proved his famous inequalities, and Aspect’s experiments proved the former were violated, showing that quantum theory provided the correct description of the phenomena. An experimental set-up, of the type studied by Aspect, consists of a source (Ca atom) located in the middle that emits simultaneously a pair of photons. One of them goes to the right, the other to the left. There are two detectors, one at each extreme. There is also a polarizer in-between each detector and the source, as depicted in Fig. 1. Let us now consider the following two propositions:

$A =$ “Left photon passes through (is detected by DA) when polarizer’s angle is $\varphi$”.

$B =$ “Right photon passes through (is detected by DB) when polarizer’s angle is $\theta$”.

Then, what we learn from experiment is that the joint probability for both photons passing through the polarizers, thus being detected, is

$$p(AB) = \frac{1}{2} \sin^2(\varphi - \theta).$$

Before exploring why classical probability is in conflict with this result, let us recall how the principles of quantum mechanics allow us to predict it.

Let $\mathcal{H}$ denote a Hilbert space which, for simplicity, will be considered to be finite dimensional. In quantum mechanics, probability distributions are obtained from state vectors $|\Psi\rangle \in \mathcal{H}$ or, more generally, by density matrices $\rho$, that is, self-adjoint positive operators of trace one. On the other hand, observables are described by self-adjoint operators. Let $A$ be such an observable. Let $\sigma(A) = \{a_1, \ldots, a_N\}$ denote its spectrum. We can then consider its spectral decomposition

$$A = \sum_j a_j E_j, \quad \sum_j E_j = \mathbb{1}, \quad E_i E_j = \delta_{ij} E_j.$$  \hfill (1.2)
If the state of the system is given by a density matrix $\rho$, the expectation value of $A$ is defined as
\[ \langle A \rangle_\rho := \text{Tr}(\rho A). \] (1.3)
In the case of a pure state, the density matrix is a rank-one projector, of the form $\rho = |\psi\rangle\langle\psi| \in \mathcal{H}$, and so (1.3) reduces to $\langle A \rangle_\psi = \langle \psi | A | \psi \rangle$. In this way we obtain a probability distribution over $\sigma(A)$, with
\[ p(a_i) = \langle E_i \rangle_\rho. \]
In fact, it follows from (1.2) and (1.3) that $0 \leq p(a_i) \leq 1$ and $\sum_i p(a_i) = 1$.

Let us use this to give a mathematical description of the experiment described above. The polarization state of a photon can be described using a 2-dimensional Hilbert space. Let $\{|x\rangle, |y\rangle\}$ denote an orthonormal basis, that can be used to describe, say, horizontal and vertical polarization states. Since we are considering a system consisting of two photons, the Hilbert space of the system can be taken to be $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ (as the photons are supposed to be far from each other at the time of detection, the symmetrization postulate can be ignored). The 2-photon state, as produced by the emission from an excited state of the Ca atom, can be described by the following state vector:
\[ |\psi\rangle = \frac{1}{\sqrt{2}} (|x\rangle \otimes |y\rangle - |y\rangle \otimes |x\rangle). \] (1.4)

For a polarizer with polarization axis pointing at an angle $\alpha$ we can use $P(\alpha)$, defined as the projector onto $\cos \alpha |x\rangle + \sin \alpha |y\rangle$. Since we have two polarizers, we introduce the following projectors (cf. Fig. 1):
\[ P_A(\phi) = P(\phi) \otimes \mathbb{1}, \quad P_B(\theta) = \mathbb{1} \otimes P(\theta). \]
It is important to remark that these two operators correspond to compatible observables, in the sense that the measurement of one of them does not affect the result of the other, i.e., they are commuting observables:
\[ [P_A(\phi), P_B(\theta)] = 0. \]

Exercise 1.2. Show that
\[ \langle \psi | P_A(\phi) | \psi \rangle = \langle \psi | P_B(\theta) | \psi \rangle = \frac{1}{2}. \]
Also show that, for the joint measurement of the two polarization states, one obtains
\[ \langle \psi | P_A(\phi) P_B(\theta) | \psi \rangle = \langle \psi | (1 - P_A(\phi))(1 - P_B(\theta)) | \psi \rangle = \frac{1}{2} \sin^2(\phi - \theta). \] (1.5)

The previous exercise shows that the predictions of quantum mechanics for this type of experiment are in accordance with what is actually measured in the laboratory. In spite of its extreme simplicity, there is an intriguing feature of this result: By appropriately arranging the polarization angles $\theta$ and $\phi$, we can obtain a total anticorrelation for the joint measurements. As we will see, this is due to the fact that the state (1.4) is an entangled state. That these kind of correlations cannot be obtained from a (local, realistic) classical theory is at the core of the original EPR controversy. For an interesting discussion of these issues in the context of an actual experimental situation, we recommend [3].

Our immediate aim will therefore be to understand where exactly classical probability fails at describing the results of such experiments. For this purpose we will
assume an approach to (classical) probability based on propositions and degrees of plausibility, following Jaynes [4].

In this setting, the objects to be considered are the following:

- A set of propositions: \{A, B, C, \ldots\}, each one of which can take on (only) two values: true or false.
- Logical operations, that can be performed on the set of propositions:
  - Conjunction, or logical product (AND): \( AB \). It is true if and only if both \( A \) and \( B \) true.
  - Disjunction, or logical sum (OR): \( A + B \). It is true if at least one of them true.
  - Negation (NOT): \( \bar{A} \), with opposite truth value as \( A \).

These logical operations are assumed to satisfy the defining rules of a Boolean algebra:

- Idempotency: \( AA = A \), \( A + A = A \)
- Commutativity: \( AB = BA \), \( A + B = B + A \)
- Associativity:
  - (A1) \( A(BC) = (AB)C = ABC \)
  - (A2) \( A + (B + C) = (A + B) + C = A + B + C \)
- Distributivity:
  - (D1) \( A(B + C) = AB + AC \)
  - (D2) \( (A + B)(A + C) = A + BC \)
- Duality (De Morgan’s laws): \( \bar{AB} = \bar{A} + \bar{B} \), \( \bar{A} + \bar{B} = \bar{A} \bar{B} \)

Exercise 1.3. Show that the proposition “\( A \Rightarrow B \)” is equivalent to “\( A = AB \)”.

Exercise 1.4. Show that (D2) follows from the other rules.

Now, given a proposition \( A \), a probability (or “degree of plausibility”, cf. [4]) \( p(A) \) can be assigned to it, under the following basic assumptions:

I. Let \( p(A) \in \mathbb{R} \) denote the probability, or degree of plausibility, of a given proposition \( A \). Then we assume that:
   - \( p(f(A_1, A_2, \ldots, A_n)) \in \mathbb{R} \), for any logical function \( f \) of the propositions \( A_1, A_2, \ldots, A_n \)
   - Using the notation \( p(A|B) \) for the conditional probability that \( A \) is true, given \( B \) is true, we assume that \( p(A|C) > p(B|C) \) whenever \( A|C \) more plausible than \( B|C \).

II. Given a proposition \( C \), let us suppose that we improve our state of knowledge, obtaining a new proposition \( C’ \). If as a result \( A \) becomes more plausible, i.e. \( p(A|C’) > p(A|C) \), but \( p(B|AC’) = p(B|AC) \), then \( p(AB|C) \geq p(AB|C) \) should hold (this is dubbed the common sense assumption by Jaynes [4]).

From I and II above we may obtain, under very general assumptions (like consistency), the following two basic rules:

- Product Rule:
  \[
  P(AB|C) = P(A|BC)P(B|C) = P(B|AC)P(A|C)
  \]  

- Sum Rule:
  \[
  P(A|C) + P(\bar{A}|C) = 1.
  \]
The reader is invited to consult Jaynes for a comprehensive exposition of this point of view, including many illustrative derivations and examples.

Now, in order to return to our experiment, let us define the following “coincidence” function $f$, for two given propositions $A$ and $B$:

$$f(A, B) := AB + \bar{A}\bar{B}.$$  

**Exercise 1.5.** Given 4 propositions $A_1, A_2, B_1, B_2$, use the product and sum rules to show that the following proposition is true:

$$f(A_1, B_1) \Rightarrow f(A_1, B_2) + f(A_2, B_2) + f(A_2, B_1).$$  

Since $p(A|X) \leq p(B|X)$ whenever $A \Rightarrow B$ holds (product rule) we obtain, from the previous exercise, “Bell’s Inequality”:

$$p(f(A_1, B_1)) \leq p(f(A_1, B_2)) + p(f(A_2, B_2)) + p(f(A_2, B_1)).$$  

Referring back to figure [let us consider the following propositions $(i, j = 1, 2)$:

$A_i =$ “Left photon passes through (is detected by $D_A$) when polarizer’s angle is $\varphi_i$.”

$B_j =$ “Right photon passes through (is detected by $D_B$) when polarizer’s angle is $\theta_j$.”

The inequality (1.10) should hold true for all choices of $\varphi_i, \theta_j$. But this then implies:

$$\sin^2(\varphi_1 - \theta_1) \leq \sin^2(\varphi_1 - \theta_2) + \sin^2(\varphi_2 - \theta_2) + \sin^2(\varphi_2 - \theta_1).$$

For the choice $\varphi_1 = 0$, $\varphi_2 = \frac{\pi}{3}$, $\theta_1 = \frac{\pi}{2}$, $\theta_2 = \frac{\pi}{6}$, this means:

$$\sin^2 \left( \frac{\pi}{2} \right) \leq \sin^2 \left( \frac{\pi}{6} \right) + \sin^2 \left( \frac{\pi}{3} - \frac{\pi}{6} \right) + \sin^2 \left( \frac{\pi}{3} - \frac{\pi}{2} \right),$$

$$\sin^2 \left( \frac{\pi}{2} \right) \leq \sin^2 \left( \frac{\pi}{6} \right) + \sin^2 \left( \frac{\pi}{6} \right) + \sin^2 \left( -\frac{\pi}{6} \right),$$

$$1 \leq \frac{3}{4}. $$

This contradiction means that the assumptions we have considered above (which are at the basis of classical probability) do not apply in the quantum realm. So, definitely, quantum theory leads to a very different type of probability theory. In the next section we will explore some of the more notorious differences between classical and quantum probabilities.

1.2. **Classical versus quantum probability.** Until now we have avoided any mention of propositions in terms of set theory, which is the basis of the Kolmogorov axiomatics. In the finite dimensional case, at least, they turn out to give equivalent structures. Let us then consider the main properties of a (classical) probability theory, formulated in terms of set theory and, for simplicity, in the finite dimensional context. Let us consider a finite set $\Omega = \{x_1, x_2, \ldots, x_N\}$, regarded here as the sample space. The event space $\mathcal{E}$ is a certain collection of subsets of $\Omega$, that must contain the empty set and be closed under complements and unions.

The set of events forms a Boolean algebra, under the standard set theoretic operations:

- **AND:** $A \cap B$, 

- **OR:** $A \cup B$, 

- **NOT:** $\bar{A}$, 

- **AND:** $A \cap B$, 

- **OR:** $A \cup B$, 

- **NOT:** $\bar{A}$.
A probability distribution is then defined as a map \( p : \mathcal{E} \rightarrow [0, 1] \subset \mathbb{R} \), such that

(i) \( p(\emptyset) = 0 \), \( p(\Omega) = 1 \),

(ii) \( p(\bigcup_{k=1}^{n} A_k) = \sum_{k=1}^{n} p(A_k) \), for \( A_1, A_2, \ldots, A_n \in \mathcal{E} \) pairwise disjoint.

**Remark 1.6.** Notice that the space of probability distributions is a convex set, for if \( p_1 \) and \( p_2 \) are two probability distributions, then \( \lambda p_1 + (1-\lambda) p_2 \) is again a probability distribution, provided \( 0 \leq \lambda \leq 1 \). But not only is the space of probability distributions a convex set, it is a special kind of convex set: a simplex. To see this, all we have to do is to consider the following “extremal” distributions, \( p^{(1)}, p^{(2)}, \ldots, p^{(N)} \), defined by

\[
p^{(i)}(x_j) := \delta_{ij}.
\]

It is clear that any \( p \) can be written as a unique convex combination of these extremal distributions, as we have

\[
p = \sum_{i} \lambda_i p^{(i)},
\]

with \( \lambda_j = p(x_j) \).

A random variable (or “observable”) is a function \( f : \mathcal{E} \rightarrow \mathbb{R} \). We call the space of all such functions \( \text{Obs}(\Omega) \). Notice that \( \text{Obs}(\Omega) \) forms a commutative algebra.

Summarizing, in the finite-dimensional case we have the following structure:

- The event space (\( \mathcal{E} \subseteq \mathcal{P}(\Omega) \)) forms a Boolean algebra.
- The space of probability distributions is convex and furthermore has the structure of a simplex: Every probability distribution \( p \) can be uniquely written as convex combination of “extremal” distributions.
- The space of observables (random variables) has the structure of a commutative algebra.

**Remark 1.7.** In cases where the sample space is not a finite set (like in classical mechanics) we need a suitable generalization of the above definitions. This is afforded by measure theory, in the following way: Sample and event spaces are now replaced by a measurable space \((\Omega, \mathcal{E})\), where \( \mathcal{E} \) is a suitable \( \sigma \)-algebra of \( \Omega \). Probability distributions are then defined as normalized, positive measures. In particular, we can now handle countable additivity:

\[
p \left( \bigcup_{k=1}^{\infty} A_k \right) = \sum_{k=1}^{\infty} p(A_k), \ \text{for} \ A_j \ \text{pairwise disjoint}.
\]

Finally, the space of observables is still a commutative algebra, for the product and sum of two measurable functions is a measurable function. A similar remark applies to the convex structure of the space of probability distributions.

How do these structures show up in classical physics? In classical mechanics, for example, the dynamics of a system can be described in terms of canonical variables “position” \( (q_i) \) and “momentum” \( (p_j) \), that give rise to the phase space of the system. It follows from Hamilton’s variational principle that if \( H(q, p) \) is the Hamiltonian of the system, the canonical variables will evolve along solutions to
Hamilton’s equations:
\[
\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad i = 1, \ldots, n. \tag{1.11}
\]

Usually the phase space is the cotangent bundle \( T^*Q \) of some configuration space \( Q \). The canonical variables \((q, p)\) are then local coordinates on \( T^*Q \) and the observables are smooth functions on phase space: \( C^\infty(T^*Q) \). Since time evolution is given by Hamilton’s equations or, at the level of observables by \( \frac{df}{dt} = \{H, f\} \), with \( \{\cdot, \cdot\} \) denoting the Poisson bracket, one would think that there is no much space for a probabilistic model here since, given a set of initial conditions, by solving the equations of motion we are able, in principle, to predict the position and momenta of all the particles. But, as we learn from classical statistical physics, for \( n \gg 1 \) (\( n \sim 10^{23} \)) we certainly need a statistical approach! Therefore we are forced to introduce probability distributions, expressed in terms of probability densities \( \rho(q, p) \), so that the average value of an observable \( f \in C^\infty(T^*Q) \) is given by
\[
\langle f \rangle = \int f(q, p)\rho(q, p)\,d\mu,
\]
where \( d\mu = d^nqd^n p \) is the Liouville measure on phase space. For instance, for the canonical ensemble (used to describe a subsystem embedded in a thermal bath at temperature \( T \)), we have \( \rho(q, p) \propto e^{-H(q, p)/k_B T} \). Now we can return to the case of a few point particles and interpret the state of the system at a given time, usually defined as just a point \((q_0, p_0)\) in phase space, as an extremal probability distribution (a “pure state”), for which the probability density is just a Dirac delta distribution: \( \rho(q, p) = \delta(q - q_0, p - p_0) \). In any case, we see that classical physics can be regarded as a special type of probability theory, where the three properties of classical probability highlighted above still hold, i.e., every classical system of point particles can be understood as a probability theory, in the Kolmogorov sense.

What about Quantum Mechanics? As discussed above, probability distributions are obtained from state vectors \(|\Psi\rangle\) in a Hilbert space \( \mathcal{H} \), or more generally from density matrices, \( \rho \), whereas observables are described by self-adjoint operators. Consider the spectral decomposition of a self-adjoint operator \( A \), as in (1.2). Assuming a non-degenerate, discrete spectrum, we notice that the projectors \( E_i \), having as spectrum the set \( \{0, 1\} \), can be regarded as “indicators of events”. Now, there is a correspondence between projections \( E : \mathcal{H} \to \mathcal{H} \) and subspaces \( V \subset \mathcal{H} \). The partial order that we naturally obtain by inclusion then gives rise to the structure of an “orthocomplemented lattice of proposition”, where the corresponding operations are defined as
\[
\text{OR: } V_1 \lor V_2 \iff \text{span}(V_1, V_2)
\]
\[
\text{AND: } V_1 \land V_2 \iff V_1 \cap V_2
\]
\[
\text{NOT: } V' \iff V^\perp.
\]
An important feature of this system is that it does not give rise to a Boolean algebra structure. The reason for this is that the orthogonal complement is not the only possibility for a complement in this lattice. This in turn implies the breakdown of the distributive law, which is part of the definition of a Boolean algebra. As in the classical case, the state space (here the space of density matrices) is a convex space.
But, in contrast to the classical case, this space is not a simplex. A consequence of this is that the representation of a density matrix as a convex sum of pure states is (highly) non-unique. Finally, in quantum theory the space of observables forms a non-commutative algebra, in contrast to the classical case, where the algebra is commutative.

It is now clear that, in principle, both approaches (classical and quantum) can be considered in order to describe physical phenomena in probabilistic terms. In fact, EPR-like arguments are in favor of a "local-realistic" point of view according to which even quantum phenomena should be explained in terms of classical probability. That this is not the case is proved by Bell's inequalities and their violation, experimentally verified by Aspect in the 80’s. So quantum theory can be regarded as a kind of "non-commutative" probability theory. One of the points of these lectures is that, when formulated in the language of operator algebras, both quantum and classical physics can be described in a unified way. We will also take advantage of this formulation to discuss a similar phenomenon, occurring in topology and geometry: In non-commutative geometry the generalization of topological/geometric notions to the non-commutative setting has been mainly achieved by first expressing them in algebraic terms and then realizing that dropping the commutativity assumption allows for vast generalizations.

2. Aspects of operator algebras in quantum physics

2.1. Observable algebras and states. Let $\mathcal{H}$ be a separable Hilbert space. Recall that, given a linear operator $T : \mathcal{H} \rightarrow \mathcal{H}$, $T$ is said to be bounded if there is some $C > 0$ such that

$$\|T(x)\| \leq C\|x\|$$

for all $x$ in $\mathcal{H}$, where the norm is the one induced by the inner product: $\|x\|^2 = \langle x, x \rangle$. If $T$ is a bounded operator, we define its norm as follows:

$$\|T\| := \sup_{x \neq 0} \frac{\|T(x)\|}{\|x\|}. $$

One then checks that for $T$ and $S$ bounded the inequalities

$$\|T + S\| \leq \|T\| + \|S\|,$$

$$\|TS\| \leq \|T\| \|S\|,$$

are satisfied. From the completeness of $\mathcal{H}$ it follows that the space

$$\mathcal{B}(\mathcal{H}) = \{ T : \mathcal{H} \rightarrow \mathcal{H} \mid T \text{ is linear and bounded} \}$$

is a complete normed space. It is also an algebra and has an involution "$*$" given by the adjoint: $T^* := T^\dagger$. We thus may call $\mathcal{B}(\mathcal{H})$ the "$*$-algebra of bounded operators on $\mathcal{H}$".

**Exercise 2.1.** Show that for $T \in \mathcal{B}(\mathcal{H})$ we have:

$$\|T^*T\| = \|T\|^2.$$

We now abstract these notions and make them independent of any underlying Hilbert space. As we will see below, a lot will be gained from this, since we will then be able to study representations of the (abstract) operator algebras, and the equivalence/inequivalence of these representations will have a deep physical meaning.
Definition 2.2. A Banach space is a normed vector space \( (V, \| \cdot \|) \) which is complete with respect to the (metric induced by) \( \| \cdot \| \).

Definition 2.3. A Banach algebra is a Banach space \( (A, \| \cdot \|) \) which is also an algebra, with the property that \( \|ab\| \leq \|a\|\|b\|, \forall a, b \in A \) (which in turn implies that multiplication is a continuous operation).

Definition 2.4. An involution on a (complex) algebra \( A \) is a map \( * : A \rightarrow A \) such that, for any \( a, b \in A \) and \( \mu, \nu \in \mathbb{C} \):

i. \( (\lambda a + \mu b)^* = \overline{\lambda} a^* + \overline{\mu} b^* \)

ii. \( (ab)^* = b^* a^* \)

iii. \( (a^*)^* = a \)

Notice that this is, basically, an abstraction of the adjoint operation on \( B(H) \).

Definition 2.5. A \( C^* \)-algebra is a Banach ∗-algebra \( (A, \| \cdot \|, *) \) with the fundamental property

\[ \|a^* a\| = \|a\|^2. \] (2.1)

Example 2.6. Let \( M \) be a compact, Hausdorff topological space and set \( A = C(M) \), the space of continuous complex functions on \( M \) and, for \( f \in C(M) \), set \( f^*(x) = \overline{f(x)} \) and \( \|f\| = \sup_{x \in M} |f(x)| \). Then \( (C(M), \| \cdot \|, *) \) is a \( C^* \)-algebra.

Example 2.7. Let \( \mathcal{H} \) be a Hilbert space. Then, as we expect, \( (B(H), \| \cdot \|, *) \) is a \( C^* \)-algebra, where the norm is the operator norm and the involution is given by the adjoint operation.

Later we will see that the list of examples of \( C^* \)-algebras is basically exhausted by the previous two examples, a remarkable fact. A motivation to work with algebras of bounded operators comes from physics since, as can be shown, the canonical commutation relations (CCR)

\[ [\hat{q}, \hat{p}] = i\hbar \mathbf{1} \]

cannot be implemented by means of bounded operators \( \hat{q} \) and \( \hat{p} \). Then, although these commutation relations have a very clear meaning from the physical point of view, mathematically they correspond to unbounded operators and hence issues like self-adjointness, domains, etc. come into play, which make them more difficult to deal with. One can, nevertheless, replace the CCR by their exponentiated (or Weyl) form, as follows. First we define operators \( U(a) \) and \( V(b) \), for \( a, b \in \mathbb{R} \), acting on wave functions as follows:

\[ (U(a)\psi)(x) := \psi(x - ha), \]
\[ (V(b)\psi)(x) := e^{-ibx}\psi(x). \] (2.2)

By Stone’s theorem, it follows that \( U(a) = e^{-ia\hat{p}} \) and \( V(b) = e^{-ib\hat{q}} \).

Exercise 2.8. Show that the operators \( U(a) \) and \( V(b) \) satisfy the following commutation relations:

\[ U(a_1)U(a_2) = U(a_1 + a_2), \]
\[ V(b_1)V(b_2) = V(b_1 + b_2), \]
\[ U(a)V(b) = e^{i\hbar a b}V(b)U(a). \] (2.3)
As we will see later on, these operators give rise to a $C^*$-algebra. In fact, we will see that to any symplectic vector space we can canonically associate a $C^*$-algebra (its Weyl $C^*$-algebra). The unitary representations of these algebras, in the case of infinite dimensional symplectic vector spaces, play a prominent role in the study of quantum field theory on curved spacetimes.

**Example 2.9.** Consider a (complex, involutive, with unit) algebra $A$ generated by elements $a_1, a_2, \ldots, a_n, 1$, subject to the following canonical anticommutation relations (CAR):

$$a_i a_j^* + a_j^* a_i = \delta_{ij} 1, \quad a_i a_j + a_j a_i = 0.$$  \hspace{1cm} (2.4)

If we want to define a $C^*$ norm on this algebra, it has to be such that the $C^*$-property (2.1) is satisfied. But from (2.4) we obtain $(a_i a_j)^2 = a_i a_j$, which along with (2.1) implies $\|a_i a_j\|^2 = \|a_i a_j\|$. The only option we have, then, is to define $\|a_i\| = 1$ for every $i \in \{1, \ldots, n\}$.

**Exercise 2.10.** Generalize the previous example to the case of a finite dimensional Hilbert space $H \cong C^n$, in the following way. Let $\langle \cdot | \cdot \rangle$ denote the inner product. For any pair of vectors, $u, v \in H$, consider generators $a(u), a(v)$ satisfying the following relations (CAR):

$$\{a(u), a(v)^*\} = \langle u | v \rangle 1, \quad \{a(u), a(v)\} = 0.$$  \hspace{1cm} where $\{A, B\} \equiv AB + BA$. How must $\|a(u)\|$ be defined in this case?

The (mathematical) notion of state for a $C^*$-algebra is also very close to the notion of quantum state. To appreciate this, consider a physical system modeled by the algebra $B(H)$ of bounded operators on a Hilbert space $H$. As mentioned in the previous section, in physics we distinguish between two kinds of states:

- **Pure states:** These are described by normalized vectors $|\psi\rangle \in H$ (actually, by rays on Hilbert space). If $A$ is an observable, then its expectation value is defined as

$$\langle A \rangle := \langle \psi | A | \psi \rangle.$$  \hspace{1cm} (2.5)

- **Mixed states:** They are described by operators $\rho : H \to H$ such that $\rho^\dagger = \rho > 0$, $\text{Tr} \rho = 1$. The expectation value is given, in this case, by

$$\langle A \rangle_\rho := \text{Tr}_H (\rho A).$$

**Exercise 2.11.** Show that the condition for a mixed state (described by a density matrix $\rho$) to be pure is $\rho^2 = \rho$. Thus, all states can be described by density matrices.

We therefore see that a state can be regarded as a mapping $A \mapsto \langle A \rangle$ from the observable algebra to the complex numbers. It must be possible, then, to express the properties $\rho > 0$ and $\text{Tr} \rho = 1$ only in terms of this mapping. This leads us to the general definition of state for a $C^*$-algebra.

**Definition 2.12.** Let $\mathcal{A}$ denote a (unital) $C^*$-algebra, with unit $1$. A positive linear functional

$$\omega : \mathcal{A} \to \mathbb{C}$$

such that $\omega(1) = 1$ is called a state. We will denote the set of all states on $\mathcal{A}$ with $\mathcal{S}_\mathcal{A}$. 

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**Exercise 2.11.** Show that the condition for a mixed state (described by a density matrix $\rho$) to be pure is $\rho^2 = \rho$. Thus, all states can be described by density matrices.

The space of all density matrices is naturally a convex space. The extremal elements then turn out to be the pure ones. Check this assertion in the simple case $H = C^2$. 

We therefore see that a state can be regarded as a mapping $A \mapsto \langle A \rangle$ from the observable algebra to the complex numbers. It must be possible, then, to express the properties $\rho > 0$ and $\text{Tr} \rho = 1$ only in terms of this mapping. This leads us to the general definition of state for a $C^*$-algebra.

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$$\omega : \mathcal{A} \to \mathbb{C}$$

such that $\omega(1) = 1$ is called a state. We will denote the set of all states on $\mathcal{A}$ with $\mathcal{S}_\mathcal{A}$. 

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Remark 2.13. In this context, positivity of $\omega$ means that $\omega(a^*a) \geq 0$ for all $a \in \mathcal{A}$.

Remark 2.14. If $\mathcal{A}$ is not unital, we can replace the normalization condition by the condition $\|\omega\| = 1$. For unital algebras, both definitions coincide.

Having in mind the example of $\mathcal{B}(\mathcal{H})$, it then makes sense to have a notion of spectrum for an abstract $C^*$-algebra. This leads, in turn, to the spectral theorem for $C^*$-algebras [6].

**Definition 2.15.** Let $a$ be an element of a unital $C^*$-algebra $\mathcal{A}$. Then its **spectrum** is defined as the set
\[
\sigma(a) := \{ \lambda \in \mathbb{C} \mid (\lambda \mathbb{1} - a) \text{ is not invertible} \}.
\]

**Definition 2.16.** Let $a$ be an element of a unital $C^*$-algebra $\mathcal{A}$. Then its **spectral radius** is defined as
\[
\rho(a) := \sup \{ |\lambda| \mid \lambda \in \sigma(a) \}.
\]

**Exercise 2.17.** Show that the space $M_n(\mathbb{C})$ of $n \times n$ matrices with complex entries is a $C^*$-algebra with respect to the norm defined as
\[
\|A\|_{\text{max}} := |\lambda_{\text{max}}|^{1/2},
\]
where $\lambda_{\text{max}}$ is the eigenvalue of $A^*A$ with the largest absolute value. Show also that this norm coincides with the operator norm.

**Remark 2.18.** The previous exercise illustrates the remarkable fact that, for a $C^*$-algebra $(\mathcal{A}, \|\cdot\|, \ast)$, the norm of any element normal $a \in \mathcal{A}$ coincides with its spectral radius:
\[
\|a\| = \sqrt{\rho(a^*a)}.
\]
This is an important fact, as it links topological properties of the algebra with algebraic ones. In particular, it implies that the norm in a $C^*$-algebra is **unique**.

The following two properties will be very useful:

**Exercise 2.19.** Let $\phi : \mathcal{A} \to \mathbb{C}$ be a positive linear functional on a $C^*$-algebra. Prove that
\[
(i) \quad \phi(a^*b) = \overline{\phi(b^*a)}.
(ii) \quad |\phi(a^*b)|^2 \leq \phi(a^*a)\phi(b^*b) \quad \text{("Cauchy-Schwarz inequality")}
\]
Hint: Consider $\phi((\lambda a + b)^*(\lambda a + b))$ as a quadratic form on $\lambda$. As an alternative, you may try deriving these relations just by thinking of $\phi(a^*b)$ as $\langle a|b \rangle$.

Another consequence of positivity is continuity:

**Proposition 2.20.** Let $\phi$ be a positive linear functional on a unital $C^*$-algebra $\mathcal{A}$. Then $\phi$ is a continuous linear functional, and $\|\phi\| = \phi(\mathbb{1})$.

**Proof (cf. [11]).** If $a$ is positive ($a = a^*$ and $\sigma(a) \subseteq \mathbb{R}_+$) then we have, from the spectral radius formula, that $\sigma(a) \subseteq [0, \|a\|]$. This means that $\|a\| - \lambda \geq 0$ for all $\lambda \in \sigma(a)$. This can be restated as follows. Define
\[
f : \sigma(a) \to \mathbb{C} \quad \lambda \mapsto f(\lambda) := \|a\| - \lambda.
\]
Then $f \in C(\sigma(a))$ and $f \geq 0$. But then it follows (from the continuous functional calculus) that $\sigma(f(\lambda)) = f(\sigma(a))$, so that $f(a) \geq 0$ or, in other words, that $\|a\| \mathbb{1} - a$ is a positive operator. Since $\phi$ is positive and linear, this implies $\phi(a) \leq \phi(\mathbb{1})\|a\|$.
Now, for an arbitrary $\alpha \in \mathcal{A}$, apply the Cauchy-Schwarz inequality from exercise 2.19 with $a = 1$ and $b = \alpha$, and use the C$^*$ property of the norm to obtain 

$$\phi(\alpha) \leq \phi(1) \|\alpha\|.$$ 

It follows that $\phi$ is continuous, with $\|\phi\| = \phi(1)$. But we also have 

$$\phi(1) = |\phi(1)| \leq \|\phi\| \|1\| = \|\phi\|,$$ 

so that $\|\phi\| = \phi(1)$. \hfill \Box

Thus, for unital C$^*$-algebras we conclude that the set of states over $\mathcal{A}$ is a convex subset of the continuous dual $\mathcal{A}^*$ of $\mathcal{A}$.

We gather from all this that it makes sense to formulate quantum physics in terms of C$^*$-algebras. The general philosophy will be to describe a given physical system in terms of its “algebra of observables”, which will be here taken to be a C$^*$-algebra $(\mathcal{A}, \|\cdot\|, \ast)$. Then we will consider the following two “dual” notions:

- A quantum state will be defined as a state (in the sense of definition 2.12) on the algebra $\mathcal{A}$.
- An observable will be an element of $\mathcal{A}$.

Furthermore, the “pairing” between an observable $a$ and a state $\omega$ will be given the physical interpretation of an expectation value, and we will write 

$$\langle a \rangle_\omega := \omega(a).$$

Regarding the distinction between pure and mixed states, we can now call a state pure if it cannot be written as a convex combination of other states; otherwise we will call it a mixed state.

2.2. The Gelfand-Naimark theorem and the GNS construction. Before discussing physical applications of the notions introduced in the previous section, we will take the opportunity to briefly review the characterization of C$^*$-algebras due to Gelfand, Naimark and Segal. The characterization of commutative C$^*$-algebras (the Gelfand-Naimark theorem) is of fundamental importance, in particular because it leads to the notion of a “noncommutative topological space” [5]. Also, the so-called GNS-construction discussed below is relevant not only because of its role in the characterization problem for noncommutative C$^*$-algebras, but also because of its striking consequences for the study of quantum systems (equilibrium states, symmetry breaking, inequivalent vacua, among others) [7, 8].

**Definition 2.21.** A character of a C$^*$-algebra $\mathcal{A}$ is a $\ast$-homomorphism $\mu : \mathcal{A} \rightarrow \mathbb{C}$. Let us denote with $\mathcal{M}_\mathcal{A}$ the set of all characters of $\mathcal{A}$.

Now, it is easy to see that if $\mu$ is a character, then $\mu(\alpha) \in \sigma(\alpha)$. This, together with the spectral radius formula (2.5), implies that $\|\mu\| \leq 1$, so that $\mathcal{M}_\mathcal{A} \subset \mathcal{A}_1^*$, where 

$$\mathcal{A}_1^* := \{\phi \in \mathcal{A}^* | \|\phi\| \leq 1\}$$

is the unit ball in the dual space. Since (by the Banach-Alaoglu theorem [9]) this ball is compact in the weak-$\ast$ topology (i.e. the one induced by the family of seminorms on $\mathcal{A}^*$: $p_\alpha(\phi) := |\phi(\alpha)|$, $\alpha \in \mathcal{A}$) then $\mathcal{M}_\mathcal{A}$ becomes a compact topological space in the subspace topology inherited from $\mathcal{A}^*$. This is quite interesting in view of example 2.6 as this is providing the converse statement. In fact, for a commutative, unital C$^*$-algebra $\mathcal{A}$, we define the Gelfand transform $\mathcal{G}$ as the map 

$$\mathcal{G} : \mathcal{A} \rightarrow C(\mathcal{M}_\mathcal{A})$$ 

$$a \mapsto \hat{a},$$
where $\hat{a}(\mu) := \mu(a)$.

**Theorem 2.22** (Gelfand-Naimark [10, 5, 11]). The Gelfand transform is an isometric $*$-isomorphism $A \cong C(M_A)$.

Rather than reviewing the proof of this theorem, we will consider some basic examples that should provide a good intuition about the correspondence between commutative $C^*$-algebras and (locally compact, Hausdorff) topological spaces.

**Example 2.23.** Consider the unital, commutative $C^*$-algebra $A$ generated by a unitary element $u$ (i.e. $u^*u = uu^* = 1$), with norm fixed by the condition $[12]$ that

$$\|1 + e^{-i\alpha}u\| = 2,$$

for all $\alpha \in [0, 2\pi)$. Theorem [2.22] states that this algebra must be the function algebra of a topological space which, as a set, is precisely the set $M_A$ of all characters of $A$. Since the algebra is generated by $u$, a character $\mu$ is fixed by its value on $u$. But $|\mu(u)|^2 = \mu(u^*u) = 1$, and so every character is of the form $\mu(u) = e^{i\theta}$, i.e. $M_A \subseteq S^1$. In order to see that actually $M_A = S^1$, we proceed as in [12] by noticing that from example [2.6] and from the uniqueness of the norm, it follows that $\|a\| = \sup_{\mu \in M_A} |\mu(a)|$, so that we must have

$$\sup_{\mu \in M_A} |1 + e^{-i\alpha}\mu(u)| = 2.$$

But this can only happen if for every $\alpha \in [0, 2\pi)$ there is a character $\mu$ with $\mu(u) = e^{i\alpha}$.

**Example 2.24.** The 2-sphere $S^2$ can also be easily characterized in terms of its algebra of continuous functions. In this case, the algebraic structure is well-known, as $C(S^2)$ is generated by the spherical harmonics $Y_{lm}$, their product being given as in the usual Clebsch-Gordan decomposition. More details on how $S^2$ can be obtained as the character space of such an algebra (this involves an appropriate definition of the norm, as in the previous example) can be found in [12].

**Example 2.25.** Take $A = C(S^2)$ as above (with the sup norm) and consider the subalgebra $A_+ \cong C(\mathbb{R}P^2)$. This fact has been exploited in studies of the spin-statistics connection in quantum mechanics [12, 13, 14, 15].

**Remark 2.26.** The isomorphism provided by theorem [2.22] is actually an equivalence between the categories of commutative $C^*$-algebras and locally compact, Hausdorff topological spaces. This means, among other things, that all information regarding the topology of $M$ is encoded in the algebra $C(M)$: An open set in $M$ can be equivalently described in terms of an ideal in $C(M)$, closed sets are described by quotient algebras, metrizability of $M$ amounts to separability of $C(M)$, and so on [10]. This is the reason why the Gelfand-Naimark theorem is considered one of the main sources for the development of noncommutative geometry [5, 11].

Now we turn to the GNS (Gelfand-Naimark-Segal) construction. Let $A$ be a $C^*$-algebra, and $\omega$ a state thereon. The GNS construction furnishes a representation of $A$ on some ($\omega$-dependent) Hilbert space. The basic idea is to use multiplication in $A$ in order to obtain a linear action of $A$ on a vector space. So we begin by regarding $A$ as a vector space $\hat{A}$ (i.e. we just “forget” multiplication). Even though the underlying spaces are equal, it will be convenient to distinguish the algebra, with
elements $a \in \mathcal{A}$, from the underlying vector space, with elements $|a\rangle \in \hat{\mathcal{A}}$. Recalling the Cauchy-Schwarz inequality (exercise 2.19), we realize that it makes sense to introduce the following sesquilinear form on $\hat{\mathcal{A}}$:

$$\langle a|b \rangle_\omega := \omega(a^*b).$$

This is “almost” an inner product, as it may happen that $\langle a|a \rangle_\omega = 0$ for some $a \neq 0$. But ignoring that fact for a moment, we notice that the product on $\mathcal{A}$ can be used to make $\mathcal{A}$ act as a linear operator on $\hat{\mathcal{A}}$:

$$\mathcal{A} \times \hat{\mathcal{A}} \longrightarrow \hat{\mathcal{A}}$$

$$a, |b \rangle \longmapsto a \cdot |b \rangle := |ab \rangle.$$

Now, in order to have a Hilbert space representation, we have to “fix” the problem with (2.6). This is done as follows.

**Exercise 2.27.** Define $\mathcal{N}_\omega := \{ a \in \mathcal{A} | \omega(a^*a) = 0 \}$, and show that it is a closed left-ideal of $\mathcal{A}$.

We therefore obtain a Hilbert space $\mathcal{H}_\omega$ given by the completion of $\hat{\mathcal{A}}/\mathcal{N}_\omega$ with respect to the inner product $\langle [a]|[b] \rangle_\omega := \omega(a^*b)$, where we use $|[a]\rangle$ to denote the equivalence class of $a$ in (the completion of) $\hat{\mathcal{A}}/\mathcal{N}_\omega$. With this we have obtained a $*$-representation of $\mathcal{A}$ by bounded operators acting on $\mathcal{H}_\omega$:

$$\pi_\omega : \mathcal{A} \longrightarrow \mathcal{B}(\mathcal{H}_\omega)$$

$$a \longmapsto \pi_\omega(a),$$

where $\pi_\omega(a)|[b]\rangle := |[ab]\rangle$.

**Exercise 2.28.** Obtain the following inequality:

$$\sqrt{\omega(a^*a)} \leq \|\pi_\omega(a)\| \leq \|a\|.$$

Although the representation $\pi_\omega$ is a $*$-homomorphism, it is not isometric. But it can be shown that for every $a \in \mathcal{A}$ there is a state $\omega$ such that $\omega(a^*a) = \|a\|^2$. Then, if we consider the direct sum

$$\mathcal{H} = \bigoplus_{\omega \in \mathcal{S}_\mathcal{A}} \mathcal{H}_\omega := \{ (\xi_\omega)_{\omega \in \mathcal{S}_\mathcal{A}} | \xi_\omega \in \mathcal{H}_\omega, \sum_{\omega \in \mathcal{S}_\mathcal{A}} \|\xi_\omega\|_\omega^2 < \infty \},$$

where in each sequence $(\xi_\omega)_{\omega \in \mathcal{S}_\mathcal{A}}$ only countable many elements are different from zero. The representations $\pi_\omega$ then give rise to a representation $\pi$ on $\mathcal{H}$ for which $\|\pi(a)\| = \|a\|$. The details of this construction can be found e.g. in [6]. The importance of this result is that any $C^*$-algebra is isometrically isomorphic to the $C^*$-algebra of bounded operators in some Hilbert space.

### 2.3. Composite systems, entanglement.

In this section, our aim will be to study certain quantum correlations that arise as a result of entanglement. This is a vast subject, and here we will only consider elementary examples, corresponding to bipartite systems. Although very simple from the mathematical point of view, these examples already contain the essence that will allow us to distinguish between classical and genuinely quantum correlations. We will also discuss a recent application of the algebraic formalism to the study of entanglement for systems of identical particles [17, 18], a topic of current interest for quantum information, condensed matter, atomic physics, and quantum optics.
We thus start by considering a composite system that is the result of coupling two subsystems 1 and 2. We will first consider quantum systems described directly in terms of Hilbert spaces. But, as will become clear, the algebraic approach based only on observable algebras and states will allow us to reformulate these ideas in more generality. This will be important for the applications to systems of identical particles. Let \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) denote the corresponding (finite dimensional, for simplicity) Hilbert spaces, and assume that the subsystems are described in terms of observable algebras \( \mathcal{A}_i \subseteq B(\mathcal{H}_i) \), \( i = 1, 2 \). Subsystems 1 and 2 are then coupled to form a composite system that will be described by \( \mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2 \).

Let now \( \omega : \mathcal{A} \to \mathbb{C} \) be a state of the composite system. Consider “partial”, or “local” measurements performed on each subsystem. This leads us to consider the restriction of \( \omega \) to \( \mathcal{A}_i \), \( i = 1, 2 \):
\[
\omega_1 := \omega|_{\mathcal{A}_1}, \quad \omega_2 := \omega|_{\mathcal{A}_2}.
\]

**Definition 2.29.** In the present context of a bipartite composite system, if \( \omega \) is a pure state on \( \mathcal{A} \), we say it is a separable state if
\[
\omega(a \otimes b) = \omega_1(a)\omega_2(b),
\]
for all \( a \in \mathcal{A}_1 \), \( b \in \mathcal{A}_2 \). A (pure) state that is not separable in the above sense is called an entangled state.

**Example 2.30.** Let \( \mathcal{H}_1 = \mathbb{C}^n \), with basis \( \{ |e_1 \rangle, \ldots, |e_n \rangle \} \) and \( \mathcal{H}_2 = \mathbb{C}^m \), with basis \( \{ |u_1 \rangle, \ldots, |u_m \rangle \} \). Let \( \mathcal{A}_1 = M_n(\mathbb{C}) \) and \( \mathcal{A}_2 = M_m(\mathbb{C}) \). The composite system is then described by the matrix algebra \( \mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2 \). Pick now a vector state \( |\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \) and set
\[
\omega_\psi : \mathcal{A} \to \mathbb{C}
\]
\[
\alpha \mapsto \langle \psi | \alpha | \psi \rangle.
\]

Then, the following three conditions are equivalent:

1. The vector state \( |\psi\rangle \) is of the form \( |\psi\rangle = |\varphi\rangle \otimes |\xi\rangle \).
2. \( S(\rho_{\psi,i}) = 0 \), \( i = 1, 2 \), where \( S(\rho_{\psi,i}) \) stands for the von Neumann entrop of the reduced density matrix \( \rho_{\psi,i} \) (see definitions below).
3. The state \( \omega_\psi \) is separable.

To see where these equivalences come from, let us expand \( |\psi\rangle \) as
\[
|\psi\rangle = \sum_{i=1}^n \sum_{j=1}^m A_{ij} |e_i\rangle \otimes |u_j\rangle.
\]

Then \( A \in M_{n,m}(\mathbb{C}) \), so we may perform a singular value decomposition and write it in the form \( A = UDV^\dagger \), with \( D \) a diagonal matrix in \( M_{n,m}(\mathbb{C}) \), \( U \in M_n(\mathbb{C}) \) and \( V \in M_m(\mathbb{C}) \). The elements of \( D \) are \( D_{kl} = \delta_{kl} \sqrt{\lambda_k} \), where the \( \lambda_k \) are called the “Schmidt coefficients”, are the eigenvalues of \( A^\dagger A \). If we define vectors
\[
|k\rangle_1 := \sum_{i=1}^n U_{ik} |e_i\rangle, \quad |k\rangle_2 := \sum_{j=1}^m V_{jk} |u_j\rangle,
\]
then we obtain
\[
|\psi\rangle = \sum_k \sqrt{\lambda_k} |k\rangle_1 \otimes |k\rangle_2.
\]

From this expression, it is clear that (i) holds precisely when there is only one non-vanishing Schmidt coefficient. Furthermore, from \( \langle \psi | \psi \rangle = 1 \) we obtain \( \sum_k \lambda_k = 1 \),
with \(0 \leq \lambda_k \leq 1\). We can, therefore, regard \(\{\lambda_k\}_k\) as a probability distribution, and compute its (Shannon) entropy, defined as

\[
H(\{\lambda_k\}_k) := -\sum_k \lambda_k \log \lambda_k.
\] (2.7)

Notice that this function vanishes precisely when \(|\psi\rangle\) is a separable state. We can relate it to the von Neumann entropy of the restricted states \(\omega_{\psi,i}\) as follows.

**Exercise 2.31.** Consider the restriction \(\omega_{\psi,i}\) of \(\omega_{\psi}\) to \(A_i \subseteq A\) (\(i = 1, 2\)). Find density matrices \(\rho_{\psi,i}\) (“reduced density matrices”) acting on \(H_i\) and such that \(\omega_{\psi}(a \otimes 1_m) = \text{Tr}_{H_i}(\rho_{\psi,1} a)\) and \(\omega_{\psi}(1_n \otimes b) = \text{Tr}_{H_2}(\rho_{\psi,2} b)\).

The von Neumann entropy of a density matrix \(\rho\) is defined as

\[
S(\rho) = -\text{Tr}(\rho \log \rho).
\]

Show that \(S(\rho_{\psi,1})\) and \(S(\rho_{\psi,2})\) coincide and are exactly equal to \(H(\{\lambda_k\}_k)\) from (2.7).

We therefore consider the quantity \(S(\rho_{\psi,i})\) (\(i = 1, 2\)) as a measure of the “amount of entanglement” of the state \(|\psi\rangle\). In order to really appreciate the meaning of this assertion, we have to understand the (very surprising, and interesting) features of quantum correlations. This can be considered as one of the starting points of quantum information theory. In quantum information theory, there are orderly ways to pose and study these type of problems where, for instance, in the (pure) bipartite case the von Neumann entropy of the reduced density matrix can be obtained as (basically) the unique entanglement measure of the state \(|\psi\rangle\), when entanglement is regarded as a physical resource and defined in operational terms \([19, 20]\). The general problem, that of multipartite entanglement, is much more complicated and involves many mathematically as well as physically interesting problems. However, our interest here will be restricted to the (pure) bipartite case. This will be enough to illustrate one of our points, which is that the algebraic framework leads to a unified description of physical systems, no matter whether they are classical or quantum. Also, the “detachment” from an a priori given Hilbert space in the quantum case allows for a more clear understanding of phenomena. As it turns out, the noncommutativity of the observable algebra can be seen as the main source of (truly quantum) correlations. This fits nicely with the relation between commutative and noncommutative spaces, as hinted above.

The next example illustrates the previous remarks.

**Example 2.32.** Let us consider the composition of two classical systems. By this we mean that the “coupling” of two systems described by (commutative) observable algebras of the form \(A_1 = C(X)\) and \(A_2 = C(Y)\) is effected by the tensor product \(A_1 \otimes A_2\). Tensor products of \(C^*\)-algebras have to be treated carefully, but assuming we have defined the appropriate tensor product, let us assume that \(C(X) \otimes C(Y) \simeq C(X \times Y)\) (a detailed discussion about tensor products can be found in \([16]\)). Hence, the composite system will be assumed to be described by the observable algebra \(A = C(X \times Y)\). Consider now a state \(\omega\) on \(A\). It is not difficult to see that it must be given by a probability distribution \(p(x, y)\) in such a way that for \(h \in A\),

\[
\omega(h) = \int_{X \times Y} h(x, y)p(x, y)dxdy.
\]
Restriction to \( A_1 \) or \( A_2 \) in this case leads to marginal distributions \( p_1(x) = \int_y p(x, y) dy \) and \( p_2(y) = \int_x p(x, y) dx \), which in turn define states \( \omega_i \) on \( A_i \). From the above definition we have that \( \omega \) is separable if, and only if,
\[
\omega(f \otimes g) = \omega_1(f)\omega_2(g), \quad \text{for all } f \in A_1, g \in A_2.
\]
But from the properties of the Gelfand transform it follows that any pure state on \( C(X \times Y) \) is of the form \( \omega(h) = h(x_0, y_0) \), i.e., they are given by point measures: \( p(x, y) = \delta_{(x_0,y_0)}(x,y) \). It follows immediately that \( \omega(f \otimes g) = \omega_1(f)\omega_2(g) \). This illustrates the fact that entanglement entails purely quantum correlations, as all pure states of a classical composite (bipartite) system are separable.

**Exercise 2.33.** The previous example was formulated in rather loosely terms. Provide the necessary details to turn it into a rigorous proof that works for locally compact spaces.

**Example 2.34.** On \( \mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2 \) consider the following family of states:
\[
|\psi_\lambda\rangle := \sqrt{\lambda} |+\rangle - \sqrt{1-\lambda} |-\rangle,
\]
and the following types of observables, acting on \( \mathbb{C}^2 \):
\[
P(a) := \frac{1}{2} (\mathbb{1} + \vec{a} \cdot \vec{\sigma}), \quad E(a) := \vec{a} \cdot \vec{\sigma},
\]
with \( \vec{a} \) a unit vector in \( \mathbb{R}^3 \) and \( \vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3) \) (Pauli matrices). Straightforward computations give
\[
\langle \psi_\lambda | E(a) \otimes E(b) | \psi_\lambda \rangle = -a_3b_3 - 2\sqrt{\lambda(1-\lambda)}(a_1b_1 + a_2b_2)
\]
and
\[
\langle \psi_\lambda | P(a) \otimes P(b) | \psi_\lambda \rangle = \frac{1}{4} \left( 1 + 2(\lambda - 1)(a_3 - b_3) - a_3b_3 - 2\sqrt{\lambda(1-\lambda)}(a_1b_1 + a_2b_2) \right).
\]
Whereas for \( \lambda = 0,1 \) we obtain separable states, for \( 0 < \lambda < 1 \) we have entangled states. In particular, for \( \lambda = 1/2 \) we obtain a maximally entangled state (Bell state), for which
\[
\langle \psi_{1/2} | P(a) \otimes P(b) | \psi_{1/2} \rangle = \frac{1}{4} \left( 1 - \vec{a} \cdot \vec{b} \right).
\]
In this case, the marginal distributions give
\[
P_A(a,+)=\frac{1}{2}=P_A(a,-),
\]
\[
P_B(b,+)=\frac{1}{2}=P_B(b,-),
\]
whereas for the joint probabilities we obtain \( (r, r' = \pm 1) \):
\[
P_{rr'} = \frac{1}{4} \left( 1 - rr'\vec{a} \cdot \vec{b} \right).
\]
In particular, for the choice \( \vec{a} \cdot \vec{b} = 1 \), we obtain total anticorrelation.

What is so special about the previous example? Consider the Clauser-Horne-Shimony-Holt (CHSH) inequality [19, 20]:
\[
\langle A(B + B') + A'(B - B') \rangle \leq 2,
\]
where \( \langle X \rangle \) denotes the expectation value of an observable \( X \), and where for the involved observables it is assumed that \(-1 \leq A, A', B, B' \leq 1 \). The inequality can
be obtained if we assume some underlying (classical) probability space \((\Omega, d\mu)\), for which the correlations above take the form
\[
\langle AB \rangle_\mu = \int_\Omega A(x)B(x)d\mu(x),
\]
or, stated in terms of algebras of observables:

Exercise 2.35. Let \(A\) be a commutative \(C^*\)-algebra, \(\omega\) a pure state thereon, and \(a, a', b, b'\) elements of \(A\), all of them with norm less or equal to one. Show that
\[
\omega(a(b + b') + a'(b - b')) \leq 2.
\]

But, in contrast to this, in example 2.34 (with \(\lambda = 1/2\)) we obtain
\[
\langle \psi_{1/2} | E(a) \otimes (E(b) + E(b')) + E(a')(E(b) - E(b')) | \psi_{1/2} \rangle = \vec{a} \cdot \vec{b} + \vec{a} \cdot \vec{b}' + \vec{a}' \cdot \vec{b} - \vec{a}' \cdot \vec{b}'.
\]

Now, it is easy to find an arrangement for the vectors \(a, a', b, b'\) such that the CHSH inequality is violated. The importance of these type of inequalities, of which Bell’s inequality was the first one, cannot be overemphasized, as they have allowed for definitive experimental tests of quantum mechanics. The CHSH inequality is also relevant in the context of hidden-variable models, and related no-go theorems [21].

In the next section we will consider the problem of entanglement for systems of identical particles, for which the tools developed in the last sections will prove very useful.

2.4. Identical particles and entanglement. When combined, two of the most intriguing features of quantum theory -the intrinsic indistinguishability of identical particles and quantum entanglement- lead to formidable conceptual issues that have been addressed for years, and for which no generally accepted framework exists. The main source of problems comes from the fact that entanglement and related concepts have been studied mainly in cases where a subsystem decomposition coincides with a tensor product decomposition of the Hilbert space. But precisely in the case of identical particles, the Hilbert space is the antisymmetric/symmetric subspace obtained from the action of the permutation group on a tensor product space. So precisely in this case decomposition into subsystems does not correspond to tensor product decomposition. This makes the use of partial trace a doubtful operation, leading to a clash with standard notions of entanglement. In [17][18][22], we have shown how, using the representation theory of operator algebras, it is possible to obtain a generalized notion of entanglement. The universality of the approach, which can be applied to particles obeying any kind of statistics including bosons, fermions, parafermions and particles obeying braid statistics, provides a unifying view of entanglement, with many potential applications.

The key idea is that, since subsystems can always be described in terms of subalgebras, the use of partial trace will be superseded by the more general notion of restriction of a quantum state \(\omega\) to a subalgebra. Then one can make use of the GNS construction in order to find a Hilbert space representation \(\pi_\omega\), as above.

Exercise 2.36. Prove that the GNS representation \(\pi_\omega\) is irreducible precisely when the state \(\omega\) is pure.

From this exercise, it follows that the condition for irreducibility of the representation \(\pi_\omega\) is precisely that the von Neumann entropy of the state \(\omega\) vanishes.
and so, given a subsystem described in terms of a subalgebra \( A_0 \subset A \), one may consider the restriction of the state \( \omega \) to \( A_0 \). This is a generalization of the notion of partial trace. Hence, a generalized notion of entanglement emerges, based on the von Neumann entropy of the restricted state. The properties of this entanglement measure are very closely tied to the GNS-representation of the subalgebra and the restricted state. In other words, one finds that entanglement depends both on the state and the subsystem of the full system. This formalism, then, lends itself to the study of problems where partial trace loses its meaning, as is the case with systems of identical particles. Let us consider a few illustrative examples.

**Example 2.37.** Consider the algebra \( A = M_2(\mathbb{C}) \) of \( 2 \times 2 \) matrices with complex entries, and let

\[
\omega_\lambda(a) = \lambda a_{11} + (1 - \lambda)a_{22}
\]

be a state on \( A \). Of course, this can only happen if \( 0 \leq \lambda \leq 1 \). Let us then see how the GNS representation is constructed, and how we can associate an entropy to the state \( \omega_\lambda \). For this purpose, let us consider the matrix units \( e_{ij} = |i\rangle\langle j| \) \((i,j = 1,2)\). They generate the algebra, and provide a basis for the underlying vector space \( \hat{A} \). They also fulfill the relations

\[
e_{ij}e_{kl} = \delta_{jk}e_{il}. \tag{2.8}
\]

Let us now check whether there will be null vectors. Writing a general element \( a \in A \) as

\[
a = \sum_{ij} a_{ij}e_{ij},
\]

we compute

\[
\omega_\lambda(aa^*) = \sum_{i,j,k} \omega_\lambda(a_{ki}a_{kj}e_{ij}) \tag{2.9}
\]

\[
= \lambda(|a_{11}|^2 + |a_{21}|^2) + (1 - \lambda)(|a_{12}|^2 + |a_{22}|^2).
\]

From this expression we recognize that, if \( \lambda \in (0,1) \), then \( \dim(\mathcal{H}_{\omega_\lambda}) = 4 \), whereas for \( \lambda = 0 \) or \( \lambda = 1 \) we obtain \( \dim(\mathcal{H}_{\omega_\lambda}) = 2 \). In fact, if \( \lambda \) is different from zero or one, we must have both \( (|a_{11}|^2 + |a_{21}|^2) = 0 \) and \( (|a_{12}|^2 + |a_{22}|^2) = 0 \). It follows that \( \mathcal{N}_{\omega_\lambda} = \{0\} \). From

\[
\pi_{\omega_\lambda}(|a\rangle\langle b|) = |ab\rangle
\]

and \( \text{[2.8]} \) we see that the representation is reducible, with 2 invariant subspaces generated, respectively, by \( \{|e_{11}\rangle, |e_{21}\rangle\} \) and \( \{|e_{12}\rangle, |e_{22}\rangle\} \). From exercise \( \text{2.36} \) we conclude that, in this case, the state has to be a mixed state. The cases \( \lambda = 0 \) and \( \lambda = 1 \) lead to a non-trivial null space, and from \( \text{[2.9]} \) we conclude that the dimension of these irreducibles is, in both cases, equal to 2. It is left to the reader to obtain a pure state on the algebra \( M_2(\mathbb{C}) \otimes M_2(\mathbb{C}) \) such that \( \omega_\lambda \) is the restriction to \( M_2(\mathbb{C}) \).

The next question we need to address is that of how to compute the entropy of the reduced state. Since our algebras will in general be unital, there is a simple way to accomplish this, namely, given a (unital) \( C^* \)-algebra \( A \) and a state \( \omega \) on it, it is always possible to find a density matrix \( \rho_\omega \) acting on the GNS space \( \mathcal{H}_\omega \), and such that

\[
\omega(a) = \text{Tr}_{\mathcal{H}_\omega}(\rho_\omega a)
\]
for all \( a \) in \( \mathcal{A} \). From the decomposition of the GNS space into irreducibles, 
\[
\mathcal{H}_\omega = \bigoplus_j \mathcal{H}_\omega^{(j)},
\]
we obtain projectors \( P^{(j)} \), with \( \sum_j P^{(j)} = \mathbb{1}_{\mathcal{H}_\omega} \). From the definition of the inner product in \( \mathcal{H}_\omega \) we have \( \omega(a) = \langle [1_A]|\pi_\omega(a)|[1_A]\rangle \). But then, using an orthonormal basis \( \{|n\rangle\}_n \) on \( \mathcal{H}_\omega \), we can write:
\[
\omega(a) = \langle [1_A]|\pi_\omega(a)|[1_A]\rangle = \langle [1_A]\sum_k P^{(k)}\pi_\omega(a)P^{(k)}|[1_A]\rangle = \langle [1_A]\sum_k P^{(k)}\pi_\omega(a)\sum_n \langle n|P^{(k)}|[1_A]\rangle \rangle = \text{Tr}_{\mathcal{H}_\omega}(\rho_\omega \pi_\omega(a)),
\]
with \( \rho_\omega \) given by
\[
\rho_\omega = \sum_k P^{(k)}|[1_A]\rangle\langle [1_A]|P^{(k)}.
\]

Consider now a composite, bipartite system for which the Hilbert space is of the form \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \). If \( \omega_\psi \) is a state on the algebra of bounded operators on \( \mathcal{H}_A \otimes \mathcal{H}_B \) that is obtained from a vector state \( |\psi\rangle \in \mathcal{H} \), then its restriction to the subalgebra \( \mathcal{A}_1 \) generated by elements of the form \( K \otimes 1_B \) gives a state
\[
\omega_1(K) \equiv \omega_{\mathcal{A}_1}(K \otimes 1_B) = \text{Tr}_{\mathcal{H}_A}(\rho_A K),
\]
where \( \rho_A \) is the reduced density matrix, defined through partial trace (cf. exercise 2.31),
\[
\rho_A = \text{Tr}_{\mathcal{H}_B}|\psi\rangle\langle \psi|.
\]
We therefore see that, for these kind of systems, partial trace equals restriction (to some subalgebra).

**Exercise 2.38.** Compute de von Neumann entropy of the density matrix \( \rho_\omega \) corresponding to the GNS space of example 2.37 and provide a physical interpretation.

The real usefulness of the algebraic approach becomes apparent only when we consider situations where the Hilbert space does not have a simple tensor product structure. This is what happens, e.g., with systems of identical particles. Because of the symmetrization postulate, the Hilbert space contains only the symmetric (for bosons) or the antisymmetric (for fermions) subspaces of the many-particle Hilbert space. As a consequence, one finds that states that from a physical point of view should not \textit{a priori} be considered to be entangled, will have reduced density matrices with non-vanishing entanglement entropy [23]. In approaches like those of [24] or [17], the description of subsystems is given by specifying suitable subalgebras. Then, the restriction of a given state to the subalgebra provides a physically sensible generalization of the notion of partial trace. Applying the GNS construction to the restricted state, it is possible to study the entropy emerging from restriction and use it as a generalized measure of entanglement.

Let us briefly discuss how this entanglement measure can be computed in concrete cases. For this purpose, consider a Hilbert space \( \mathcal{H}^{(1)} = \mathbb{C}^d \), assumed to
correspond to the space of 1-particle states of a fermionic system. The full Hilbert space is then the antisymmetric Fock space $\mathcal{F}$ obtained from $\mathcal{H}^{(1)}$. It decomposes as a direct sum of spaces of fixed number of particles. The $k$-particle Hilbert space $\mathcal{H}^{(k)}$ is just the antisymmetrized $k$-fold tensor product of $\mathcal{H}^{(1)}$. This is a kind of “toy model” for a fermionic quantum field theory, but many important features of a quantum field theory can be seen to appear already at this level. One of these features is the connection to the representation theory of Clifford algebras, as explained in full detail in [11]. As is well-known, the Clifford algebra of $\mathcal{H}^{(1)}$ acts naturally on the exterior algebra $\bigwedge^*(\mathcal{H}^{(1)})$ which, in turn, is related to the Fock space construction in the following way.

Let $\{e_n\}_n$ denote an orthonormal basis for $\mathcal{H}^{(1)}$, and denote with $a_n^{(i)}$ the corresponding annihilation (creation) operators (cf. exercise 2.10). Then, there is a vector space isomorphism between $\mathcal{F}$ and $\Lambda^*(\mathcal{H}^{(1)})$, furnished by the correspondence

$$e_{i_1} \wedge e_{i_2} \wedge \cdots \wedge e_{i_k} \leftrightarrow a_1^\dagger a_2^\dagger \cdots a_k^\dagger |0\rangle,$$

(2.10)

This correspondence is behind the famous quote by E. Nelson: “first quantization is a mystery, but second quantization is a functor”. In fact, given a self-adjoint operator $A$ on $\mathcal{H}^{(1)}$ (that is, a 1-particle observable), we obtain (by functoriality) an operator $d\Gamma(A)$ acting on Fock space, whose restriction to the $k$-particle sector $\mathcal{H}^{(k)}$ is given by

$$d\Gamma^{(k)}(A) := (A \otimes I_d \otimes \cdots \otimes I_d) +$$

(2.11)

$$+ (I_d \otimes A \otimes \cdots \otimes I_d) + \cdots + (I_d \otimes \cdots \otimes I_d \otimes A).$$

Taking the correspondence (2.10) into account, we obtain the following expression for $d\Gamma(A)$ in terms of creation/annihilation operators,

$$d\Gamma(A) = \sum_{i,j} A_{ij} a_i^\dagger a_j,$$

(2.12)

where $A_{ij} = \langle e_i | A | e_j \rangle$. In the physics literature, the operator $d\Gamma(A)$ is referred to as the second quantization of $A$.

In the present quantum-mechanical context, where the number of particles is kept fixed, we want to focus our attention on the operator $d\Gamma^{(k)}(A)$. One of the properties of this operator is that it preserves the symmetries of $\mathcal{H}^{(k)}$. Furthermore, the map $A \rightarrow d\Gamma^{(k)}(A)$ allows us to study subalgebras of 1-particle observables.

The simplest example we can consider in order to illustrate entanglement issues for systems of identical particles is that of just two fermions. Let us then consider, as done in [25] and in [17], a 2-fermion system, where each fermion can be in a linear superposition of 4 basic states which, for the sake of physical interpretation, will be divided into internal and external degrees of freedom. So we describe 1-particle states in terms of a set of (fermionic) creation/annihilation operators $a_\lambda^{(i)}, b_\lambda^{(i)}$, where $a$ stands for “left”, $b$ for “right” (the external degrees of freedom) and $\lambda = 1, 2$ for spin up and down (the internal degrees of freedom). Hence, in this case we have $\mathcal{H}^{(1)} = \mathbb{C}^4$ and, for the 2-fermion space, $\mathcal{H}^{(2)} = \bigwedge^2 \mathbb{C}^4$. An orthonormal basis for $\mathcal{H}^{(2)}$ is given by the vectors

$$a_1^{\dagger} a_2^{\dagger} |0\rangle, \quad b_1^{\dagger} b_2^{\dagger} |0\rangle, \quad a_1^{\dagger} b_2^{\dagger} |0\rangle \quad \text{and} \quad a_2^{\dagger} b_1^{\dagger} |0\rangle.$$

The two-particle algebra $\mathcal{A}$ of observables is thus isomorphic to the matrix algebra $M_6(\mathbb{C})$. 
For $|\psi_\theta\rangle = (\cos \theta a^\dagger_1 b^\dagger_2 + \sin \theta a^\dagger_2 b^\dagger_1)|\Omega\rangle$, the corresponding state $\omega_\theta$ is given by $\omega_\theta(a) = \langle \psi_\theta | a | \psi_\theta \rangle$ for $a \in \mathcal{A}$. We choose the subalgebra $\mathcal{A}_0$ to be the one generated by $1_{\mathcal{A}}$, $n_{12} = a^\dagger_1 a_1 a^\dagger_2 a_2$, $N_a = a^\dagger_1 a_1 + a^\dagger_2 a_2$ and $T_{i=1,2,3} = (1/2) a^\dagger_1 (\sigma_i)^{\lambda\lambda^\prime} a_{\lambda^\prime}$. Physically, it corresponds to the subalgebra of one-particle observables corresponding to measurements at the left location.

Exercise 2.39. Consider the restriction of $\omega_\theta$ to $\mathcal{A}_0$ and study the GNS representation corresponding to this choice. For $\theta = 0, \pi/2$ you should obtain vanishing entropy, in contrast to the result $S = \log_2 2$ obtained via partial trace for states with Slater rank one [17, 18, 26, 23].

3. Spin Chains

3.1. The transverse Ising chain. The Hamiltonian for the (quantum) Ising chain in a transverse field is given by

$$H = -\sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x - \lambda \sum_{i=1}^{N} \sigma_i^z. \quad (3.1)$$

An important aspect when solving the model and studying its solution is the type of boundary conditions considered. We will be interested in both open as well as periodic boundary conditions. The first step in the solution of this model is the so-called Wigner-Jordan transformation, that allows us to express all spin operators in terms of fermionic creation/annihilation operators:

As can be easily checked, the operators defined by

$$a_i = \sigma^z \otimes \cdots \otimes \sigma^z \otimes \sigma^+,$$
$$a_i^\dagger = \sigma^z \otimes \cdots \otimes \sigma^z \otimes \sigma^-,$ \quad (3.2)$$

where $\sigma^\pm = \frac{1}{2}(\sigma^x \pm i \sigma^y)$, are fermionic operators.

Exercise 3.1. Check that the operators defined above indeed satisfy the CAR algebra:

$$\{a_i, a_j^\dagger\} = 0 = \{a_i^\dagger, a_j\}.$$ 

The inverse transformation is given by

$$\sigma_i^z = 1 - 2a_i^\dagger a_i,$$
$$\sigma_i^x = \left( \prod_{m<i} (1 - 2a_m^\dagger a_m) \right) (a_i^\dagger + a_i), \quad (3.3)$$
$$\sigma_i^y = i \left( \prod_{m<i} (1 - 2a_m^\dagger a_m) \right) (a_i^\dagger - a_i).$$

Exercise 3.2. Check that (3.3) is the inverse transformation to (3.2).

With this we obtain, for the interaction terms of the Hamiltonian,

$$\sigma_i^x \sigma_{i+1}^x = (a_i^\dagger - a_i)(a_{i+1}^\dagger + a_{i+1}),$$

and so $H$ the takes the form

$$H = -\sum_{i=1}^{N-1} (a_i^\dagger - a_i)(a_{i+1}^\dagger + a_{i+1}) - \lambda \sum_{i=1}^{N} (1 - 2a_i^\dagger a_i). \quad (3.4)$$

The term containing the external field $\lambda$ is diagonal in this basis. The constant term $-\lambda N$ coming from the last sum is usually disregarded, because its only effect
is to shift the energy spectrum. We will nevertheless keep all terms, in order to be able to compare with numerical solutions in the spin basis, for small values of $N$.

Expanding all terms in (3.4) and moving all creation operators to the left, we obtain (cf. Eq. (10.14) in [27]):

$$H = -\sum_{i=1}^{N-1} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1}^\dagger - a_i a_{i+1}) + 2\lambda \left( \sum_{i=1}^{N} a_i^\dagger a_i \right) - \lambda N.$$  

The point of using the Wigner-Jordan transformation for this model is that the Hamiltonian becomes “almost” diagonal. By this we mean that it is a sum of local, quadratic expressions in the creation and annihilation operators. As we will see, such models can be exactly solved. We now write $H$ in a suggestive matrix notation. Arranging all creation and annihilation operators in rows and columns, we can write $H$ as a kind of quadratic form. For example, we have, for $N = 2$,

$$(a_1^\dagger, a_2^\dagger) \begin{pmatrix} 2\lambda & -1 \\ -1 & 2\lambda \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = -a_1^\dagger a_2 - a_2^\dagger a_1 + 2\lambda a_1^\dagger a_1 + 2\lambda a_2^\dagger a_2.$$  

The expression corresponding to the same term for $N = 4$ is then

$$\begin{pmatrix} a_1^\dagger, a_2^\dagger, a_3^\dagger, a_4^\dagger \end{pmatrix} \begin{pmatrix} 2\lambda & -1 & 0 & 0 \\ -1 & 2\lambda & -1 & 0 \\ 0 & -1 & 2\lambda & -1 \\ 0 & 0 & -1 & 2\lambda \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = -a_1^\dagger a_2 + a_2^\dagger a_1 - a_2^\dagger a_3 - a_3^\dagger a_2 - a_3^\dagger a_4 - a_4^\dagger a_3 + 2\lambda \sum_{i=1}^{4} a_i^\dagger a_i.$$  

For arbitrary $N$, we may define the following $N \times N$ matrices:

$$A = \begin{pmatrix} 2\lambda & -1 & 0 & 0 & \cdots \\ -1 & 2\lambda & -1 & 0 & \cdots \\ 0 & -1 & 2\lambda & -1 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}, \quad B = \begin{pmatrix} 0 & -1 & 0 & 0 & \cdots \\ 1 & 0 & -1 & 0 & \cdots \\ 0 & 1 & 0 & -1 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}.$$  

The matrix elements of these two matrices can be written as follows:

$$A_{ij} = 2\lambda \delta_{i,j} - (\delta_{i+1,j} + \delta_{i,j+1}), \quad B_{ij} = -(\delta_{i+1,j} - \delta_{i,j+1}).$$

Hence, the Hamiltonian takes the following form:

$$H = \sum_{i,j=1}^{N} \left[ a_i^\dagger A_{ij} a_j + \frac{1}{2} \left( a_i^\dagger B_{ij} a_j^\dagger - a_i a_j a_i^\dagger a_j \right) \right] - \lambda N.$$  

### 3.2 Open boundary conditions

For several reasons, including the study of edge states, it is instructive to explore the explicit solution of this model for open boundary conditions. We start with the Ising Hamiltonian written in the form (3.6). Any model that can be written as a quadratic form can be expressed in this way, the “only” difference being the explicit form of the matrices $A$ and $B$ (notice that, in order for $H$ to be Hermitian, $A$ has to be symmetric and $B$ antisymmetric). In principle, thus, the method presented below (following the work of Lieb, Schultz and Mattis [28]) can be applied to any such model.

For periodic boundary conditions, it is usually more convenient to take into account translation invariance and hence to introduce Fourier transformed operators.
But for open boundary conditions, translation invariance is “broken” and then it is a good idea to start right away with a Bogoliubov transformation, as explained below.

Recall that the operators \( a_i, a_i^\dagger \) defined in (3.2) obey fermionic canonical anti-commutation (CAR) relations (cf. exercise 3.1):

\[
\{ a_i, a_j^\dagger \} = \delta_{ij}, \quad \{ a_i, a_j \} = 0 = \{ a_i^\dagger, a_j^\dagger \}.
\]

In general, a Bogoliubov transformation is a mapping induced by a change of basis on the one-particle Hilbert space (unitary transformation), its main effect being to provide a new set of creation/annihilation operators for which the Hamiltonian (3.6) becomes diagonal. Consider, then, a new set of operators given by

\[
c_k = \sum_{i=1}^{N} (g_{ki} a_i + h_{ki} a_i^\dagger), \quad c_k^\dagger = \sum_{i=1}^{N} (\bar{g}_{ki} a_i^\dagger + \bar{h}_{ki} a_i),
\]

where \( g \) and \( h \) are \( N \times N \) matrices to be chosen so that

(i) The new operators satisfy the same CAR algebra:

\[
\{ c_k, c_l^\dagger \} = \delta_{kl}, \quad \{ c_k, c_l \} = 0 = \{ c_k^\dagger, c_l^\dagger \}.
\]

(ii) The Hamiltonian becomes diagonal in the new basis:

\[
H = \sum_k \Lambda_k c_k^\dagger c_k + \mu \tag{3.9}
\]

(with \( \mu \) some constant).

**Exercise 3.3.** Show that the requirement (3.8) leads to the following conditions:

\[
\begin{align*}
g g^\dagger + h h^\dagger &= 1_N, \\
g h^\dagger + h g^\dagger &= 0.
\end{align*}
\]

**Exercise 3.4.** Compute the trace of \( H \) in two different ways, in order to show that the constant term in (3.9) is given by

\[
\mu = \frac{1}{2} \left( \text{Tr} A - \sum_k \Lambda_k \right) - \lambda N.
\]

The second condition above, Eq. (3.9), will lead to an eigenvalue problem for \( g \) and \( h \), the solution of which amounts in principle to the solution of the full problem.

Now we compute the commutator \([c_k, H]\) in two different ways, once using (3.6) and once using (3.9). This leads to the following set of equations:

\[
g_{ki} \Lambda_k = \sum_{j=1}^{N} (g_{kj} A_{ji} - h_{kj} B_{ji}), \quad h_{ki} \Lambda_k = \sum_{j=1}^{N} (g_{kj} B_{ji} - h_{kj} A_{ji}). \tag{3.11}
\]

In order to solve this eigenvalue problem, it proves convenient to introduce new matrices \( \Phi \) and \( \Psi \), as follows:

\[
\Phi := g + h, \quad \Psi := g - h.
\]

If we now define for each \( k \) a vector \( |\Phi_k\rangle \), the \( i^{th} \) component of which is given by \( \Phi_{ki} \), and similarly for \( \Psi \), we find that (3.11) can be written as follows:

\[
(A - B)|\Psi_k\rangle = \Lambda_k |\Phi_k\rangle, \quad (A + B)|\Phi_k\rangle = \Lambda_k |\Psi_k\rangle,
\]
or, equivalently, as

\[
(A - B)(A + B)\ket{\Phi_k} = \Lambda^2_k \ket{\Phi_k}
\]

\[
(A + B)(A - B)\ket{\Psi_k} = \Lambda^2_k \ket{\Psi_k}.
\]  

(3.12)

With this we have reduced our problem from the diagonalization of a $2^N \times 2^N$ matrix to that of diagonalizing two $N \times N$ ones. As mentioned before, this would be a very easy task if we would have chosen periodic boundary conditions. The reason being that for periodic boundary conditions the matrices $(A \pm B)(A \mp B)$ are Toeplitz. But for open boundary conditions the matrices $A$ and $B$ are given by (3.5), so that

\[
\frac{1}{4}(A - B)(A + B) = \begin{pmatrix}
\lambda^2 & -\lambda & \cdots & -\lambda \\
-\lambda & 1 + \lambda^2 & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots \\
-\lambda & \cdots & \cdots & 1 + \lambda^2
\end{pmatrix}
\]  

(3.13)

and

\[
\frac{1}{4}(A + B)(A - B) = \begin{pmatrix}
1 + \lambda^2 & -\lambda & \cdots & -\lambda \\
-\lambda & 1 + \lambda^2 & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & 1 + \lambda^2 & -\lambda & \cdots & -\lambda
\end{pmatrix}
\]  

(3.14)

In order to solve (3.12), we propose the following ansatz:

\[
\Psi_{kl} = \alpha e^{ikl} + \beta e^{-ikl},
\]

(3.15)

with $\alpha$ and $\beta$ constants to be determined. The eigenvalue equation will then give 3 independent equations. The first one is obtained by equating the $j^{th}$ component of $(A + B)(A - B)\ket{\Psi_k}$ with $\Lambda^2_k \Psi_{kj}$, for $j = 2, \ldots, N - 1$. All these choices of $j$ yield the same equation (by enforcing the vanishing of the coefficients of $\alpha$ and $\beta$), namely,

\[
\left(\frac{\Lambda_k}{2}\right)^2 = \lambda^2 + 1 - 2\lambda \cos k.
\]  

(3.16)

This is (almost) the spectrum of our problem. We still need to find what are the allowed values of the label “$k$”. This is done by considering the two other cases ($j = 1$ and $j = N$), that give a system of equations for $\alpha$ and $\beta$:

\[
0 = \alpha + \beta,
\]

\[
0 = \left(\lambda e^{ik(N+1)} - e^{ikN}\right)\alpha + \left(\lambda e^{-ik(N+1)} - e^{-ikN}\right)\beta.
\]

The non-trivial solution $\alpha = -\beta$ is obtained provided the determinant of this matrix vanishes. This condition is equivalent to $k$ being solution of the following transcendental equation, for which $\lambda \neq 0$ has to be assumed:

\[
\sin kN = \lambda \sin k(N + 1).
\]  

(3.17)
Notice that, since we must have $N$ eigenvectors, we expect this equation to have $N$ roots. The behavior of these roots as a function of $\lambda$ is quite relevant; comparison with the periodic chain allows for the recognition of edge states.

3.3. Periodic boundary conditions. In the case of periodic boundary conditions, we extend the sums in (3.1) to $i = N$, adopting the convention that $\sigma^\alpha_N \equiv \sigma^\alpha_1 \ (\alpha = x, y, z)$. This generates a boundary term that couples the first spin operator to the last one:

$$H = -\sum_{i=1}^{N-1} \sigma^x_i \sigma^x_{i+1} - \frac{\lambda}{N} \sum_{i=1}^{N} \sigma^z_i \sigma^z_{N}.$$

(3.18)

We already know how to write the first two terms of this Hamiltonian in terms of creation and annihilation operators. Let us therefore consider the last term: $\sigma^x_N \sigma^x_1$.

Here it is convenient to consider the parity operator, $e^{i\pi N}$, where $N = \sum_j a_j^\dagger a_j$ is the number operator. Using the identities

$$1 - 2a_j^\dagger a_j = e^{i\pi a_j^\dagger a_j}, \quad (e^{i\pi a_j^\dagger a_j})^2 = 1, \quad e^{i\pi a_j^\dagger a_j} (a_j + a_j^\dagger) = (a_j - a_j^\dagger),$$

and (3.3) we obtain:

$$\sigma^x_N \sigma^x_1 = \left( \prod_{m=1}^{N-1} (1 - 2a_m^\dagger a_m) \right) (a_N^\dagger + a_N) (a_1^\dagger + a_1)$$

$$= \left( \prod_{m=1}^{N-1} e^{i\pi a_m^\dagger a_m} \right) (a_N^\dagger + a_N) (a_1^\dagger + a_1)$$

$$= \left( \prod_{m=1}^{N} e^{i\pi a_m^\dagger a_m} \right) e^{i\pi a_N^\dagger a_N} (a_N^\dagger + a_N) (a_1^\dagger + a_1)$$

$$= e^{i\pi N} (a_N - a_N^\dagger) (a_1^\dagger + a_1)$$

$$= (a_N - a_N^\dagger) (a_1^\dagger + a_1) e^{i\pi N}.$$

With this we can write $H$ in terms of fermionic operators:

$$H = -\sum_{i=1}^{N-1} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} - a_i a_{i+1}) + 2\lambda \sum_{i=1}^{N} a_i^\dagger a_i$$

$$-\lambda N + e^{i\pi N} (a_N^\dagger a_1 + a_1^\dagger a_N + a_N^\dagger a_1^\dagger + a_1 a_N).$$

(3.19)

An important fact (that can be easily checked) is that the parity operator commutes with $H$:

$$[H, e^{i\pi N}] = 0.$$

Thus, it is possible to diagonalize the Hamiltonian separately in sectors of even and odd numbers of “particles”. The eigenvalues of $e^{i\pi N}$ are of the form $\sigma = \pm 1$, with the plus sign for states with an even number of particles and the minus sign for states with an odd number of particles. We can, as in the previous case, write $H$ as a quadratic form in the fermion operators (cf. (3.6)), the only difference being
the explicit form of the matrices $A$ and $B$, for which we now get:

$$
A = \begin{bmatrix}
2\lambda & -1 & 0 & \cdots & \sigma \\
-1 & 2\lambda & -1 & 0 & \cdots \\
0 & -1 & 2\lambda & -1 & \cdots \\
\vdots & 0 & -1 & 2\lambda & \cdots \\
\sigma & \vdots & \vdots & \vdots & \ddots
\end{bmatrix},
B = \begin{bmatrix}
0 & -1 & 0 & \cdots & -\sigma \\
1 & 0 & -1 & 0 & \cdots \\
0 & 1 & 0 & -1 & \cdots \\
\vdots & 0 & 1 & 0 & \cdots \\
\sigma & \vdots & \vdots & \vdots & \ddots
\end{bmatrix}
$$  \hspace{1cm} (3.20)

In contrast to (3.12) or (3.14), the matrix $(A \pm B)(A \mp B)$ is now Toeplitz:

$$
\frac{1}{4}(A \pm B)(A \mp B) = \begin{bmatrix}
1+\lambda^2 & -\lambda & 0 & \cdots & \sigma \lambda \\
-\lambda & 1+\lambda^2 & -\lambda & 0 & \cdots \\
0 & -\lambda & 1+\lambda^2 & \cdots \\
\vdots & 0 & \ddots & \ddots & -\lambda \\
\sigma \lambda & \vdots & \vdots & \vdots & 1+\lambda^2
\end{bmatrix}
$$  \hspace{1cm} (3.21)

The eigenvalue problem (3.12) can again be solved using the ansatz (3.15). The eigenvalues are again given by (3.16), with the difference that the allowed values of $k$ can now be explicitly given as follows from the following exercise.

**Exercise 3.5.** Show that, in the even parity sector ($\sigma = 1$), the allowed values of $k$ are given by

$$
k_m = \frac{(2m + 1)}{N} \pi, \quad (m = 0, 1, \ldots, N - 1),
$$

whereas in the odd parity sector ($\sigma = -1$) they are given by

$$
k_m = \frac{2m}{N} \pi, \quad (m = 0, 1, \ldots, N - 1).
$$

**Exercise 3.6.** Explain how the $k$’s can be made to take positive and negative values and how then we obtain an explicit solution for the matrix $\Phi$, of the form

$$
\Phi_{k,l} \sim \begin{cases}
\sin(kl), & k > 0 \\
\cos(kl), & k < 0.
\end{cases}
$$

It should by now be clear that the solution of the eigenvalue problem is much easier in the periodic case. We have chosen to discuss the open chain mainly because of the role that boundary effects play in connection to symmetry breaking and also for studies of surface effects [29, 30]. Now we are going to take advantage of the translational symmetry in the periodic case. As discussed below, if instead of applying a Bogoliubov transformation right after transforming the spin operators to fermion operators via the Jordan-Wigner transformation, we perform a Fourier transformation as an intermediate step, we quickly obtain a much more elegant solution, that can be easily generalized to treat the limiting case of an infinite chain. Here we will again make use of the fact that the Hamiltonian commutes with the parity operator.

Looking back at (3.19), we realize that it is possible to express $H$ in a more compact form if we introduce boundary conditions of the fermion operators, depending on the parity sector we are interested in. In fact, notice that if we choose $\sigma = -1$, 

\[^3\text{This stands in contrast to the case of open boundary conditions, where they are given by the solutions of the transcendental equation 3.17.}\]
then the boundary term can be included in the first sum, just by setting \( a_{N+1} \equiv a_1 \).

But if we want to do the same in the sector \( \sigma = +1 \), we will need \( a_{N+1} \equiv -a_1 \).

In view of our previous discussion, it is clear that the choice \( \sigma = -1 \) is more convenient computationally (the matrices \((A \pm B)(A \mp B)\) are circulant in that case). But if we are interested in the ground state, then we must consider the other choice \((\sigma = 1)\). This can be seen if we compare the ground state energies of the fermionic Hamiltonian in each sector. As can be easily checked, the lowest energy eigenvalue indeed comes from the sector \( \sigma = 1 \). The difference between them decreases with increasing \( N \) and eventually disappears in the thermodynamic limit. It is for this reason that the boundary term is usually disregarded. We nevertheless feel that the price to pay if we keep all terms is actually very low, and in return we can have complete control over the spectrum and its degeneracies [31].

**Exercise 3.7.** Making use of the solution of the eigenvalue problem for both periodic and antiperiodic boundary conditions, plot the lowest energy eigenvalues for \( \sigma = \pm 1 \) as functions of \( \lambda \) and \( N \).

We therefore define

\[
a_{N+1} := -e^{i\pi N} a_1.
\]

In this way the Hamiltonian becomes

\[
H = -\sum_{i=1}^{N} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i - a_i a_{i+1}^\dagger - 2\lambda a_i^\dagger a_i) - \lambda N.
\]

Notice that the sum now goes over \( 1 \leq i \leq N \). So we see that we can describe both sectors using the same quadratic form, the choice of parity being now encoded in the boundary conditions for the fermion operators. It should be remarked that when we consider anti-periodic boundary conditions for the fermions we are still considering periodic boundary conditions for the spin chain. Anti-periodicity for the fermions in this context is only related to the choice of a negative eigenvalue for the parity operator.

Let us now introduce the Fourier transformed operators

\[
d_k := \frac{1}{\sqrt{N}} \sum_{l=1}^{N} a_l e^{-i\phi_k l}.
\]

The choice of the phases \( \phi_k \) must be made in such a way that the CAR algebra is preserved, but in addition it has to imply the boundary condition \( a_{l+N} = -e^{i\pi N} a_l \).

Therefore, the phases \( \phi_k \) will also depend on the parity sector.

**Exercise 3.8.** Show that in the even parity sector \((\sigma = 1, a_{l+N} = -a_l)\), the phases are given by

\[
\phi_k = \left( \frac{2k + 1}{N} \right) \pi,
\]

whereas in the odd parity sector \((\sigma = -1, a_{l+N} = a_l)\) they are given by

\[
\phi_k = \left( \frac{2k + 2}{N} \right) \pi.
\]

A word of caution is perhaps in order: In principle, \( k \) is an integer that takes values in the range \( 1 \leq k \leq N \). Nevertheless, due to the translational symmetry, \( k \) actually belongs to a “Brillouin zone”, meaning with this that there is no difference
between $k$ and $k \pm N$. So, for instance, for $\sigma = 1$ we have that $e^{i(\phi_k + \phi_{k'})} = 1$ whenever $2\pi(k + k' + 1)/N$ is an integer or, in other words, when

$$k + k' + 1 = 0 \pmod{N}. \quad (3.24)$$

For this reason, even if the allowed values of $k$ are originally in the range $\{1, \ldots, N\}$, we will allow $k$ to take any integer value, provided we interpret this (for $\sigma = 1$) in the sense of (3.24). With this convention we then obtain, for example:

$$\phi_{-k-1} = -\phi_k.$$ 

A similar remark applies to the case $\sigma = -1$. For the remaining part of this section we will confine ourselves to the even parity sector and so $\sigma = 1$ will be tacitly assumed.

We can now go back to the Hamiltonian (3.22) and insert there the new operators defined by (3.23). As a result, we obtain the following form of the Hamiltonian:

$$H = \sum_{k=1}^{N} \left[ 2(\lambda - \cos \phi_k)d_k^\dagger d_k - i \sin \phi_k(d_k^\dagger d_{-k-1}^\dagger + d_k d_{-k-1}) - \lambda \right]. \quad (3.25)$$

This form of the Hamiltonian is indeed very convenient as it suggests that a diagonalization by means of a Bogoliubov transformation that only mixes $d_k^{(1)}$ with $d_{-k-1}^{(1)}$ should be possible. For this reason we propose the following transformation:

$$c_k = \alpha_k d_k + \beta_k d_{-k-1}^\dagger, \quad (3.26)$$

with $\alpha_k, \beta_k$ (possibly complex) coefficients to be found. Imposing the condition $\{c_k, c_{k'}^\dagger\} = \delta_{k,k'}$ we readily obtain $|\alpha_k|^2 + |\beta_k|^2 = 1$. Furthermore, it is easy to check that the choices

$$\alpha_{-k-1} = \alpha_k, \quad \beta_{-k-1} = -\beta_k,$$

enforce $\{c_k, c_{k'}\} = 0$. Inverting (3.26) and inserting the result in (3.25), we obtain:

$$H = \sum_{k=1}^{N} \left( c_k^\dagger c_k \right) \left[ 2(\cos \phi_k - \lambda)\alpha_k \beta_k - i \sin \phi_k(\alpha_k^2 + \beta_k^2) \right] + \text{h.c.} + 2 \sum_{k=1}^{N} c_k^\dagger c_k \left( \lambda - \cos \phi_k \right)(|\alpha_k|^2 - |\beta_k|^2) + i \sin \phi_k(\alpha_k \beta_k - \beta_k \alpha_k) \\
+ \sum_{k=1}^{N} \left[ 2(\lambda - \cos \phi_k)|\beta_k|^2 + i \sin \phi_k(\alpha_k \beta_k - \beta_k \alpha_k) - \lambda \right]. \quad (3.27)$$

Vanishing of the coefficients in the first sum leads to

$$\frac{\sin \phi_k}{\lambda - \cos \phi_k} = \frac{2i\alpha_k \beta_k}{\alpha_k^2 + \beta_k^2}. \quad (3.28)$$

Recalling that $|\alpha_k|^2 + |\beta_k|^2 = 1$, we see that the right hand side of this expression simplifies if we parameterize $\alpha_k$ and $\beta_k$ as follows:

$$\alpha_k = \cos \frac{\theta_k}{2}, \quad \beta_k = -i \sin \frac{\theta_k}{2}.$$ 

In fact, with this choice (3.28) simplifies to

$$\tan \theta_k = \frac{\sin \phi_k}{\lambda - \cos \phi_k}.$$
We can now introduce a normalization factor $\Lambda_k^4$ by means of
\[
\sin \theta_k = \frac{\sin \phi_k}{(\Lambda_k/2)}, \quad \cos \theta_k = \frac{\lambda - \cos \phi_k}{(\Lambda_k/2)}.
\]
This leads to
\[
\Lambda_k = 2\sqrt{(\lambda - \cos \phi_k)^2 + \sin^2 \phi_k}.
\]
With these definitions, the remaining terms in (3.27) simplify further yielding the desired diagonal form for the Hamiltonian:
\[
H = \sum_{k=1}^{N} \Lambda_k \left( c_k^\dagger c_k - \frac{1}{2} \right).
\]

Exercise 3.9. Verify all the computations leading from (3.22) to (3.29).

The Ground State. Having brought the Hamiltonian to the diagonal form (3.29), we now proceed to find an expression for the ground state. Since $\Lambda_k$ has been chosen to be positive (or zero) for all values of $k$, the ground state $|\Omega(\lambda)\rangle$ will be given by the condition $c_k|\Omega(\lambda)\rangle = 0, \quad \forall k \in \{1, \ldots, N\}$. Let $|0\rangle$ be the “vacuum” state for the operators $d_k$, defined by the condition $d_k|0\rangle = 0$. Observe now that if we define
\[
B_k := \cos \frac{\phi_k}{2} + i \sin \frac{\phi_k}{2} d_k^\dagger d_{k-1}^\dagger,
\]
then we get $c_k B_k |0\rangle = 0$ for all $k$. Since $[B_k, B_k^\dagger] = 0$, one would think that $\prod_{k=1}^{N} B_k |0\rangle$ does the job, but we must take into account that $B_{k'} = B_k$ whenever $k' + k + 1 = 0 \pmod{N}$. If $N$ is even, this means that each $B_k$ appears twice in $\prod_{k=1}^{N} B_k$ and then an easy calculation shows that $c_{k'} \prod_{k=1}^{N} B_k |0\rangle$ does not vanish. Hence, we must be careful to include in the product only one instance of each $B_k$.

To do this, we distinguish two cases: $N$ even and $N$ odd. Restricting the domain of $\phi_k$ to the interval $(-\pi, \pi)$ we get, for $N$ even, $0 < \phi_k < \pi$ for $1 \leq k \leq N/2 - 1$ (also for $k = N$) and $-\pi < \phi_k < 0$ for $N/2 \leq k \leq N - 1$. Now, for each $k$ such that $0 < \phi_k < \pi$, there is exactly one $k'$ with $-\pi < \phi_{k'} < 0$ and such that $B_k = B_{k'}$. In fact, let $k$ be such that $0 < \phi_k < \pi$ and put $k' = N - k - 1$. It follows that $-\pi < \phi_{k'} < 0$ and $k' + k + 1 = 0 \pmod{N}$, so that $B_k = B_{k'}$. We therefore see that, for even $N$, the ground state is given by
\[
|\Omega(\lambda)\rangle = \prod_{0 < \phi_k < \pi} B_k |0\rangle.
\]
Writing $N = 2M$, we may as well consider $k$ to be such that $-M \leq k \leq M - 1$. The ground state, then, takes the form $|\Omega(\lambda)\rangle = \prod_{k=0}^{M-1} B_k |0\rangle$.

For the case $N$ odd, write $N = 2M + 1$. In this case all the $B_k$ appear twice in $\prod_{k=1}^{N} B_k$, except when $k = M$. When $k = M$ we have $\phi_k = \pi$. This, together with the fact that $d_M^\dagger = d_{M-1}^\dagger$, implies that $B_M \equiv 0$, so we must exclude it from the product. In analogy to the previous case, for each $k$ for which $0 < \phi_k < \pi$ we can find exactly one $k'$ such that $-\pi < \phi_{k'} < 0$ and $B_k = B_{k'}$, namely $k' = 2M - k$. Now, for $0 \leq K \leq M - 1$, we have $0 < \phi_k < \pi$, whereas for $M + 1 \leq k \leq 2M$, we have $\phi_k \in (-\pi, 0)$. The result is that, for odd $N$, the ground state is given by
\[
|\Omega(\lambda)\rangle = \prod_{0 < \phi_k < \pi} B_k d_M^\dagger |0\rangle.
\]

\[\text{In section 3.5, we will multiply } H \text{ by a factor } 1/2, \text{ in order to simplify some expressions.}\]
The operator $d_M^\dagger$ has to be included in (3.30) in order to ensure that $c_M|\Omega(\lambda)\rangle = 0$ (recall that in this case $c_M = -id_M^\dagger$).

3.4. **Entanglement properties of the ground state.** Having obtained the exact spectrum of the model, as well as the ground state both for open and periodic boundary conditions, it is now possible -in principle- to obtain all relevant correlation functions and relate them to physical observables like magnetization, susceptibilities, and so on. As is well-known, the quantum Ising chain does not present any phase transition at finite temperature, but it certainly is one of the paradigmatic examples of a system displaying a quantum critical point. In fact, in the thermodynamic limit there is a quantum phase transition occurring when the external field $\lambda$ approaches the critical value $\lambda_c = 1$. In this notes we will review an approach to the study of this quantum phase transition from the point of view of entanglement. We will also be interested in certain geometric and topological properties of the ground state that are relevant for this quantum phase transition.

Let us start by considering the model (3.1) for an open, two-site chain ($N = 2$). Putting $\alpha = \sqrt{1 + 4\lambda^2}$, we find that the ground state is given in the spin basis by

$$|\Omega(\lambda)\rangle = \frac{1}{\sqrt{2\alpha(\alpha - 2\lambda)}} \left(|++\rangle + (\alpha - 2\lambda)|-\rangle \right).$$

(3.31)

Taking the partial trace with respect to one of the sites, we obtain

$$\rho = \text{Tr}_1|\Omega(\lambda)\rangle\langle\Omega(\lambda)| = \frac{1}{2\alpha(\alpha - 2\lambda)} \left(|++\rangle\langle++| + (\alpha - 2\lambda)^2|--\rangle\langle--| \right),$$

which in terms of the basis $\{|+, -\rangle\}$ takes the following simple matrix form:

$$\rho = \begin{pmatrix} \frac{1}{2} + \frac{\lambda}{\alpha} & 0 & 0 & \frac{\lambda}{2} \\ 0 & \frac{1}{2} - \frac{\lambda}{\alpha} & 0 & 0 \\ 0 & 0 & \frac{1}{2} - \frac{\lambda}{\alpha} & 0 \\ \frac{\lambda}{2} & 0 & 0 & \frac{1}{2} + \frac{\lambda}{\alpha} \end{pmatrix}. \quad (3.32)$$

Figure 2 displays a plot of the eigenvalues of $\rho$ as a function of $\lambda$. As we shall see, the behavior of this entanglement spectrum as the size of the chain increases will provide important information regarding the quantum phase transition in this model.
Exercise 3.10. Follow the steps outlined in section 3.2 to show that for \( N = 2 \)
the matrices \( g \) and \( h \) introduced in (3.7) are given by
\[
g = \frac{1}{\sqrt{8\alpha}} \left( \begin{array}{cc}
\frac{2\lambda + \alpha - 1}{2\sqrt{\alpha + 1}} & \frac{2\lambda + \alpha - 1}{2\sqrt{\alpha + 1}} \\
\frac{-2\lambda - \alpha - 1}{\sqrt{\alpha + 1}} & \frac{-2\lambda - \alpha - 1}{\sqrt{\alpha + 1}}
\end{array} \right),
\]
\[
h = \frac{1}{\sqrt{8\alpha}} \left( \begin{array}{cc}
\frac{2\lambda - \alpha + 1}{2\sqrt{\alpha + 1}} & \frac{\alpha - 1 - 2\lambda}{\sqrt{\alpha + 1}} \\
\frac{-2\lambda - \alpha + 1}{\sqrt{\alpha + 1}} & \frac{-\alpha + 1 - 2\lambda}{\sqrt{\alpha + 1}}
\end{array} \right).
\]
Use this in order to show that the condition \( c_k |\Omega(\lambda)\rangle \rangle = 0 \) \( (k = 1, 2) \)
leads exactly to (3.31).

As we have seen, in this simple case \( (N = 2) \) the density matrix for the reduced state
can be easily computed. In spite of the fact that the model can be exactly solved,
the computation of correlation functions (as those involved in the computation
of the reduced density matrix) for arbitrary values of \( N \) is a non-trivial task.
We will therefore present, following [32], a method that allows us to obtain
the spectrum of \( \rho \) for arbitrary values of \( N \) and that can be used for any quadratic Hamiltonian.
As a preparation for the general case, we first explain the idea using
our very simple example of a two-site chain, where all calculations can be explicitly carried out.

Let \( A \) be the CAR algebra generated by the two fermionic operators \( a_1, a_2 \) and
the unity \( 1 \). We consider the “Fock representation” where
\( a_1^\dagger \) acts on the state \( |0\rangle \equiv |++\rangle \). This state is cyclic and therefore we can write the ground state
(3.31) in terms of it (cf. exercise 3.10):
\[
|\Omega(\lambda)\rangle = \frac{1}{\sqrt{2\alpha(\alpha - 2\lambda)}} \left( |0\rangle + (\alpha - 2\lambda)a_1^\dagger a_2^\dagger |0\rangle \right).
\] (3.33)
As discussed in section 2.1 we can use it to define a state \( \omega_\lambda \) in the algebraic sense:
\[
\omega_\lambda : A \rightarrow \mathbb{C}, \quad A \mapsto \omega_\lambda (A) := \langle \Omega(\lambda)| A |\Omega(\lambda)\rangle.
\]
This is, of course, a pure state. Nevertheless, if we restrict it to the subalgebra \( A_1 \)
that is generated by \( 1 \) and \( a_1 \) (“a half-chain”), then we find that in general the resulting state \( \omega_\lambda|A_1\rangle \)
will be a mixed state. Let us consider this restriction in more detail. Defining \( \omega_{\lambda,1} := \omega_\lambda|A_1\rangle \),
we expect that for any \( A \in A_1 \)
\[
\omega_{\lambda,1}(A) = \text{Tr}(\rho A) \tag{3.34}
\]
will hold, with
\[
\rho = e^{-\varepsilon_1 a_1^\dagger a_1} Z^{-1},
\]
\( Z = \text{Tr} e^{-\varepsilon_1 a_1^\dagger a_1} \), both traces being taken on the Hilbert space
corresponding to the half-chain (which in this case has a basis given by \( \{|0\rangle, a_1^\dagger |0\rangle\}\)). Finding \( \varepsilon_1 \)
amounts to finding the spectrum of \( \rho \) and this, in turn, can be used to compute the entanglement entropy.
The specific form of \( \rho \) as the exponential of a quadratic form is to be expected in view of the fact that the ground state is Gaussian.
In order to find \( \varepsilon_1 \), we notice that it is possible to compute the left hand side of (3.34).
The only relevant case is \( A = a_1^\dagger a_1 \), so let us define \( C_1 := \omega_{\lambda,1}(a_1^\dagger a_1) \). Using (3.33),
we get:

\[
C_1 = \omega_{\lambda,1}(a_1^\dagger a_1) = \omega_{\lambda}(a_1^\dagger a_1) = \frac{1}{2} - \frac{\lambda}{\alpha},
\]

where we still keep the notation \(\alpha = \sqrt{1 + 4\lambda^2}\). On the other hand, we have

\[
\text{Tr}(\rho a_1^\dagger a_1) = \frac{1}{1 + e^{\varepsilon_1}}.
\]

It follows that

\[
1 - 2C_1 = \frac{2\lambda}{\alpha} = \tanh \frac{\varepsilon_1}{2}
\]

or, equivalently,

\[
\varepsilon_1 = \ln \left( \frac{1/2 + \lambda/\alpha}{1/2 - \lambda/\alpha} \right).
\]

Since \(\rho\) is already diagonal in the basis \(\{|0\}, a_1^\dagger|0\rangle\), we obtain:

\[
\rho = \left( \begin{array}{cc}
1 & 0 \\
0 & 1 + e^{\varepsilon_1}
\end{array} \right) = \left( \begin{array}{cc}
\frac{1}{2} + \frac{\lambda}{\alpha} & 0 \\
0 & \frac{1}{2} - \frac{\lambda}{\alpha}
\end{array} \right),
\]

which coincides with (3.32). Notice, in passing, that \(C_1\) can also be obtained directly from \(h\). In fact, a small computation shows that \(C_1 = (h^t h)_{11}\).

This last remark gives a hint towards the solution for the general case: As we shall see, the spectrum of \(\rho\) in the general case can be extracted from an eigenvalue problem that uses the matrices \(h\) and \(g\) as input. Let us, then, start by considering the algebra \(\mathcal{A}\) generated by \(1\) and by all operators \(a_i\), with \(i = 1, \ldots, N\). Again, the ground state \(|\Omega(\lambda)\rangle\) gives rise to a state \(\omega_\lambda : \mathcal{A} \to \mathbb{C}\). We are interested in the restriction of this state to the subalgebra \(\mathcal{A}_L\) generated by \(\{1, a_1, \ldots, a_L\}\). By the same argument as before, we expect this new state \(\omega_{\lambda,L} := \omega_\lambda|_{\mathcal{A}_L}\) to be of the form \(\omega_{\lambda,L}(A) = \text{Tr}(\rho A)\) \((A \in \mathcal{A}_L)\), with

\[
\rho = e^{-H_\rho} Z, \quad Z = \text{Tr} e^{-H_\rho}
\]

and

\[
H_\rho = \sum_{i,j=1}^L \left( a_i^\dagger K_{ij} a_j + \frac{1}{2}(a_i^\dagger M_{ij} a_j - a_i M_{ij} a_j) \right).
\]

For the Ising model, the matrices \(K\) and \(M\) (yet to be determined) will be real, so that \(K\) has to be symmetric, and \(M\) antisymmetric. Now we define \(32\), for \(i, j = 1, \ldots, L\) the correlation functions

\[
C_{ij} := \omega_{\lambda,L}(a_i^\dagger a_j), \quad F_{ij} := \omega_{\lambda,L}(a_i^\dagger a_j^\dagger).
\]

Using \(3.7\) one shows that \(C_{ij} = (h^t h)_{ij}\) and \(F_{ij} = (h^t g)_{ij}\). Let us first consider the simpler case \(M = 0\). In this case \(H_\rho\) can be diagonalized by a simple transformation of the form

\[
b_l = \sum_{i=1}^L \gamma_{li} a_i, \quad l = 1, \ldots, L,
\]

where the matrix \(\gamma\) is such that \(\gamma^t \gamma = 1_L\). Solving the eigenvalue problem

\[
K(|\phi_l\rangle) = \varepsilon_l |\phi_l\rangle
\]
and introducing the convention \( |i\rangle = (0, 0, \ldots, 1, \ldots, 0) \) (1 in the \( i \)th entry and 0 everywhere else), we set \( \gamma_i := \langle i|\varphi_i \rangle \), i.e., the rows of \( \gamma \) are the eigenvectors \( |\varphi_i \rangle \).

We then obtain
\[
H_\rho = \sum_{l=1}^L \varepsilon_l |b_l\rangle \langle b_l|.
\]

It follows that \( Z = \prod_{l=1}^L (1 + e^{-\varepsilon_l}) \), so that \( \omega_{KL} |b_l\rangle = \gamma_i = \delta_{ij} (1 + e^{\varepsilon_l})^{-1} \). Using (3.36) we then obtain \( C_{ij} = \sum_{l=1}^L \gamma_i \gamma_j (1 + e^{\varepsilon_l})^{-1} \), which is equivalent to the matrix identity \( C = (1 + e^K)^{-1} \). This can also be written in the following form:
\[
1 - 2C = \tanh \frac{K}{2}.
\]

If \( M \neq 0 \), we replace (3.36) by
\[
b_l = \sum_{i=1}^L (\gamma_i a_i + \eta_i a_i^\dagger),
\]
where now we require (cf. exercise 3.3):
\[
\gamma^t \gamma + \eta^t \eta = 1,
\]
\[
\gamma^t \eta + \eta^t \gamma = 0.
\]

Once again, the matrices \( \gamma \) and \( \eta \) should be such that \( \rho \) becomes diagonal, i.e., \( H_\rho = \sum_{l=1}^L \varepsilon_l |b_l\rangle \langle b_l| \) should hold. The eigenvalue problem to be solved is
\[
(K - M) |\psi_l \rangle = \varepsilon_l |\varphi_l \rangle, \\
(K + M) |\varphi_l \rangle = \varepsilon_l |\psi_l \rangle.
\]

Using these eigenvectors as rows for the matrices \( \psi \) and \( \varphi \) and putting
\[
\gamma = \frac{1}{2} (\varphi + \psi), \quad \eta = \frac{1}{2} (\varphi - \psi),
\]
we obtain the desired diagonal form for \( H_\rho \). As in the previous case, we can now write all correlation functions that involve the operators \( a_i \) in terms of correlation functions that only involve the operators \( b_l \).

**Exercise 3.11.** Obtain the following two relations:
\[
C_{ij} = \sum_{l=1}^L \left( \gamma_i \gamma_l + \eta_i \eta_l \frac{1}{1 + e^{\varepsilon_l}} \right),
\]
\[
F_{ij} = \sum_{l=1}^L \left( \gamma_i \eta_l + \eta_i \gamma_l \frac{1}{1 + e^{-\varepsilon_l}} \right),
\]
and use them in order to prove the following identity:
\[
\frac{1}{1 + e^{(K \pm M)}} - \frac{1}{1 + e^{-(K \pm M)}} = 2C - 1_L \pm 2F,
\]
where \( C \) and \( F \) are the \( L \times L \) matrices with components given by (3.35).

From this exercise we obtain, making use of (3.37),
\[
(2C - 1_L - 2F)(2C - 1_L + 2F) |\varphi_l \rangle = \tanh \frac{\varepsilon_l}{2} |\varphi_l \rangle.
\]

We will now make use of this expression in order to obtain the entanglement spectrum and the entanglement entropy of the ground state of the Ising chain when \( L = N/2 \), for various values of \( N \) and \( \lambda \). In Fig. 3 we plot the entanglement...
spectrum (in logarithmic scale) for a chain of $N = 10$ sites, when the ground state is restricted to a half-chain. We notice that, in contrast to the case $N = 2$, the gap between the first two eigenvalues is now closed for almost all values of $\lambda$ below $\lambda_c = 1$.

In Fig. 4 we compare the entanglement spectrum for an Ising chain of $N = 10$ sites against the spectrum of a chain of $N = 100$ sites. It is apparent that for $N = 100$ the gap near $\lambda_c$ has almost closed.

This gap, when evaluated at the critical value $\lambda_c$, bears the name of Schmidt gap. We will use the notation $\Delta_S$ for the Schmidt gap. De Chiara and collaborators have shown, using finite-size scaling, that the Schmidt gap can be interpreted as an order parameter. In fact, from a finite size scaling analysis, one can in fact obtain numbers $\mu_1$ and $\mu_2$ such that when we plot $\Delta_S N^{\mu_1}$ versus $|\lambda - \lambda_c| N^{\mu_2}$, all points collapse to a single curve, irrespective of the value of $N$ chosen. This result was obtained in [33] using a DMRG algorithm. Figure 5, obtained by C. Rivera using the same DMRG technique [34] depicts the resulting curve, for which points corresponding to different lengths of the chain (ranging from $N \approx 700$ to $N = 8000$) are seen to collapse to a single curve. The values of $\mu_1$ and $\mu_2$ for which this is achieved give values for the critical exponents which are very close to the actual values ($\nu = 1$ and $\beta = 1/8$). The entanglement spectrum can also be used to compute the entanglement entropy and its dependence on the size of the subsystem chosen. A numerical evaluation of this entropy gives the result expected from conformal field theory, that is, at the critical point, the entanglement entropy follows a logarithmic behavior, of the form

$$ S(l) \sim \frac{c}{3} \log l, $$

where $c$ denotes the central charge of the corresponding CFT. In this case (Ising chain), numerical evaluation of the entropy for different chain sizes gives a value of $c = 1/2$, in accordance with the predictions of CFT.

![Figure 3](image.png)

**Figure 3.** Entanglement spectrum for an Ising chain of $N = 10$ sites as a function of the external field $\lambda$. 

3.5. The XY model. The XY model is a generalization of the Ising model. The model also represents a spin chain with nearest-neighbor interactions. Its Hamiltonian is given by

\[ H = -\frac{1}{2} \sum_{j=1}^{N} \left( \frac{1+\gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1-\gamma}{2} \sigma_j^y \sigma_{j+1}^y + \lambda \sigma_j^z \right). \]

There are two parameters in this model. As in the Ising case, \( \lambda \) represents an external field. The parameter \( \gamma \) is an anisotropy parameter. Notice that if \( \gamma = 1 \), we recover, up to an overall factor of 1/2, the Ising Hamiltonian (3.1). Our interest in this model lies in the fact that according to the values of the parameters \( \gamma \) and \( \lambda \), we may study critical regions corresponding to different universality classes: If \( \gamma > 0 \), there is a critical line determined by \( \lambda = 1 \) that corresponds to the Ising universality class, with central charge \( c = 1/2 \). On the other hand, for \( \gamma = 0 \) the whole line \( 0 < \lambda < 1 \) corresponds to the XX universality class, with central charge \( c = 1 \).
3.6. Solution of the model. The solution of this model can be obtained in the same fashion as we did in the case of the Ising model. The first step, then, consists in using the Wigner-Jordan transformation to bring the Hamiltonian to a quadratic form in fermionic operators. The result one obtains is

\[ H = -\frac{1}{2} \sum_j (a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j + \gamma a_j^\dagger a_{j+1} - \gamma a_{j+1} a_j) \quad (3.39) \]

\[ + \lambda \left( N - \frac{N}{2} \right), \]

with \( N \equiv \sum_j a_j^\dagger a_j \), the fermionic number operator. Since we are interested in the ground state, we consider the even parity sector and proceed, as with the Ising model, with a Fourier transformation, followed by a Bogoliubov transformation.

For odd \( N (= 2M + 1) \) and with

\[ d_k = \frac{1}{\sqrt{N}} \sum_{l=1}^N a_l e^{-i\phi_k l}, \quad \phi_k := \left( \frac{2k + 1}{N} \right) \pi, \quad -M \leq k \leq M, \]

we obtain:

\[ H = \sum_k ((\lambda - \cos \phi_k) d_k^\dagger d_k - \frac{i\gamma}{2} \sin \phi_k (d_k^\dagger d_{k-1}^\dagger + d_{k-1} d_k)) - \frac{\lambda N}{2}. \]

We can now consider a Bogoliubov transformation, as in (3.26),

\[ c_k = \cos \frac{\theta_k}{2} d_k - i \sin \frac{\theta_k}{2} d_{k-1}^\dagger, \quad \tan \theta_k = \frac{\gamma \sin \phi_k}{\lambda - \cos \phi_k}, \]

and obtain the following diagonal form for the Hamiltonian:

\[ H = \sum_{k=-M}^M \Lambda_k \left( c_k^\dagger c_k - \frac{1}{2} \right), \]

with

\[ \Lambda_k = \sqrt{(\lambda - \cos \phi_k)^2 + \gamma^2 \sin^2 \phi_k}. \]

Defining \( B_k := \cos \frac{\phi_k}{2} + i \sin \frac{\phi_k}{2} d_k^\dagger d_{k-1}^\dagger \) we obtain the following explicit form for the ground state \( |\Omega(\lambda, \gamma)\rangle \):

\[ |\Omega(\lambda, \gamma)\rangle = \left( \prod_{0 \leq k < M} B_k \right) d_M^\dagger |0\rangle, \]

where \( |0\rangle \) is the vacuum state with respect to the operators \( d_k \).

3.7. Criticality. The XY model has a rich phase diagram, and this provides an opportunity to check the behavior of entanglement entropy at the critical point and its relation to the central charge. In the previous section we focused on a finite-size scaling analysis for the Ising model, which in turn brought up the difficulty of having to compute correlation functions for finite size chains. In this section, we will only be interested in properties in the thermodynamic limit, i.e., we will discuss the behavior of the entanglement entropy of a sub-chain of length \( L \), considered as a subsystem of a chain of infinite length, or the geometric phase of the ground state associated to closed loops around the critical point. Calculations in the thermodynamic limit are greatly simplified because discrete sums become integrals that
can be readily evaluated. Let us now very briefly describe how to obtain the entanglement entropy of a sub-chain of size $L$ in the thermodynamic limit. We will follow the approach of Vidal et al. [35], which amounts to the real (e.g. Majorana) version of the method discussed in section 3.4. We begin by replacing the fermion operators $(a_i)$ appearing in (3.39) by new, Majorana fermion operators ($\tilde{c}_i$), defined as follows:

$$\tilde{c}_{2n-1} := (a_n + a_n^\dagger)$$
$$\tilde{c}_{2n} := i(a_n^\dagger - a_n).$$

These Majorana operators satisfy commutation relations of the form $\{\tilde{c}_m, \tilde{c}_n\} = 2\delta_{mn}$. Now, consider the correlation matrix $\langle \tilde{c}_m \tilde{c}_n \rangle = \delta_{mn} + i\Gamma_{mn}$, where the expectation value is taken with respect to the ground state. The matrix $\Gamma$ can be expressed as a block matrix, with the block $(i,j)$ being given by the $2 \times 2$ matrix $\Pi_{j-i}$ ($i$ and $j$ range from 0 to $N-1$, $N$ being the size of the full chain), where

$$\Pi_l := \begin{pmatrix} 0 & g_l \\ -g_l & 0 \end{pmatrix}.$$

In the thermodynamic limit ($N \to \infty$) the coefficient function $g_l$ takes the following compact form:

$$g_l = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-il\phi} \left( \frac{\cos \phi - \lambda - i\gamma \sin \phi}{|\cos \phi - \lambda - i\gamma \sin \phi|} \right).$$

The restriction of the correlation matrix to the sites belonging to a sub-chain of size $L$ is then a $L \times L$ matrix $\Gamma_L$ which is obtained just by deleting the entries of $\Gamma$ that do not correspond to sites in the sub-chain.

**Exercise 3.12.** Following the method of section 3.4 as well as Vidal et al. [35], show that the entanglement entropy corresponding to the restriction of the full chain to a sub-chain of $L$ sites is given by the formula

$$S(L) = \sum_{m=0}^{L-1} H \left( \frac{1 + \nu_m}{2} \right),$$

(3.40)

where $H$ denotes the Shannon entropy as defined in (2.7) and $\{\nu_m\}_m$ are the positive eigenvalues of $i\Gamma_L$.

Figure 6 displays the behavior of the entropy as a function of $L$. One of the curves (dashed) shows the results for the XX chain, which corresponds to $\gamma = 0$. From the logarithmic dependence of the entropy we extract the value $c = 1$ for the central charge in this model. The continuous curve shows the entropy for the critical case $\lambda = 1, \gamma = 0.5$, which belongs to the Ising universality class. In this case, the value obtained for the central charge is $c = 1/2$. The dots correspond to the non-critical case $\lambda = 0.5, \gamma = 0.5$. We can see that in this case the entropy saturates with $L$. Thus, the results confirm the expected behavior of the entropy as predicted by CFT.

4. **Quantum fields**

4.1. **The scalar field.** In section 2 we mentioned that the canonical commutation relations (CCR) lead to a $C^*$-algebra, whose representation theory plays a very important role in quantum field theory. Let us recall that the operators $U(a)$ and $V(b)$ defined in (2.2) satisfy the so-called Weyl form of the CCR (cf. exercise 2.8).
The first thing we want to do is to recognize that any implementation of the CCR in their Weyl form corresponds in fact to the construction of a representation of a certain group (the Heisenberg group). The Heisenberg group of $\mathbb{R}^n$, whose underlying set is $(\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R})$, is the group defined by the following operation:

$$(\vec{a}_1, \vec{b}_1, r_1) \cdot (\vec{a}_2, \vec{b}_2, r_2) := (\vec{a}_1 + \vec{a}_2, \vec{b}_1 + \vec{b}_2, r_1 + r_2 + \frac{1}{2}(\vec{a}_1 \cdot \vec{b}_2 - \vec{a}_2 \cdot \vec{b}_1)).$$

**Exercise 4.1.** Study the Lie algebra of the Heisenberg group and explain how this Lie algebra is related to the CCR.

**Exercise 4.2.** Show that the operators $\mathcal{R}(\vec{a}, \vec{b}, r)$ defined through

$$\mathcal{R}(\vec{a}, \vec{b}, r) := V(\vec{b})U(\vec{a})e^{i\hbar(r + \frac{1}{2}r\vec{b})},$$

with $U$ and $V$ as in (2.2), furnish a representation of the Heisenberg group.

The key point regarding these commutation relations is actually their relation to the (canonical) symplectic structure of the underlying classical phase space, $T^*\mathbb{R}^n$. In fact, if for $u = (\alpha, \beta) \in T^*\mathbb{R}^n$ we define

$$W(\alpha, \beta) := e^{-i(\alpha\vec{q} + \beta\vec{p})},$$

we obtain the following identity:

$$W(u)W(v) = e^{-\frac{i}{\hbar}\sigma(u,v)}W(u + v),$$

where $u$ and $v$ denote elements of the symplectic vector space $T^*\mathbb{R}^n$, and $\sigma$ the standard symplectic form. Notice that we have the following relations between all...
these operators:

\[ W(\alpha, \beta) = e^{i\frac{\alpha \beta}{\hbar}} V(\alpha) U(\beta) = R(\beta, \alpha, 0). \]

**Definition 4.3.** (cf. [36]) Let \( V \) be a real vector space and \( \sigma : V \times V \to \mathbb{R} \) a symplectic form (i.e. a bilinear, skew-symmetric, non-degenerate form). A \(*\)-algebra \( W(V, \sigma) \) is called a Weyl \(*\)-algebra of \((V, \sigma)\) if there is a family \( \{W(u)\}_{u \in V} \) of “generators” such that

1. \( W(u)W(v) = e^{-\frac{i}{2}\sigma(u,v)} W(u + v), \quad W(u)^* = W(-u), \quad u, v \in V. \)
2. \( W(V, \sigma) \) is generated by the family \( \{W(u)\}_{u \in V} \), i.e., it is the span of finite linear combinations of finite product of the \( W(u) \).

In [36] it is proved that every symplectic vector space \((V, \sigma)\) determines uniquely a Weyl \(*\)-algebra, up to \(*\)-isomorphism. Also, if \( \phi : V_1 \to V_2 \) is a symplectomorphism between two symplectic vector spaces, then the corresponding Weyl \(*\)-algebras are isomorphic. A most important fact is that \( W(V, \sigma) \) can be completed to a \( C^* \) algebra, the Weyl \( C^* \)-algebra.

It is a fundamental result, due to Stone and von Neumann, that when the dimension of \( V \) is finite (and hence necessarily even), there is essentially only one representation of the CCR, which can be taken to be the standard Schrödinger representation [36]. But in infinite dimensions uniqueness is lost, and so inequivalent representations do exist. This fact is closely related to the non-uniqueness of a vacuum state for a free quantum field in a curved spacetime background. The following example illustrates how the construction of a (free, bosonic) quantum field runs in parallel to the previous discussion of CCR, the “only” (!) difference here being that the symplectic vector space we are dealing with is infinite dimensional.

**Example 4.4** (The Klein-Gordon field, cf. [37]). Let \((M, g)\) denote a globally hyperbolic spacetime, and consider the Klein-Gordon equation on that background:

\[ (\Box_g + m^2) \phi = 0. \]

Let \( \Sigma_0 \) denote a fixed Cauchy surface, to which the initial data for the solutions of the Klein-Gordon equation will be referred and consider the following vector space, a space of solutions of the K-G equation:

\[ S := \{ \phi \in C^\infty(M, \mathbb{R}) : (\Box_g + m^2) \phi = 0 \text{ and } \phi|_{\Sigma_0} \in C^\infty_0(\Sigma_0) \}. \]

It is a most remarkable fact that the classical field equation comes equipped with a natural symplectic structure. In fact, if \( \Sigma \) is any space-like (Cauchy) hypersurface, and \( n \) denotes the unit normal, then on the vector space \( S \) defined above we can define the following symplectic form:

\[ \sigma(\phi_1, \phi_2) := \int_\Sigma (\phi_1 \nabla_\mu \phi_2 - \phi_2 \nabla_\mu \phi_1) n_\mu d\text{vol}_g. \]

For \( f \in C^\infty_0(M) \), let \( A \) and \( R \) denote the advanced and retarded fundamental solutions of the K-G equation. That is, for \( f \in C^\infty_0(M) \) we have

\[ (\Box_g + m^2) Af = f, \quad (\Box_g + m^2) Rf = f, \]

where the support of \( Af \) lies in the causal past of the support of \( f \) (and analogously for \( Rf \)). Then \( E := A - R \) gives a map

\[ E : C^\infty_0(M) \to S. \]
The CCR for the quantum field (in its smeared form) then take the form
\[ [\hat{\varphi}(f), \hat{\varphi}(g)] = -i\sigma(E_f, E_g). \]

Just as in non-relativistic quantum mechanics, the operators obeying CCR are unbounded, and so it is convenient to go to the Weyl form, which leads us back to the Weyl C*-algebra, this time the one corresponding to the infinite dimensional vector space \((\mathcal{S}, \sigma)\).

### 4.2. Fermionic second quantization and Clifford algebras

Representation spaces for the Weyl algebra of the previous example are bosonic Fock spaces. For the classical Dirac field, the transition to the corresponding quantum description can be performed in a completely analogous way, only that in this case, instead of an antisymmetric form, a symmetric one is used which, again, comes “for free” as part of the structure of the (vector space) of solutions of the classical field equation. It is an interesting fact that the existence of a natural bilinear antisymmetric form in the scalar field case (and of a symmetric one in the case of the Dirac field) leads to quantum fields that obey the physically correct relation between spin and statistics.

In very general terms, quantization of free fields can be formulated as follows. Suppose we are given a real vector space \(V\) together with a non-degenerate (anti-)symmetric bilinear form \(s : V \times V \to \mathbb{R}\). If in addition we choose a complex structure \(J\) which is compatible with \(s\) (meaning \(s(u, v) = s(Ju, JV)\) holds), we can complexify and obtain a complex vector space \(V_J\). The bilinear form \(s\) can then be used to define an inner product on \(V_J\), making it a Hilbert space. According to whether the bilinear form is symmetric or antisymmetric, one then considers the antisymmetric or the symmetric subspace of the tensor algebra of \(V_J\), call it \(F_J\). Endomorphisms of \(V_J\) may be lifted to \(\text{End}(F_J)\) in a natural (i.e. functorial) way. These liftings are then interpreted as the “second quantization” of observables (self-adjoint operators in \(V_J\)) and symmetries (unitary operators).

In this section we will focus on the fermionic case, following the beautiful treatment of the subject presented in [11], which makes strong use of Clifford algebras and spin group representations. In the next section we will explore the connection between second quantization (as presented here) and quantum criticality in spin chains (as discussed previously). Let us start by first considering the simple case where \(\dim V < \infty\). If \(V\) is a finite dimensional real vector space, and \(g\) a positive definite symmetric bilinear form on it, we can construct the corresponding Clifford algebra \(Cl(V, g)\). As shown in [11], it is possible to obtain a concrete realization of the complexified Clifford algebra \(\mathbb{C}l(V)\) as a subalgebra of \(\text{End}(\Lambda^V)\), but the corresponding representation is not irreducible. The situation changes if we assume \(V\) has even dimension, say \(2m\). Then we may choose an orthogonal complex structure, that is, a linear operator \(J \in \text{End}_\mathbb{C}(V)\) such that \(J^2 = -1\) and \(g(Ju, JV) = g(u, v)\) for all \(u, v \in V\), and regard \(V\) as a complex vector space \(V_J\) of dimension \(m\). The scalar product on \(V_J\) is given by \((u|v) = g(u, v) + ig(Ju, v)\). It then turns out that the exterior algebra \(\Lambda^V\) is an irreducible Clifford module. We call this module the Fock space and use the notation \(F_J(V)\) for it. The action of \(\mathbb{C}l(V)\) on \(F_J(V)\) is obtained by defining “creation” and “annihilation” operators.

\[5\] We urge the reader to consult [11] for details and explicit computations.
From these definitions, we obtain the anti-commutation relations
\[ a_j^\dagger, a_j : V \to \text{End}(\mathcal{F}_f(V)) \] acting on \( \mathcal{F}_f(V) \) as follows:
\[
a_j(v)(u_1 \wedge \ldots \wedge u_k) := \sum_{j=1}^k (-1)^{j-1} (v|u_j)J_{j} u_1 \wedge \ldots \wedge \widehat{u}_j \wedge \ldots \wedge u_k,
\]
\[
a_j^\dagger(v)(u_1 \wedge \ldots \wedge u_k) := v \wedge u_1 \wedge \ldots \wedge u_k, \quad a_j(v)(1) := 0.
\]

From these definitions, we obtain the anti-commutation relations
\[
\{a_j^\dagger(u), a_j(v)\} = \langle u|v \rangle_J, \quad \{a_j(u), a_j(v)\} = 0 = \{a_j^\dagger(u), a_j^\dagger(v)\},
\]
from which \((a_j^\dagger(v) + a_j(v))^2 = \langle v|v \rangle_J\) follows. Hence, the map
\[
\pi_j : V \to \text{End}(\Lambda^*_V)
\]
may be extended to \(\mathbb{C}l(V)\) by making use of the universal property of the Clifford algebra. The scalar product \(\langle | \rangle_J\) on \(V_J\) induces one on \(\mathcal{F}_f(V)\), which on basis elements is given by
\[
\langle u_1 \wedge \ldots \wedge u_k | v_1 \wedge \ldots \wedge v_{k'} \rangle = \delta_{kk'} \det \langle u_i|v_j \rangle_J,
\]
thus making \(\mathcal{F}_f(V)\) a (finite dimensional) Hilbert space. It may be checked that \(a_j^\dagger(v)\) is really the adjoint of \(a_j(v)\), with respect to this scalar product. Our interest is to lift (or quantize) operators \(A \in \text{End}(V_J)\) to operators acting on Fock space. In the present context, this is done by means of maps \(\Gamma, \ d\Gamma : \text{End}(V_J) \to \text{End}(\mathcal{F}_f(V))\) defined as the graded operators obtained from
\[
\Gamma^{(k)}A(u_1 \wedge \ldots \wedge u_k) := Au_1 \wedge \ldots \wedge Au_k
\]
and
\[
d\Gamma^{(k)}A(u_1 \wedge \ldots \wedge u_k) := \sum_{j=1}^k u_1 \wedge \ldots \wedge u_{j-1} \wedge (Au_j) \wedge u_{j+1} \wedge \ldots \wedge u_k.
\]

**Exercise 4.5.** Check the correspondence between the definition of \(d\Gamma\) given here and the one given by (2.11) and (2.12).

**Exercise 4.6 (cf. [11]).** Derive the following identity: \([d\Gamma(A), a_j^\dagger(v)] = a_j^\dagger(Av)\).

Given any \(x \in V\) and \(v \in V^C\) any unitary vector, we see that \(\phi(v)(x) := \chi(v) \cdot x \cdot v = x - 2g(v,x)v\), i.e. the twisted conjugation by \(v\) using the grading automorphism \(\chi\) is a reflection on the hyperplane perpendicular to \(v\). But reflections generate the orthogonal group \(O(V,g)\) so that the map \(\phi\), being defined for all invertible elements of the Clifford algebra, when restricted to the subgroup generated by all products of an even number of unitary vectors (\(\text{Spin}^+(V)\)), reduces to a homomorphism onto \(SO(V)\). This homomorphism may be restricted to \(\text{Spin}(V)\).

Let us recall that there is a canonical vector space isomorphism between the Clifford algebra and the exterior algebra, given explicitly in terms of an orthonormal basis by:
\[
Q : \Lambda V^C \to \mathbb{C}l(V)
\]
\[
v_1 \wedge \ldots \wedge v_k \mapsto v_1 \cdot v_2 \cdots v_k.
\]
Direct computation then shows that $\mathfrak{spin}(V)$ coincides with $Q(\Lambda^2 V)$ and hence $Q(\Lambda^2 V) \cong \mathfrak{so}(V)$, the isomorphism being given by

$$\text{ad} : \quad Q(\Lambda^2 V) \longrightarrow \mathfrak{so}(V)$$

$$a \quad \mapsto \quad [a, \cdot]$$

Let $c : \mathcal{C}(V) \rightarrow \text{End}(S)$ be an irreducible representation of $\mathcal{C}(V)$. Since $\mathfrak{spin}(V)$ is realized as a subspace of $\mathcal{C}(V)$, we can compose $c$ with the isomorphism $\text{ad}^{-1}$ to obtain a representation, called the infinitesimal spin representation, of $\mathfrak{so}(V)$ on $S$. Setting $\hat{B} := \text{ad}^{-1}(B)$:

$$\hat{\mu} : \quad \mathfrak{so}(V) \rightarrow Q(\Lambda^2 V) \hookrightarrow \mathcal{C}(V) \rightarrow \text{End}(S)$$

$$B \quad \mapsto \quad \hat{B} \quad \mapsto \quad \hat{\mu}(\hat{B}) \quad \mapsto \quad c(\hat{B}),$$

i.e.,

$$\hat{\mu}(B) := c(\hat{B}), \quad B \in \mathfrak{so}(V).$$

The infinitesimal spin representation satisfies the following basic relation:

$$[\hat{\mu}(B), c(v)] = c(Bv). \quad (4.3)$$

Comparing (4.3) with the identity from exercise 4.6 one realizes that $dT$ and $\hat{\mu}$ must be closely related. In order to express this relation, note that any real linear operator $R$ on $V$ can be written as $R = R_+ + R_-$, with $R_+$ linear in $V$ and $R_-$ antilinear and skewsymmetric (in $(V_j, \langle \cdot, \cdot \rangle_j)$). Then, it can be shown that for any $B \in \mathfrak{so}(V)$, the following relation holds:

$$\hat{\mu}(B) = d\Gamma(B_+) + \frac{1}{2} (a^\dagger B_+ a^\dagger - aB_- a) - \frac{1}{2} \text{Tr}B_+, \quad (4.4)$$

where $a^\dagger B_- a^\dagger := \sum_{k,l} \langle u_k | B_- u_l \rangle j_k^a j_l^a$ and $aT a := \sum_{k,l} \langle Tu_l | u_k \rangle j_k^a j_l^a$ (with $\{u_k\}_k$ any orthonormal basis in $V_j$). This equation plays an important role for the definition of the quantization map in the infinite dimensional case, discussed below.

In the infinite dimensional context, we begin with a separable real vector space $V$ on which a positive definite symmetric bilinear form $g$ is defined. It is assumed that $V$ is complete in the metric induced by $g$, so that $(V^\mathbb{C}, \langle \cdot, \cdot \rangle)$ is a separable Hilbert space, where $\langle \langle u|v \rangle \rangle := 2g(\bar{u}, v)$. The Clifford algebra is constructed as follows. Consider the algebra $\mathcal{C}_{\text{fin}}(V)$ obtained from the union of all algebras $\mathcal{C}(W)$, where $W$ runs through all finite dimensional subspaces of $V$. There is a unique trace $\tau$ on $\mathcal{C}_{\text{fin}}(V)$, inherited from the traces on each $\mathcal{C}(W)$. The scalar product induced by the trace makes $\mathcal{C}_{\text{fin}}(V)$ a prehilbert space. Its completion $\mathcal{H}_+^\mathbb{C}$ allows one to represent $\mathcal{C}_{\text{fin}}(V)$ as a subalgebra of $\mathcal{B}(\mathcal{H}_+)$ via the GNS construction. The closure of this algebra is then a $C^*$-algebra, which is defined to be the Clifford algebra $\mathcal{C}(V)$. The universal property remains valid in this context and in particular an orthogonal map $h \in O(V, g)$ extends to a $C^*$-algebra automorphism $\theta_h$ of $\mathcal{C}(V)$ (Bogoliubov automorphism).

In order to construct a representation of the Clifford algebra on Fock space we need, as before, an orthogonal complex structure $J$. The Fock space $\mathcal{F}_J(V)$ is now defined as the completion of the exterior algebra $\Lambda^\bullet V_J$ with respect to the scalar product $\langle \cdot, \cdot \rangle$. The action of $\mathcal{C}(V)$ on the exterior algebra is defined as in the finite dimensional case, its extension giving rise to an irreducible representation $\pi_J : \mathcal{C}(V) \rightarrow \text{End}(\mathcal{F}_J(V))$. As in the finite dimensional case, the action of the
orthogonal group $O(V)$ on the set of orthogonal complex structures is transitive, for given two complex structures $J$ and $K$, there is a unitary map $h : V_J \to V_K$ such that $K = hJh^{-1}$. As can be shown, if the Bogoliubov automorphism $\theta_h$ is implementable by a unitary operator on Fock space, then $\pi_J$ and $\pi_K$ are equivalent. In general however, they will be inequivalent. The converse also holds: Implementability of $\theta_h$ follows from equivalence of the representations. Necessary and sufficient conditions on $h$ for $\theta_h$ to be implementable are afforded by the Shale-Stinespring theorem (cf. [11], thm. 6.16), namely that the antilinear part $\frac{1}{2}(h + JhJ)$ of $h$ be Hilbert-Schmidt. In terms of the representations, it says that $\pi_J$ and $\pi_K$ are unitarily equivalent if and only if $(J - K)$ is Hilbert-Schmidt.

**Exercise 4.7.** Provide a physical interpretation of the Shale-Stinespring theorem. Hint: Try relating the vacua associated to two complex structures $J$ and $K$.

For the construction of quantized currents (like the charge or the number operator) we need a map taking self-adjoint operators on $H$ : $= V_C$ to self-adjoint operators on $F_J(V)$. The explicit construction of this map, which can be found in [11], will not be presented here. Instead, we will try to describe some of the motivations behind the construction.

Recall that $O(V)$ acts transitively on the set of orthogonal complex structures, $\mathcal{J}(V)$. Since we have chosen a fixed complex structure $J$ to construct the representation $\pi_J$ on Fock space, then any other complex structure will be given in terms of $J$ and of an element $h \in O(V)$ $(J' = hJh^{-1})$. Recall also that an element of the unitary group $U_J(V)$ is just an orthogonal map $h \in O(V)$ that commutes with $J$. A unitary transformation $U \in U_J(V)$ is implemented in Fock space by a map $\Gamma_J$ such that:

$$\Gamma_J(U)\pi_J(v)\Gamma_J(U)^{-1} = \pi_J(Uv).$$

Now, the observables of the 1-particle theory correspond to elements of the Lie algebra $\mathfrak{o}_J(V)$ of the restricted orthogonal group, which is defined as $O_J(V) := \{ h \in O(V) \mid [h, J] \text{ is Hilbert-Schmidt}\}$. If an element $X \in \mathfrak{o}_J(V)$ is such that $[X, J] = 0$, then it follows that $XJ$ is self-adjoint on $V_J$ and it can be quantized by means of $d^* J$. The question of (unitary) equivalence of the quantization obtained by means of $J$ on one side and by means of $J' = hJh^{-1}$ on the other, may be formulated as follows. The complex structure $J'$ is determined by $h$. The map $v \mapsto \pi_J(hv)$ extends to an automorphism of the Clifford algebra and the question is then whether this automorphism is implementable on Fock space. So, given $h \in O(V)$, we are looking for a unitary operator $\mu(h)$ on Fock space such that:

$$\mu(h)\pi_J(v)\mu(h)^{-1} = \pi_J(hv).$$

In view of the inclusion $U_J(V) \subseteq O(V)$, we see that we are looking for an extension of $\Gamma_J$ to $O(V)$. If $[J, h]$ is Hilbert-Schmidt, that is, if $h \in O_J(V)$, then the map $\mu$ can be constructed (it is the pin representation of $O_J(V)$ on Fock space). Its restriction to $SO_J(V)$ is the spin representation, from which an infinitesimal version $\hat{\mu}$ can be defined on a dense domain of Fock space and turns out to be given by (4.4) without the trace term and, therefore, it is not a Lie algebra homomorphism. This gives rise the so-called Schwinger term, defined as

$$\alpha(A, B) := [\hat{\mu}(A), \hat{\mu}(B)] - \hat{\mu}([A, B]).$$

The Schwinger term is a cocycle that gives an obstruction for $\hat{\mu}$ to be a Lie algebra homomorphism. As explained in [11], the Schwinger term is related to anomalies in
quantum field theory and also to noncommutative geometry. It appears naturally when studying the Virasoro algebra, and therefore is also related to the notion of central charge in conformal field theory. As we have seen, central charges do also appear when we study entanglement entropy in spin chains that display critical behavior. Our aim in the next section is to give an idea of how all these concepts are interrelated. This will allow us to close the circle by providing a new topological interpretation of quantum criticality, for which the underlying geometry is not anymore the geometry of the space of external parameters, but a geometry in the sense of noncommutative geometry. This geometric interpretation of anomalies, central charges, Schwinger cocycles etc., has been known for several decades (to the best of my knowledge the first person to realize this was Araki \cite{39, 40}). But the connection to quantum critical phenomena does not seem to have been exploited.

4.3. Cyclic cocycles and quantum criticality. Previously in these notes we discussed the Gelfand-Naimark theorem, which serves as a motivation for the notion of a noncommutative space. It turns out that the Schwinger term described in the previous section also has a nice geometric interpretation, in the context of noncommutative geometry \cite{11, 41}. In order to give at least a glimpse of how this interpretation appears we will present, following \cite{5}, a very basic (yet instructive) example, namely the Gauss-Bonnet theorem, in the language of noncommutative geometry. But before that we quickly review some aspects of the geometry of surfaces, following the beautiful presentation of the subject by Pressley \cite{42}. We thus start with a given 2-dimensional surface, described locally through a parametrization

\[ \sigma : U \subseteq \mathbb{R}^2 \longrightarrow \mathbb{R}^3 \\
(u, v) \longmapsto \sigma(u, v) = (x(u, v), y(u, v), z(u, v)). \]

At each point, the tangent plane is generated by \( \sigma_u \equiv \frac{\partial \sigma}{\partial u} \) and \( \sigma_v \equiv \frac{\partial \sigma}{\partial v} \) and we can define the normal unit vector as

\[ n := \frac{\sigma_u \times \sigma_v}{\| \sigma_u \times \sigma_v \|}. \]

The infinitesimal length element on the surface is given by

\[ ds^2 = Edu^2 + 2Fdu dv + Gdv^2, \]

where

\[ E = (\sigma_u, \sigma_u), \quad F = (\sigma_u, \sigma_v), \quad G = (\sigma_v, \sigma_v) \]

are the components of the first fundamental form:

\[ F_I = \begin{pmatrix} E & F \\ F & G \end{pmatrix}. \]

Recall that the first and second fundamental forms enter the definition of Gaussian curvature of a surface, which we now recall, starting from the curvature of a curve. For a plane curve, parametrized by \( \gamma(t) \) with unit speed (\( ||\dot{\gamma}(t)|| = 1 \)), let \( n(t) \) denote the unit normal at \( \gamma(t) \). Then the (signed) curvature \( \kappa \) is defined through the relation

\[ \ddot{\gamma} = \kappa n. \]

The curvature gives us an idea of how much the curve deviates from a straight line \cite{42}. In fact, we may compute

\[ (\gamma(t + \Delta t) - \gamma(t)) \cdot n \approx (\dot{\gamma}(t) \Delta t + \frac{\ddot{\gamma}(t)}{2} \Delta t^2 + \cdots) \cdot n = \frac{1}{2} \kappa \Delta t^2. \]
Now we repeat the same reasoning, but with a surface. That is, we want to compute 
\[ (\sigma(u + \Delta u, v + \Delta v) - \sigma(u, v)) \cdot n, \]
where now \( n \) denotes the unit normal to the surface. From a second order Taylor expansion and using the fact that 
\[ \sigma_u \cdot n = 0 = \sigma_v \cdot n, \]
we get
\[ \sigma(u + \Delta u, v + \Delta v) - \sigma(u, v) \approx \frac{1}{2}(L\Delta u^2 + 2M\Delta u\Delta v + N\Delta v^2) = \frac{1}{2}(\Delta u, \Delta v) \begin{pmatrix} L & M \\ M & N \end{pmatrix} \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}, \]
where \( L = \sigma_{uu} \cdot n \), \( M = \sigma_{uv} \cdot n \) and \( N = \sigma_{vv} \cdot n \) are the coefficients of the second fundamental form:
\[ F_{II} = \begin{pmatrix} L & M \\ M & N \end{pmatrix}. \]

Now, for any smooth curve \( \gamma \) we have a decomposition of the form
\[ \ddot{\gamma} = \kappa_n n + \kappa_g g \times \dot{\gamma}, \]
where \( \kappa_n \) and \( \kappa_g \) denote, respectively, the normal and geodesic curvatures of \( \gamma \). To define the curvature of the surface we need to consider only curves with \( \kappa_g = 0 \), for which the normal curvature takes the form
\[ \kappa_n = \ddot{\gamma} \cdot n = Lu^2 + 2Mu\dot{v} + Nv^2. \]
The value of \( \kappa_n \) changes depending on the direction of the curve at the evaluation point, and it is clear it must attain maximum and minimum values. They are the principal curvatures, denoted as \( \kappa_1 \) and \( \kappa_2 \). The Gaussian curvature is defined as \( K := \kappa_1\kappa_2 \). We can obtain several useful formulas for the curvature using the fundamental forms. The principal curvatures \( \kappa_1 \) and \( \kappa_2 \) are obtained from an extremization problem, where we look for extremal values of the principal curvature as we change the direction of the curve -given by \( (\dot{u}, \dot{v}) \)- subject to the unit-speed restriction \( \|\dot{\gamma}\| = 1 \). So, with \( x = (x_1, x_2), \ x_1 = \dot{u}, x_2 = \dot{v}, \) we want to extremize
\[ Q : \mathbb{R}^2 \rightarrow \mathbb{R} \\
\quad x \mapsto x^t F_{II} x, \]
subject to the restriction \( \|\dot{\gamma}\|^2 = 1 \). But we also have
\[ \|\dot{\gamma}\|^2 = Eu^2 + 2F\dot{u}\dot{v} + Gv^2 = x^t F_I x. \]

**Exercise 4.8.** Solve the extremization problem posed above, subject to the constraint \( \|\dot{\gamma}\|^2 = 1 \), and show that the solution is given by the solution of the eigenvalue problem
\[ (F_{II}^{-1} F_I) x = \lambda x, \]
where the eigenvalue \( \lambda \) is the Lagrange multiplier of the problem. Show furthermore that, for a given solution \( (x, \lambda) \), the corresponding normal curvature coincides precisely with \( \lambda \) and conclude that the Gaussian curvature can be expressed as follows:
\[ K = \kappa_1\kappa_2 = \text{det} (F_{II}^{-1} F_I) = \frac{LN - M^2}{EG - F^2}. \]

There are other ways we can characterize \( K \). One of them uses the Gauss map: For any point \( p \) in the surface, consider the unit normal, \( n_p \). Regarding this vector as a point in the unit sphere, we obtain a map \( p \mapsto n_p \) from the surface to the unit sphere, the Gauss map. As we go around a small loop centered at \( p \), the Gauss map produces an image loop on the unit sphere. The quotient of the areas enclosed
by the loops converges, in the limit where the original loop shrinks to a point, to the Gaussian curvature. Yet another way to obtain the Gaussian curvature is by means of the Weingarten map. First notice that we have \( n_u \cdot \sigma_u = -L \), \( n_u \cdot \sigma_v = -M \) and \( n_v \cdot \sigma_v = -N \). This can be easily checked; for instance, the first relation is obtained by taking the partial derivative of \( \sigma_u \cdot n = 0 \) with respect to \( u \). The others are obtained in the same way.

The Weingarten map \( \mathcal{W} \) is most easily defined in the basis \( \{ \sigma_u, \sigma_v \} \), where it has a matrix given by \( F^{-1} \mathcal{F} \mathcal{I} \). In fact, if we define \( \mathcal{W}(\sigma_u) = -n_u \), \( \mathcal{W}(\sigma_v) = -n_v \) and write

\[
-n_u = \lambda_{11} \sigma_u + \lambda_{12} \sigma_v, \\
-n_v = \lambda_{21} \sigma_u + \lambda_{22} \sigma_v,
\]

then it follows that

\[
\Lambda := \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix} = F^{-1} \mathcal{F} \mathcal{I}.
\]

Now we compute

\[
n_u \times n_v = (\det \Lambda) \sigma_u \times \sigma_v = (\det F^{-1} \mathcal{F} \mathcal{I}) \sigma_u \times \sigma_v,
\]

from which the following identity is obtained:

\[
n \cdot (n_u \times n_v) = K ||\sigma_u \times \sigma_v||.
\]

Now, as the components of the unit normal \( n = (n_1, n_2, n_3) \) are smooth functions of \( (u,v) \), we can compute their exterior derivatives

\[
dn_i = (\partial_u n_i) du + (\partial_v n_i) dv,
\]

in order to obtain

\[
\varepsilon_{ijk} n_k dn_i \wedge dn_j = 2n \cdot (n_u \times n_v) du \wedge dv.
\]

This leads to the following formula for the Euler characteristic:

\[
\chi(\Sigma) = \frac{1}{4\pi} \int \varepsilon_{ijk} n_k dn_i \wedge dn_j.
\]

This formula is particularly well suited to explain the noncommutative viewpoint, to which we now turn, following the example presented by Connes in \[5\]. Let us consider an algebra \( A \) (without assuming other properties, for the moment being) together with a trilinear map

\[
\tau : A \times A \times A \to \mathbb{C}
\]

such that

\[
\tau(a_0, a_1, a_2) = \tau(a_2, a_0, a_1) \tag{4.5}
\]

and

\[
\tau(a_0a_1, a_2, a_3) - \tau(a_0, a_1a_2, a_3) + \tau(a_0, a_1, a_2a_3) - \tau(a_3a_0, a_1, a_2) = 0. \tag{4.6}
\]

Now let \( t \mapsto e_t \) be a (continuous) family of idempotents, \( e_t^2 = e_t \). Then it can be shown that the quantity \( \tau(e_t, e_t, e_t) \) does not depend on \( t \), providing an “invariant”
of the algebra. A quick way to see what is going on is to assume that we can differentiate with respect to $t$. In this case we have

$$\dot{e}_t = [x_t, e_t],$$

with $x_t = [\dot{e}_t, e_t]$. Using this fact and (4.5), we obtain

$$\frac{d\tau}{dt}(e_t, e_t, e_t) = 3\tau([x_t, e_t], e_t, e_t).$$

But the last expression vanishes exactly. To see this, we put

$$a_0 = x_t$$

and $a_1 = a_2 = a_3 = e_t$ in (4.6) and use $e_t = e_t$. Now, coming back to Gauss-Bonnet, if we take the algebra to be $A = C^\infty(\Sigma)$, we see that the trilinear map $(f_0, f_1, f_2) \mapsto \int_\Sigma f_0 df_1 \wedge df_2$ satisfies (4.5) and (4.6) above, provided $\partial \Sigma = \emptyset$. But, as explained in [5], in this algebra there are no interesting idempotents. This can be remedied by adding a “bit of noncommutativity” to this algebra, that is, by replacing it by the following one:

$$A = C^\infty(\Sigma) \otimes M_2(\mathbb{C}).$$

Now, recalling the Gauss map, we realize that we can use the normal to the surface in order to obtain an idempotent, namely

$$e = \frac{1}{2} (1 - n \cdot \sigma),$$

where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$, a “vector” whose components are the Pauli matrices. Then, if we define -following [5] -

$$\tau(f_0 \otimes M_0, f_1 \otimes M_1, f_2 \otimes M_2) := \left( \int_\Sigma f_0 df_1 \wedge df_2 \right) \text{Tr}(M_0 M_1 M_2),$$

we obtain (an algebraic version of) the Euler characteristic.

**Exercise 4.9.** Prove the last statement, i.e., compute $\tau(e, e, e)$ and show that it is (up to a constant factor) precisely $\chi(\Sigma)$.

What we learn from the previous example is that it seems plausible to encode geometry and topology in algebraic structures related to a manifold $M$. This is precisely the way noncommutative geometry works. After establishing such algebraic and operator-theoretic characterization of certain geometric or topological structures, one can try to keep the algebraic version, but now dropping the commutativity assumption. Such is the case with differential calculus. Let us then quickly list the main properties of de Rham cohomology and see whether they can be formulated for more general algebras. Given a compact manifold $M$, the space of 1-forms $\Omega^1(M)$ consists of elements of the form $fdg$, where $f$ and $g$ are smooth functions on $M$, and $dg = \sum_i (\partial_i g) dx_i$ is the exterior derivative of $g$. Differential forms of order $k$, $\Omega^k(M)$, are generated locally by expressions of the form $dx_I \equiv dx_{i_1} \wedge \ldots \wedge dx_{i_k}$ so that, in general, the exterior derivative $d : \Omega^k(M) \rightarrow \Omega^{k+1}(M)$ can be defined through $d(f dx_I) := df \wedge dx_I$. The exterior derivative satisfies the Leibniz rule

$$d(\omega \wedge \eta) = d\omega \wedge \eta + (-1)^{\|\omega\|} \omega \wedge d\eta$$

and fulfills the basic identity $d^2 = 0$, from which we obtain the (de Rham) cohomology “groups”:

$$H^k(M) = \text{Ker } d^{k+1}/\text{Im } d^k,$$

that contain important information about the topology of $M$. Finally, we also have Stoke’s theorem:

$$\int_{\partial M} \omega = \int_M d\omega.$$

Now suppose we are given a unital algebra $A$. Thinking of it as given by some space of functions on a “virtual” (i.e. noncommutative) space, we may try to define a
In order to define the space of 1-forms, we consider the map $d : A \to A \otimes A$ defined as $da := 1 \otimes a - a \otimes 1$. Its usefulness comes from the fact that it acts as a derivation:

$$d(ab) = (da)b + a(db).$$

But $A \otimes A$ is “too big” to be regarded as a space of 1-forms. We want to have a closer resemblance to $\Omega^1(M)$. Recalling that 1-forms can always be put in the form $\theta = f dg$, we consider the restriction to the subspace of $A \otimes A$ generated by elements of the form $adb$. Noticing that $adb = a(1 \otimes b - b \otimes 1) = a \otimes b - ab \otimes 1$,

we arrive at the following definition:

$$\Omega^1 A := \ker(m) \cong A \otimes \overline{A} \quad (\overline{A} \equiv A/\mathbb{C}) ,$$

where $m : A \otimes A \to A$ is the multiplication map $m(a \otimes b) = ab$. Then, starting from $\Omega^1 A = A \otimes \overline{A}$ we can go on and define $\Omega^k A := A \otimes \overline{A} \otimes \ldots \otimes \overline{A}$ for $k \geq 1$. The exterior derivative, then, is simply given by

$$d(a_0 \otimes \overline{a}_1 \otimes \cdots \otimes \overline{a}_k) := 1 \otimes \overline{a}_0 \otimes \overline{a}_1 \otimes \cdots \otimes \overline{a}_k.$$

From these definitions we get, as can be easily checked:

(i) $d^2 = 0$ and Leibniz rule: $d(\omega_k \eta) = d\omega_k \eta + (-1)^k \omega_k d\eta$,

(ii) $\Omega^k A \cdot \Omega^l A \subseteq \Omega^{k+l} A$.

This means that in any complex algebra we can find an analog of the space of differential forms (i.e., a graded differential algebra). The importance of this construction lies in the fact that it satisfies a universal property, as any derivation of $A$ into a bimodule factors through a bimodule morphism from $\Omega^l A$.

We also want to have a notion of integration. In this context this is achieved through the introduction of cycles. An $n$-dimensional cycle is a complex graded differential algebra $(\Omega^\bullet = \bigoplus_{k \leq n} \Omega^k, d)$, along with an “integral”, i.e. a linear map $\int : \Omega^\bullet \to \mathbb{C}$, such that:

$$\int \omega = 0 \quad (\text{for } k < n), \quad \int \omega_k \omega_l = (-1)^{kl} \int \omega_l \omega_k \quad \text{and} \quad \int d\omega_{n-1} = 0.$$

The third requirement is tantamount to Stokes’ theorem for the case of spaces without boundary. Now, given an algebra $A$, a cycle over $A$ is a cycle $(\Omega^\bullet, d, \int)$ together with a homomorphism $\rho : A \to \Omega^0$ [11, 5]. A basic example is afforded by the de Rham complex on a compact manifold without boundary.

Given a cycle over $A$ we may now define, for $a_0, a_1, \ldots, a_n \in A$,

$$\tau(a_0, \ldots, a_n) := \int \rho(a_0)d(\rho(a_1)) \cdots d(\rho(a_n)).$$

As shown in [3], this map satisfies (the generalization to $n$ of) the relations (4.5) and (4.6), i.e., it is a cyclic cocycle.

**Definition 4.10.** Given a complex algebra $A$, an odd Fredholm module over $A$ is given by a representation $\sigma : A \to B(H)$ on the algebra of bounded operators on a Hilbert space, together with a self-adjoint operator $F : H \to H$, such that $F^2 = 1$ and such that $[F, \sigma(a)]$ is a compact operator for each $a$ in $A$. An even
Fredholm module contains, in addition to the structure of an odd Fredholm module, an additional grading of $\mathcal{H}$, say $\gamma$, such that $\gamma F = -\gamma F$ and $[\gamma, \sigma(a)] = 0, a \in \mathcal{A}$.

On a Fredholm module one can introduce the structure of a graded differential algebra defining the differential as

$$d(\sigma(a)) := i[F, \sigma(a)].$$

Letting $\Omega^1$ be spanned by elements of the form $a_0 da_1$, and so on, we arrive at the formula $d\omega = i[F, \omega]|_\pm$ as a suitable definition for $d$, where the bracket denotes a supercommutator (depending on the degree of $\omega$).

**Example 4.11 (Quasi-free Representations).** An important class of examples for cyclic-cocycles is afforded by the so-called Schwinger terms (as defined in the previous section) in quantum field theory. In the context of charged fermionic fields, we start with a real vector space $V$ (given as a certain space of solutions to the classical field equation), a symmetric bilinear form $g$ on $V$ and a compatible (orthogonal) complex structure $J$. Physically, $J$ is determined by the spectrum of the Hamiltonian. From the data $(V, J, g)$ one then defines a complex Hilbert space which is the complexification of $V$ using $J$ as the complex structure. So we get a Hilbert space $\mathcal{H} = (V_J, \langle \cdot | \cdot \rangle_J)$, where the inner product is given by

$$\langle u | v \rangle_J := g(u, v) + ig(Ju, v).$$

We also have a representation of the field algebra on Fock space,

$$\hat{\pi}_J : \mathcal{C}l(V) \to \text{End}(F_J(V)).$$

Now, the point is that the Schwinger term

$$\alpha(A, B) = [\hat{\mu}(A), \hat{\mu}(B)] - \hat{\mu}[A, B] = \frac{i}{8} \text{Tr} (J[J, A][J, B]), \quad (4.7)$$

defines a cyclic 1-cocycle. A geometric interpretation of this cocycle is then made possible in the context of non-commutative geometry described above.

When discussing the entanglement properties of spin chains, we found that the entanglement entropy of a sub-chain of length $L$, at the critical point, scales logarithmically with $L$. We mentioned that the constant in front of the logarithm was related to the central charge of the corresponding conformal field theory. These central charges can also be understood as anomalies appearing in the quantization process of the effective field theories describing the spin chains. As an example, let us consider the Ising chain:

$$H = -\frac{1}{2} \sum_{n=1}^{N} \left( \sigma_{n}^{x} \otimes \sigma_{n+1}^{x} + \lambda \sigma_{n}^{z} \right).$$

Using the Wigner-Jordan transformation and then defining the (Majorana) operators $[43]$

$$\chi_1(n) = (a_n^\dagger + a_n), \quad \chi_2(n) = i(a_n^\dagger - a_n),$$

we obtain

$$H = \frac{i}{2} \sum_n \left( \chi_2(n) \chi_1(n+1) + \lambda \chi_1(n) \chi_2(n) \right).$$

We can go to the continuum limit by assuming the sites in the chain are separated by a unit length $l_0$ and defining $x_n = l_0 n$. Then, to first order in $l_0$, we have:

$$\chi_\alpha(x_{n\pm 1}) \approx \chi_\alpha(x_n) \pm l_0 \partial_x \chi_\alpha(x_n).$$
Defining the “chiral” components \( \chi_{\pm} = (\chi_1 \pm \chi_2)/2 \) and the corresponding spinor\
\[
\psi = \begin{pmatrix} \chi_+ \\ \chi_- \end{pmatrix},
\]
one obtains, using Heisenberg’s equations of motion,
\[
(i\gamma^\mu \partial_\mu - m) \psi = 0,
\]
(4.8)
where \( m = m(\lambda) \) is such that \( m(\lambda_c) = 0 \).

**Exercise 4.12.** Defining light-cone coordinates \( x_{\pm} = x^0 \pm x^1 \), show that, at the critical point \((m = 0)\), the Dirac equation (4.8) is equivalent to \( \partial_+ \chi_- = 0 = \partial_- \chi_+ \).

**Exercise 4.13.** In the massless case, (4.8) can be obtained from the Lagrangian
\[
\mathcal{L} = i\bar{\psi} \gamma^\mu \partial_\mu \psi.
\]
Considering the spatial coordinate \( x_1 \) to be defined on \( S^1 \) (which amounts to imposing periodic boundary conditions on the spin chain), expand the chiral fields in Fourier modes and then express the Hamiltonian density \( \mathcal{H} = \bar{\psi} \frac{\partial \mathcal{L}}{\partial \psi} - \mathcal{L} \), and the energy function \( H = \int_{S^1} dx_1 \mathcal{H}(x_0, x_1) \) in terms of the Fourier modes.

As the previous calculations show, when \( m = 0 \) the two chiral fields are completely decoupled from each other. Thus, we may study them separately. Let us consider \( \chi_+ \), for which the mode expansion must be of the form
\[
\chi_+(t, x) = \sum_{n \in \mathbb{Z}} a_n e^{in(t+x)}.
\]
Imposing canonical anticommutation relations to the field (which is real), we obtain:
\[
\{a_n, a_m\} = \delta_{n+m,0}, \quad a_n^* = a_{-n}.
\]
From the previous exercise, we see that the contribution of \( \chi_+ \) to the (second quantized) Hamiltonian will be
\[
H_+ = \sum_{n \in \mathbb{Z}} n : a_{-n} a_n : ,
\]
where normal ordering has been introduced. Now, how do we define normal ordering depends on what we regard as the “vacuum state”. This has important consequences for the commutation relations of the (Fourier components of the) stress-energy tensor.

**Exercise 4.14.** Decomposing the stress-energy tensor
\[
T_{\mu\nu} = \frac{1}{4}(\bar{\psi} \gamma_\mu \partial_\nu \psi + \bar{\psi} \gamma_\nu \partial_\mu \psi)
\]
in light-cone components \( T_{++}, T_{--}, T_{+-}, T_{-+} \) and \( T_{+-} \), show that \( T_{++} = T_{--} = 0 \), and that the Fourier components \( (L_n) \) of \( T_{++} \) satisfy the following commutation relations (Virasoro algebra):
\[
[L_m, L_n] = (m - n)L_{m+n} + \frac{c}{12} (m^3 - m) \delta_{m+n,0},
\]
with \( c = 1/2 \).

The correct solution of the previous exercise depends crucially in a careful handling of the normal ordering prescription. This in turn is related to the “filling-up of the Dirac sea” which, in mathematical terms, can be reduced to the problem
of quantizing a linear system with an appropriately chosen complex structure. In fact, writing the Hamiltonian density in terms of the spinor $\psi$, we obtain

$$H = -i\psi^\dagger \sigma_3 \partial_x \psi.$$  

This means that the 1-particle Hamiltonian (which is defined on the Hilbert space $L^2(S^1) \otimes \mathbb{C}^2$) is given by $H^{(1)} = -i\sigma_3 \partial_x$. As we have seen, the splitting of the 1-particle Hilbert space into positive and negative energy states gives rise to a complex structure, which is the one that should be used for quantization. When this is done, one obtains the anomalous term of the Virasoro algebra as an anomaly (Schwinger term) given precisely as a cyclic 1-cocyle of the form (4.7). Now, the relevance of this fact in the context of quantum phase transitions is that there are already some geometric characterizations of the critical point in terms of, e.g., Berry phases [44, 45]. This has also been related to the behavior of certain Chern numbers associated to the parameter space of the spin chain [46]. Now, using Araki’s self-dual formalism, it should also be possible to compute the cocycle outside the critical point. The behavior of the cocycle as a function of the model’s external parameters may provide a new geometric characterization of the critical point.

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