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One-dimensional Cellular Automata in Quantum and Fermionic Theories

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Chapter 1

Introduction

The first axiomatization of quantum mechanics by means of Hilbert spaces is due to Hilbert, von Neumann, and Norheim in ref. [HNN28], along with the monumental work of Neumann [Neu32]. The works first laid the foundation for a rigorous mathematical description of quantum phenomena and prepared the ground for the subsequent development of quantum theory (QT). However, these axioms gave neither some physical insights into the theory nor reasons why the world must be quantum.

Our comprehension about quantum mechanics has profoundly changed since the debut of quantum information. The studies on quantum algorithms and communication along with the striking results of cryptography [BB84; Eke91], teleportation [Ben+93], and dense coding [BW92] to name but a few, radically upended the old consensus. Quantum mechanics is no longer considered a contrived version of its classical counterpart, but it is rather a modern and powerful theory to describe physical phenomena. Some reasons for preferring a quantum world over a classical one have been accurately collected and laboriously translated into new axioms, which in turn are now able to shed light on the key features of the theory.

A crucial role in the investigation of the structure and fundamentals of quantum physics has indeed been played by information theory. Many aspects of physical phenomena can be formulated in terms of information. For instance, if we consider information as a measure of the different configurations in which a system can be, we can interpret the entropy of the system as a quantification of our ignorance of its microscopic description. The well-known thermodynamic quantity has then been reinterpreted as information content of the system state by Shannon in refs. [Sha48; SW49], where he introduced the concept of bit as elementary information carriers. Many decades later, Schumacher proved an analogous to the noiseless coding theorem for quantum theory in ref. [Sch95], where the term *qubit*

has been coined as the elementary information carrier of quantum systems. This is the birth of the theory of information of quantum systems, i.e. quantum information, whose privileged subjects are the quantification of the information content of physical systems, and a suitable description of how this is processed by physical transformations.

The informational paradigm is based on the idea that information plays, at a fundamental level, a crucial role in the description of natural phenomena. Accordingly, since the 2000s a wide community embarked upon the enterprise of deriving the quantum mechanics principles from axioms based on the recent results of quantum information and providing a clear operational interpretation, see refs. [Fuc01; Har01; Fuc02; DAr06; CDP11]. Following the same intuitions, many concepts that were previously equivocal and convoluted have been clarified, such as e.g. the notion of entanglement, complementarity, purification, holism and non-locality.

Many technical problems have been overcome in the quantum information by focusing only on finite dimensional systems. Such a restriction might seem too restrictive, but allowed the introduction of robust models for describing quantum computation [Chi93; MW19], quantum algorithms [DJ92; Sho94; Gro96; Cle+98], and error correction [Per85; Sho95]. For an extensive dissertation, see ref. [NC10]. However, from a theoretical point of view, we may be interested in defining rigorously the concept of computation on infinitely many systems, as well as to introduce some notion of locality for this kind of transformations. From the quantum information viewpoint, it very clear how to define the possible operations on some quantum systems and how to describe the protocol through quantum circuits. Nonetheless, the same models do not apply for a transformation that acts on a lattice of quantum systems: both the definitions of quantum states and quantum operations do not behave as expected if applied straight to an infinite number of systems.

The task of characterization of transformations onto countably-infinitely many systems is also motivated by the *desideratum* to simulate and describe quantum fields. Indeed, the quantum field theory (QFT) is the most detailed description of the dynamics of physical systems available nowadays. Despite its impressive predictive power, the QFT still lacks a satisfactory interpretation and the conceptual aspects behind its mathematical structure are discussed topics both in physics and in philosophy of science [Kuh20]. Among the interpretative issues of QFT we can mention the ultraviolet divergences, the causality violation due to the Hamiltonian description leading to the wave-function superluminal tails [Tha92] and the localization problem [RS61; Kuh20].

In this context, the class of quantum cellular automata (QCAs) naturally

emerges as a theoretical tool for simulating and describing quantum fields. Indeed, QCAs are the quantum analogues of classical cellular automaton (CA), namely an algorithm that defines the local evolution of a grid, which is a finitely-generated group and whose sites can have a state out of finitely many. A CA is actually the *evolution rule* of the grid and its accurate definitions for locality, homogeneity—or translation invariance,—isotropy, reversibility, and universality make it an excellent candidate model for describing physical phenomena. However, its classical nature forbids every application to fundamental physics. For this reason, the quantum cellular automata have been introduced by replacing the sites of a classical CA with quantum systems. The framework have been rigorously defined in ref. [SW04] and a QCA on an accordingly defined grid is a function that maps observables into observables in the customary Heisenberg picture. In so doing, quantum cellular automata are models for *parallel* quantum computation over infinite many systems. They are in fact dual to the quantum Turing machine, and so to quantum circuit by equivalence, where information is processed sequentially.

The same procedure for defining QCAs can be applied for other theories of physical relevance, in particular to the Fermionic quantum theory (FQT). In this case, qubits are replaced with local Fermionic modes,[1] and the automaton must preserve valid Fermionic observables. Thereby, we expect to rigorously derive features so that we can describe and simulate Fermionic quantum fields with a safe and sound toolset.

The study of quantum cellular automata in other theories than the quantum one is clearly motivated by the fact that the fundamental quantum fields are indeed Fermionic or Bosonic. However, cellular automata are the test field for comparing different theories with their respective features, in particular the notion of locality. The concept of CA and QCA have been generalized in the works of refs. [Per20; Per21], where a meticulous definition has been provided in the more general framework of operation probabilistic theories. Thereby, one may generalize cellular automata for theories such as the quantum theory, Fermionic quantum theory, the real quantum theory, the classical theory, and classical theories with entanglement refs. [DEP20a; DEP20b].

Aside from the theoretical interest, physical realizations of quantum cellular automata have been considered as quantum simulators of physical systems with the aim to harness the computational speedup provided by quantum algorithms. The interest of the scientific community is devolved

[1] The elementary information carrier for the Fermionic information theory is however the *febit*, see refs. [PTV21; PTV22].

to the development of technological platform capable of implementing QCAs. However, their strongly interacting evolution over the field operators have prohibited any such control so far. Efforts then moved to implement linear QCAs, also known as quantum walks (QWs). Several platforms ranging from cold atoms [Kar+09], trapped ions [Sch+09; Zäh+10], to photonics systems [Owe+11; San+12; Kit+12; Car+15; Bou+16], have been employed to implement QWs. Although limited by the non-interacting regime, such setups allows us to simulate phenomena otherwise out of reach. Indeed, in the recent paper,[2] we simulated the evolution of a particle according to the Dirac equation onto a photonic platform. In particular, we observed the *Zitterbewegung* effect of states in superposition of particle and antiparticles, namely the trembling motion of the expectation value of the position operator.

Outline of the thesis

The work presented in this thesis is threefold:

- We introduce new quantum cellular automaton definition in terms of supermaps and the so called T-operator, i.e. a local operator that incorporates all the necessary information for defining a QCA.
- We classificate all nearest-neighbor Fermionic quantum cellular automaton (FQCA) over the one-dimensional lattice consisting of one local Fermionic mode per site.
- We report the experimental realization of a photonic platform to simulate the evolution of a one-dimensional QW, specifically to observe the *Zitterbewegung* of a particle satisfying the Dirac dispersion relation.

In the present chapter, both the quantum theory and Fermionic quantum theory are introduced. Their definition is given in the canonical fashion and fixes the notation for the whole work. However, for what pertains the quantum theory, in § 1.1.2 a brief introduction to the higher-order quantum theory is given. Namely, the notion of supermap is provided as transformation from quantum operations to quantum operations. On the other hand, the Fermionic quantum theory is introduced along with two representations of the canonical anticommutation relations (CAR): through the

[2] Under review: Alessia Suprano, Danilo Zia, Emanuele Polino, Davide Poderini, Gonzalo Carvacho, Fabio Sciarrino, Matteo Lugli, Alessandro Bisio, and Paolo Perinotti "Quantum Simulation of *Zitterbewegung* via a Photonic Dirac Cellular Automaton."

creation and annihilation operators in § 1.2.1 and through the self-adjoint representation in § 1.2.4.

In chapter 2, a dissertation over the well established theory of quantum cellular automata is presented. In particular, we first review some underlying notions of classical cellular automata. We then move to the definition of quasi-local observable algebra and that of QCA as homomorphism between them. Among others, the relevant result of the structure theorem and the index theorem are presented.

Once all prerequisites have been given, in chapter 3 we introduce a new notion of QCA as a supermap between transformations onto the grid, such that it preserves their locality. This new definition is then proved to be equivalent to the well-known one of literature. Thereby, the T-operator is described and characterized as a local object that completely describes the rule of the automaton. Indeed, some necessary and sufficient properties of the T-operator are given for it to represent a valid QCA.

In the next chapter 4, the classification of FQCA is reported in the particular case of nearest-neighbors, one-dimensional lattice, and one local Fermionic mode per site. We briefly describe the differences between the index theorem introduced in chapter 2 for QCA and FQCA. The dissertation then continues with the analysis of two relevant cases: the first one strongly resembles a particular subclass of quantum cellular automata, whilst the second case is a *unicum* of FQCA. Indeed, due to a different notion of locality in the Fermionic quantum theory, a new class of FQCA has been found to have no quantum counterparts.

We present in chapter 5 an experimental implementation through a photonic platform of a quantum walk. In a collaboration between the theoretical group of the University of Pavia and the experimental one of the University of Rome "La Sapienza," we devised an experiment to simulate the *Zitterbewegung* of a particle through the implementation of a quantum walk. The positional state of the particle is encoded in the orbital angular momentum (OAM) of light whereas the internal degree of freedom, also known as coin, is represented by the polarization of the photon. We describe the theoretical background of quantum walks along with that of the *Zitterbewegung* effect. The result of the experiment are then concisely presented.

Finally, in chapter 6 we draw the conclusions of the work and present some future prospetives of the field.

1.1 Quantum theory

We firstly introduce the quantum theory of information. The fundamental axioms of the theory are defined according to von Neumann on finite-dimensional Hilbert spaces and illustrated along with the mathematical notation to describe quantum systems and operations. We build up the theory starting from three postulates, as presented in ref. [DCP16]:

1. To each system A we associate a complex Hilbert space $\mathcal{H}_A$. To the composition AB of systems A and B we associate the tensor product $\mathcal{H}_{AB} \coloneqq \mathcal{H}_A \otimes \mathcal{H}_B$.

2. To each state of system A corresponds a positive operator $\rho \in \mathrm{St}(\mathcal{H}_A)$ on $\mathcal{H}_A$ with $\mathrm{Tr}[\rho] \leq 1$.

3. Any map that satisfies all mathematical requirements for representing a transformation within the theory will actually be an admissible quantum transformations of the theory.

From all three assumptions we derive the well-know properties of the theory and the structure of state, effect and transformation sets, which we introduce hereafter.

Any state $\rho \in \mathrm{St}(\mathcal{H}_A)$, also known as a preparation of the system, is a positive operator $\rho \geq 0$ on the Hilbert space $\mathcal{H}_A$ such that $\mathrm{Tr}[\rho] \leq 1$. The set $\mathrm{St}(\mathcal{H}_A)$ boasts both a conic and convex structure. The states satisfying $\mathrm{Tr}[\rho] = 1$ are called *deterministic* and belongs to $\mathrm{St}_1(\mathcal{H}_A)$. We define a preparation test as a collection of preparations $\{\rho_i : \rho_i \in \mathrm{St}(\mathcal{H}_A)\}$ such that the *coarse graining*, i.e.

$$\rho = \sum_i \rho_i,$$

is deterministic. Moreover, the conic structure emerges as soon as we consider a collection of sub-deterministic preparations $\{\rho_i : \mathrm{Tr}[\rho_i] < 1\}$ and conically combine them to attain

$$\sigma = \sum_i p_i \rho_i \quad \text{for} \quad p_i \geq 0,$$

where σ is a new preparation and must fulfill $\mathrm{Tr}[\sigma] \leq 1$. On the other hand, we define the *pure* states as those featuring rank equal to one, namely the projectors onto a one-dimensional subspace of $\mathcal{H}_A$. In the Dirac notation, we denote the pure preparations as $\rho = |\psi\rangle\langle\psi|$, for $|\psi\rangle \in \mathcal{H}_A$. Mixed states,

on the contrary, have rank larger than one and are inherently linked to the convex combination of preparations

$$\tau = \sum_i p_i \rho_i \quad \text{for} \quad 0 \leq p_i \leq 1, \ \sum_i p_i = 1$$

where ρ_i are some states and $\tau \in \mathrm{St}(\mathcal{H}_A)$.

Linear functionals on states are called effects and labeled as $E \in \mathrm{Eff}(\mathcal{H}_A)$. They are represented by positive operators dominated by the identity, that is $0 \leq E \leq I$; the identity, in turn, represents the deterministic effect. We denote the pairing between the state ρ and effect E on the same system through the Born rule as

$$\Pr = (E|\rho) = \mathrm{Tr}[E\rho],$$

that represents the probability of measuring E given the preparation ρ. Effects may be labeled as *atomic* when their rank is equal to one. We define as positive-operator valued measure (POVM) or effect test the collection of effects $\{E_i : 0 \leq E_i \leq I\}$ such that the coarse graining is the deterministic effect, namely $I = \sum_i E_i$.

1.1.1 Quantum Transformations

We conclude our introduction to the quantum theory with the definition of quantum transformation $\mathcal{C} \in \mathrm{Transf}(A \to B)$ as the linear, completely-positive and trace-non-increasing map $\mathcal{C} : \mathrm{St}(\mathcal{H}_A) \to \mathrm{St}(\mathcal{H}_B)$. Both states and effects may be seen as transformations from and to the trivial system, respectively. Transformations that are trace-preserving, i.e. $\mathrm{Tr}[\mathcal{C}(\rho)] = \mathrm{Tr}[\rho]$, are called deterministic transformations or *quantum channels* and belongs to $\mathrm{Transf}_1(A \to B)$, whereas those that are only trace-non-increasing are usually named quantum operations. Thanks to Kraus' theorem, see ref. [Sti55], we describe any transformation $\mathcal{C}$ through the set of operators $\{K_i : \mathcal{H}_A \to \mathcal{H}_B | \sum_i K_i K_i^\dagger \leq I\}$, also known as the Kraus operators, such that $\mathcal{C}$ can be described both in the Schrödinger picture and in the Heisenberg picture, namely

$$\mathcal{C}(\rho) = \sum_i K_i \rho K_i^\dagger, \qquad \mathcal{C}^\dagger(E) = \sum_i K_i^\dagger E K_i,$$

respectively, where $\rho \in \mathrm{St}(A)$ and $E \in \mathrm{Eff}(B)$. We denote by $\mathrm{Lin}(\mathcal{H}_A \to \mathcal{H}_B)$ the space of linear operators from $\mathcal{H}_A$ to $\mathcal{H}_B$. The maps featuring only one Kraus operator are called atomic. A collection of transformations $\{\mathcal{T}_i\}$

for which $\mathcal{C} = \sum_i \mathcal{C}_i$ is trace preserving is called a quantum instrument or transformation test. Quantum theory features the relevant property that any deterministic and atomic transformation $\mathcal{C} \in \mathrm{Transf}(A \to A)$ is reversible, i.e. its only Kraus operator belongs to the set of unitary matrices $\mathsf{SU}(\mathcal{H}_A)$. On the other hand, any Kraus operator of $\mathrm{Transf}(A \to A)$ live in the full-matrix algebra $\mathfrak{M}(\mathcal{H}_A)$, that is the C*-algebra of endomorphisms $\mathrm{End}(\mathcal{H}_A)$ over $\mathcal{H}_A$.

For every set $\mathrm{St}(A)$, $\mathrm{Transf}(A \to B)$, $\mathrm{Eff}(A)$ of states, quantum operations, and effects, respectively, on system A, B we denote with the subscript $\mathbb{R}$ the real span thereof. In particular, $\mathrm{Eff}_{\mathbb{R}}(A) \coloneqq \mathrm{Span}_{\mathbb{R}}(\mathrm{Eff}(A))$ is the C*-algebra of observables over system A, whereas $\mathrm{Transf}_{\mathbb{R}}(A \to B) \coloneqq \mathrm{Span}_{\mathbb{R}}(\mathrm{Transf}(A \to B))$ is the algebra of quantum operations from system A to system B.

Remark. Theories whose transformation are defined by Kraus operators belonging to some algebra are generally called quantum theories. Some notable examples are the quantum theory itself, the Fermionic quantum theory, cf. § 1.2, and the real quantum theory.

Kraus isomorphism Every linear operator $C : \mathcal{H}_A \to \mathcal{H}_B$ onto Hilbert spaces $\mathcal{H}_A$, $\mathcal{H}_B$ describes the action of an atomic transformation $\mathcal{C} : \rho \mapsto C\rho C^\dagger$ if we relax the trace-non-increasing condition. However, the reverse is not true as atomic quantum operations are mapped to their Kraus operators *modulo a phase*. Let A, B be two quantum systems, we define the Kraus map $\mathfrak{K} : \mathrm{Transf}_a(A \to B) \longrightarrow \mathrm{Lin}(\mathcal{H}_A \to \mathcal{H}_B)/\mathsf{U}(1)$ from the atomic transformations to their Kraus operators modulo a phase. Please note that such a transformation is not linear since the combination of two quantum operations is not equivalent to combination of their Kraus operators, unless they are linearly dependent. In the particular case of $A = B$, we have that the Kraus isomorphism

$$\mathfrak{K} : \mathrm{Transf}_a(A \to A) \longrightarrow \mathrm{Lin}(\mathcal{H}_A)/\mathsf{U}(1), \tag{1.1}$$

is a monoidal isomorphism between the atomic quantum operations and their Kraus operators modulo a phase, namely it preserves both the identity and the product. Indeed, the composition of atomic transformations is represented by the product of their Kraus operators, whereas the identity transformation $\mathcal{I}$ is represented by the identity operator I.

Choi-Jamiołkowski isomorphism The conic structure of quantum operations can be probed through the Choi-Jamiołkowski isomorphism $\mathfrak{C}$, cf. refs. [Jam72; Cho75]. Let us first introduce the double-ket notation: given

a bounded linear operator $A : \mathcal{H} \to \mathcal{V}$ between Hilbert spaces we denote with

$$|A\rangle\!\rangle := \sum_{ij} A_{ij} |i\rangle \otimes |j\rangle$$

the vector of $\mathcal{H} \otimes \mathcal{V}$, where $\{|i\rangle\}$, $\{|j\rangle\}$ are bases for $\mathcal{H}$, $\mathcal{V}$, respectively, and A_{ij} are matrix entries of operator A in that bases. For any two bounded linear operators $A : \mathcal{H} \to \mathcal{H}'$, $B : \mathcal{K} \to \mathcal{K}'$ and a vector $|C\rangle\!\rangle \in \mathcal{H} \otimes \mathcal{K}$ it holds

$$A \otimes B|C\rangle\!\rangle = |ACB^{\perp}\rangle\!\rangle \in \mathcal{H}' \otimes \mathcal{K}', \qquad \langle\!\langle A|B\rangle\!\rangle = \mathrm{Tr}[A^{\dagger}B].$$

Thereby, we represent with ease the maximally entangled state

$$|I\rangle\!\rangle\langle\!\langle I| = \sum_i |i\rangle\langle i| \otimes |i\rangle\langle i|,$$

for any system Q and $\{|i\rangle\}$ a basis of $\mathcal{H}_Q$. The Choi-Jamiołkowski transformation $\mathfrak{C}$ is an isomorphism of cones and maps every transformation $\mathcal{C} \in \mathrm{Transf}(A \to B)$ to a state $\rho_{\mathcal{C}} \in \mathrm{St}(AB)$, which is known as the Choi operator of $\mathcal{A}$. The Choi-Jamiołkowski isomorphism then reads

$$\begin{aligned} \mathfrak{C} : \mathrm{Transf}(A \to B) &\to \mathrm{St}(AB) \\ \mathcal{C} &\mapsto \rho_{\mathcal{C}} := (\mathcal{C} \otimes \mathcal{I})\, |I\rangle\!\rangle\langle\!\langle I|, \end{aligned}$$

the isomorphism is in fact linear and preserves atomic maps. Indeed, if $\mathcal{C}$ is atomic then C is its only Kraus operator and the Choi operator of the transformation is

$$\mathfrak{C}(\mathcal{C}) = (\mathcal{C} \otimes \mathcal{I})\, |I\rangle\!\rangle\langle\!\langle I| = (C \otimes I)\, |I\rangle\!\rangle\langle\!\langle I|\, (C^{\dagger} \otimes I) = |C\rangle\!\rangle\langle\!\langle C|.$$

On the other hand, any quantum operation $\mathcal{C}$ of Kraus operators $\{C_i\}$ is mapped to $\mathfrak{C}(\mathcal{C}) = \sum_i |C_i\rangle\!\rangle\langle\!\langle C_i|$.

1.1.2 Higher-order Quantum Theory

We briefly introduce the reader to the higher-order quantum theory, cf. refs. [CDP09; BP19]. One may wonder how one can define functions that map admissible quantum operation to admissible quantum operations. In particular, we would like to describe the whole class of such maps and gather some criteria to detect whether a given one respects the axioms of the quantum theory.

We observe that dealing with quantum operations $\mathrm{Transf}(A \to B)$, where A, B are some quantum systems, is the same as dealing with states $\mathrm{St}(AB)$,

thanks to the Choi-Jamiołkowski isomorphism $\mathfrak{C}$. Hence, let A, B, C, and D be some quantum systems, the supermap

$$\mathscr{A} : \text{Transf}(A \to B) \longrightarrow \text{Transf}(C \to D)$$

can be expressed as a quantum operation

$$\mathcal{A} : \text{St}(AB) \to \text{St}(CD) \tag{1.2}$$

by conjugating the supermap with the Choi-Jamiołkowski isomorphism, i.e.

$$\mathcal{A} = \mathfrak{C}\mathscr{A}\mathfrak{C}^{-1}. \tag{1.3}$$

This procedure allows us to relate supermaps $\mathscr{A}$ and quantum operations $\mathcal{A}$ by preserving their cone structure. Indeed, the positivity of $\rho \in \text{St}(AB)$ is a necessary and sufficient condition for $\mathfrak{C}^{-1}(\rho) \in \text{Transf}(A \to B)$ being a completely positive map (CP-map). In so doing, the necessary condition so that $\mathscr{A}$ maps CP-maps to CP-map is that $\mathcal{A}$ maps positive states into positive states. However, this is granted by the fact that $\mathcal{A}$ is a quantum operation. The relation between the supermap $\mathscr{A}$ and the transformation $\mathcal{A}$ can be seen through the following commutative diagram:

$$\begin{array}{ccc} \mathcal{T} & \xrightarrow{\mathscr{A}} & \mathcal{T}' \\ {\scriptstyle \mathfrak{C}^{-1}}\uparrow & & \downarrow{\scriptstyle \mathfrak{C}} \\ T & \xrightarrow{\mathcal{A}} & T' \end{array}$$

where $T \in \text{St}(AB)$, $\mathcal{T} \in \text{Transf}(A \to B)$, $T' \in \text{St}(CD)$, $\mathcal{T}' \in \text{Transf}(C \to D)$.

The Choi-Jamiołkowski is linear, thus $\mathscr{A} = \mathfrak{C}^{-1}\mathcal{A}\mathfrak{C}$ is linear as well. We still need to prove that the transformed operations are still trace-non-increasing. Let $I \in \text{Eff}(CD)$ be the deterministic effect for system CD, we readily notice that $0 \leq (\mathcal{T}')^{\dagger}(I) = \text{Tr}_0[\rho_{T'}] \leq I$. We are then ready to give a definition of supermap.

Definition (Supermap)**.** Let A, B, C, and D be quantum systems, the map

$$\mathscr{A} : \text{Transf}(A \to B) \longrightarrow \text{Transf}(C \to D)$$

is an admissible supermap if it is linear and preserves positivity, even when applied locally on a bipartite map $\text{Transf}(AC \to BC)$ for some system C.

It is then possible to reduce every higher-order transformation such as $A \to ((B \to C) \to D)$ recursively to a map onto states $\text{St}(ABCD)$. This tells us that the cone generated by probabilistic higher-order operations is the whole cone of positive operators. Essentially, the above result implies that the only relevant cone in quantum mechanics is that of positive operators.

Theorem 1. *Let A, B, C, and D be quantum systems and*

$$\mathscr{A} : \mathrm{Transf}(A \to B) \longrightarrow \mathrm{Transf}(C \to D)$$

be a supermap that preserves the conic structure of quantum operations, i.e. it preserves the atomicity of transformations, then the action of $\mathscr{A}$ onto the Kraus operators

$$\alpha : \mathrm{Lin}(\mathcal{H}_A \to \mathcal{H}_B) \to \mathrm{Lin}(\mathcal{H}_C \to \mathcal{H}_D)$$

is linear.

Proof. In the following, we combine the Kraus map $\mathfrak{K}$ and the Choi-Jamiołkowski isomorphism $\mathfrak{C}$ of § 1.1.1 to describe the action of the supermap $\mathscr{A}$ through the quantum operation $\mathcal{A} : \mathrm{St}(AB) \to \mathrm{St}(CD)$ of eqs. (1.2) and (1.3) over the Choi operators. Indeed, a Kraus operator $C \in \mathrm{Lin}(\mathcal{H}_A \to \mathcal{H}_B)$ represents an atomic quantum operation $\mathcal{C} \in \mathrm{Transf}_a(A \to B)$ whose Choi operator is $|C\rangle\!\rangle\langle\!\langle C| \in \mathrm{St}(AB)$. The action of the transformation $\mathcal{A}$ is atomic as the supermap $\mathscr{A}$ preserves atomicity by assumption, therefore $\mathcal{A}$ maps every Choi operator $|C\rangle\!\rangle\langle\!\langle C|$ to $A|C\rangle\!\rangle\langle\!\langle C|A^\dagger$ where $A \in \mathrm{Lin}(\mathcal{H}_A \otimes \mathcal{H}_B \to \mathcal{H}_C \otimes \mathcal{H}_D)$ is the only Kraus operator of $\mathcal{A}$. We readily observe that the action of $\mathcal{A}$ onto the Kraus C is linear as A is linear onto the Kraus vector $|C\rangle\!\rangle$. The construction hitherto provided is hereafter depicted as the diagram

$$\begin{array}{ccccccc}
C & \xrightarrow{\mathfrak{K}^{-1}} & \mathcal{C} & \xrightarrow{\mathfrak{C}} & |C\rangle\!\rangle\langle\!\langle C| & \xrightarrow{\mathcal{P}} & |C\rangle\!\rangle \\
\downarrow{\scriptstyle \alpha} & & \downarrow{\scriptstyle \mathscr{A}} & & \downarrow{\scriptstyle \mathcal{A}} & & \downarrow{\scriptstyle A} \\
C' & \xleftarrow[\mathfrak{K}]{} & \mathcal{C}' & \xleftarrow[\mathfrak{C}^{-1}]{} & |C'\rangle\!\rangle\langle\!\langle C'| & \xleftarrow[\mathcal{P}]{} & |C'\rangle\!\rangle
\end{array}$$

where $\mathcal{P}$ is the map from a rank one operator $|C\rangle\!\rangle\langle\!\langle C|$ to the vector $|C\rangle\!\rangle$ of its one-dimensional support space. Please note that $\mathcal{P}$ is a map along rays of the state cone and A is a Kraus operator of $\mathcal{A}$ defined modulo a phase.

Finally, we define $\alpha := \mathfrak{K}\mathscr{A}\mathfrak{K}^{-1}$ and show that the image of every operator in $\mathrm{Lin}(\mathcal{H}_A \to \mathcal{H}_B)$ is unique. Indeed, the Kraus map $\mathfrak{K}$ links an atomic quantum operation to its Kraus operator modulo a phase. We now prove that such degree of freedom is immaterial and that we can define a map α between linear operators as a bijection. Let α, β be two maps of Kraus operators such that

$$\beta(C) = \alpha(C)e^{i\phi(C)}$$

for $C \in \mathrm{Lin}(\mathcal{H}_A \to \mathcal{H}_B)$ and phase ϕ. We then consider some quantum operations $\mathcal{P}$, $\mathcal{M} \in \mathrm{Transf}(A \to B)$ with Kraus operators $L + R$, $L - R \in$

$\mathrm{Lin}(\mathcal{H}_A \to \mathcal{H}_B)$, respectively, and evaluate the image of the transformation $\mathcal{C} = \mathcal{P} - \mathcal{M}$ under the supermap $\mathscr{A}$. Let $\rho \in \mathrm{St}(A)$, we have

$$\mathcal{C}(\rho) = (L+R)\rho(L+R)^\dagger - (L-R)\rho(L-R)^\dagger = 2(L\rho R^\dagger + R\rho L^\dagger),$$

so that if we apply the maps α, β thereto we attain

$$\begin{aligned}\mathscr{A}(\mathcal{C})(\sigma) &= 2(\alpha(L)\ \sigma\ \alpha(R)^\dagger + \alpha(R)\ \sigma\ \alpha(L)^\dagger),\\ &= 2(\alpha(L)\ \sigma\ \alpha(R)^\dagger e^{i(\phi(L)-\phi(R))} + \alpha(R)\ \sigma\ \alpha(L)^\dagger e^{i(\phi(R)-\phi(L))}).\end{aligned}$$

The last two equations must equal for every $\sigma \in \mathrm{St}(C)$. We readily see that for $L \not\propto R$ there always exists some vector $|\psi\rangle \in \mathcal{H}_C$ such that $\alpha(L)|\psi\rangle \not\propto \alpha(R)|\psi\rangle$. Thus for $\sigma = |\psi\rangle\langle\psi|$,

$$\begin{aligned}\alpha(L)|\psi\rangle\langle\psi|\alpha(R)^\dagger e^{i(\phi(L)-\phi(R))} + \alpha(R)|\psi\rangle\langle\psi|\alpha(L)^\dagger e^{i(\phi(R)-\phi(L))} =\\ \alpha(L)|\psi\rangle\langle\psi|\alpha(R)^\dagger + \alpha(R)|\psi\rangle\langle\psi|\alpha(L)^\dagger\end{aligned}$$

only iff $\phi(L) = \phi(R)$. On the other hand, for $L \propto R$ we have that L has the same phase as every other non-proportional operator R', which in turn must have the same phase as R. □

1.2 Fermionic quantum theory

In the 1980s, R. Feynman wondered whether it is possible to simulate the behavior of Fermionic systems through quantum qubits [Fey82]. Since then, the properties of Fermions have been thoroughly investigated both in terms of computational capabilities and operational features. On the one hand, the former aspect sheds light on the underlying informational structure of the theory, with the striking result that the Fermionic theory and quantum theory of qubits are computationally equivalent, as proved by ref. [BK02]. On the other hand, the latter leads to a deeper understanding of the physical traits of the Fermionic theory, especially to the notions of locality and entanglement.

Fermions are half-integer spin particles that undergo the Pauli exclusion principle, i.e. two Fermionic particles cannot occupy the same state at the same time. We present the theory in the second quantization formalism as a superselection of the quantum one. In particular, FQT treats local Fermionic modes as elementary systems, which represents the counterpart of qubits in quantum theory. From the computational point of view, a local Fermionic mode is a system which can be either empty or occupied by a

single "excitation." Within this framework, the Fermionic parity superselection rule as been derived as a consistency constraint of the Fermionic probabilistic theory, see ref. [DAr+14]. We then describe some correspondences to the quantum theory through the Jordan-Wigner transformation. Eventually, we show an alternative representation of the Fermionic algebra due to ref. [Der06], which comes in handy for the classification of Fermionic Quantum Cellular Automata in chapter 4.

As we shall further see in the following, the differences between the quantum theory and the Fermionic quantum theory are profound, and as such the two should not be mistaken. In particular, in § 1.2.3 it is clear that the two theories have distinct notions of locality. This has consequences in many features of the theory such as discrimination [LPT20; LPT21], Violation of local tomography and entanglement monogamy [DAr+14].

1.2.1 The Fermionic algebra

The notion of locality in the FQT is rigorously defined through the Fermionic algebra $\mathfrak{F}$. For n local Fermionic modes, we consider the annihilation and creation operators φ_i, $\varphi_i^\dagger$ as those satisfying the CAR

$$\{\varphi_i, \varphi_j^\dagger\} = \delta_{ij} I \quad \text{and} \quad \{\varphi_i, \varphi_j\} = 0, \tag{1.4}$$

where $i, j = 1 \dots n$. We further inspect the properties of the underlying Hilbert space if we introduce the number operators as $N_i = \varphi_i^\dagger \varphi_i$. From the anticommutation relations of eq. (1.4), we conclude that their spectrum is

$$\sigma(N_i) = \{0, |0\rangle_i ; 1, |1\rangle_i\},$$

i.e. $\varphi_i^\dagger \varphi_i |0\rangle_i = 0$ and $\varphi_i^\dagger \varphi_i |1\rangle_i = |1\rangle_i$. Moreover, the annihilation and creation operators φ_i, $\varphi_i^\dagger$ satisfy the relevant properties of

$$\varphi_i |1\rangle_i = |0\rangle_i , \tag{1.5}$$

$$\varphi_i^\dagger |0\rangle_i = |1\rangle_i , \tag{1.6}$$

due to eq. (1.4).

The Fermionic operators φ_i, $\varphi_i^\dagger$ are the generator of the Fermionic algebra $\mathfrak{F}(n)$ for n local Fermionic modes while eqs. (1.5) and (1.6) allow us to interpret them as lowering and raising operators, respectively, for the number operator $\varphi_i^\dagger \varphi_i$. Furthermore, the operators $\varphi_i^\dagger \varphi_i$ mutually commute and are simultaneously diagonalizable. We define the vacuum state $|\Omega\rangle$ as the unique shared eigenvector whose eigenvalue is equal to zero, namely

$$\varphi_i^\dagger \varphi_i |\Omega\rangle = 0 \quad \forall i = 1 \dots n.$$

Starting from the vacuum vector $|\Omega\rangle$ and accordingly applying the creation operators $\varphi_i^\dagger$, we introduce the Fock basis of elements

$$|s_1 s_2 \dots s_n\rangle := (\varphi_1^\dagger)^{s_1}(\varphi_2^\dagger)^{s_2}\cdots(\varphi_n^\dagger)^{s_n}|\Omega\rangle, \quad s_i = 0,1 \tag{1.7}$$

which span the antisymmetric Fock space

$$\mathcal{F}^n := \mathrm{Span}_{\mathbb{R}}\{|s_1 s_2 \dots s_n\rangle : s_i = 0,1\}$$

of dimension equal to 2^n. The term s_i is the occupation number of the i-th mode and corresponds to the eigenvalue of the number operator $\varphi_i^\dagger\varphi_i$. Finally, we point out that a vector of eq. (1.7) represents a Slater determinant in the first quantization formalism.

1.2.2 The parity superselection rule

One of the most distinctive traits of the Fermionic quantum theory is the parity superselection rule. In ref. [WWW52], the authors extensively describe the notion of superselection rule, namely a restriction of all the admissibile measurements of a theory, and derive the parity superselection rule as a consequence of the time inversion symmetry.

In the present section we introduce an axiomatization of FQT, see ref. [DAr+14]. In such a framework, the parity superselection rule can be derived from first principles. The theory deals with systems made of finitely many local Fermionic modes and is derived starting from the superselected states of the quantum theory of qubits. We then require the atomic and local transformations to act on their systems through the Fermionic operators of the algebra F we introduced above. This defines the notion of locality for Fermionic quantum operations. As a consequence, the FQT manifests new and distinctive traits ranging from a different structure of state and effect sets, an alternative notion of entanglement to the parity superselection rule. We begin by assuming the following postulates:

1. The Fermionic quantum theory is causal.
2. The states of n local Fermionic modes are represented by density matrices on the antisymmetric Fock space $\mathcal{F}^n$.
3. The transformations on n local Fermionic modes are represented by linear Hermitian-preserving maps.
4. For a composite system $Q = AB$ of n modes, the local transformations on the subsystem A of the first $1\dots m < n$ modes have Kraus operators generated by the Fermionic operators $\varphi_j, \varphi_j^\dagger \in \mathsf{F}(m)$ for $j = 1\dots m$.

5. Local transformations on a system retain the same Kraus representation when other systems are added or discarded.

6. The transformation of Kraus operators $X_i = \varphi_i + \varphi_i^\dagger \ \forall i = 1 \dots n$ is physical, namely it is an admissible map of the theory.

7. The paring between states and effects is given by the Born rule

$$\mathrm{Pr} = (a|\rho) = \mathrm{Tr}[a\rho].$$

8. On a single mode the pairing between the deterministic effect e and the state ρ is $(e|\rho) = \mathrm{Tr}[\rho]$.

The Fermionic algebra takes here the crucial role of defining the locality of transformations. Indeed, in assumption 4 we require the Kraus operator of an atomic and local transformation to belong to the algebra of the Fermionic modes the map is acting upon. Moreover, assumptions 4 and 6 let us derive a relevant property of any transformation between n local Fermionic modes, namely that each Kraus operator is a combination of either an even or odd number of field operators.

The previous results lead to the following two fundamental features of the Fermionic theory, see ref. [DAr+14], which allow us to characterize both the sets of preparations and effects.

Theorem (Parity superselection)**.** *States of FQT satisfy the parity superselection rule, i.e. their density matrices commute with the parity operator*

$$P := \frac{1}{2}\left[I + \prod_{i=0}^{n}\left(\varphi_i\varphi_i^\dagger - \varphi_i^\dagger\varphi_i\right)\right].$$

Theorem (Fermionic effects)**.** *Effects of the FQT are positive operators made of products of an even number of fields operators.*

The former theorem restricts the set of possible pure states for Fermionic systems only to those having a well-defined parity. The antisymmetric Fock space of n modes decomposes into the direct sum

$$\mathcal{F}^n = \mathcal{F}_0^n \oplus \mathcal{F}_1^n,$$

the subscript indicating the eigenvalue of the parity operator, and the set of states also decomposes as well in

$$\mathrm{St}(\mathcal{F}^n) = \mathrm{St}(\mathcal{F}_0^n) \oplus \mathrm{St}(\mathcal{F}_1^n).$$

If we consider vectors in the form of eq. (1.7), the parity is the sum of the excitations modulo two

$$s := \sum_{i=0}^{n} s_i \mod 2$$

or, equivalently, whether the total occupation number $s = \sum_i s_i$ is even or odd.

We point out that the set structure of Fermionic states is strongly shaped by the parity superselection rule and irreversibly altered from the original quantum one. Since convex-only combinations between vectors of different parity are allowed, the particular case of a single isolated mode surprisingly reduces to the classical bit

$$\mathrm{St}(\mathcal{F}^1) = \{p\,|0\rangle\langle 0| + (1-p)\,|1\rangle\langle 1| : p \in [0,1]\}.$$

Beside, the whole set of states $\mathrm{St}(\mathcal{F}^n)$ is spanned by the convex combinations of the even and odd preparations as depicted in fig. 1.1, where the case of two local Fermionic modes is considered. For two modes, the even and odd states separately have the supports lying on a bidimensional space, shown as two Bloch spheres in the figure. The states represented on the spheres are pure, whereas those inside the balls and the convex combination between them are the Fermionic mixed states.

Generally, the vector space of parity-defined vectors is isomorph to that of $n-1$ qubits, where n is the number of local Fermionic modes. On the other hand, the linear span of states and effects corresponds to the space of $2^n \times 2^n$ hermitian matrices

$$\mathrm{St}_{\mathbb{R}}(\mathcal{F}^n) = \mathrm{Eff}_{\mathbb{R}}(\mathcal{F}^n) = \mathrm{Herm}((\mathbb{C}^2)^{\otimes n}),$$

whose dimension is 2^{2n}. Once we reordered the Fock basis so that the even vectors precede the odd ones, we obtain $\forall \rho \in \mathrm{St}(n)$ and $\forall a \in \mathrm{Eff}(n)$ that

$$\rho = \left(\begin{array}{c|c} \rho_0 & \\ \hline & \rho_1 \end{array}\right), \qquad \rho_0, \rho_1 \geq 0 \quad \text{and} \quad \mathrm{Tr}[\rho_0 + \rho_1], \leq 1$$

$$a = \left(\begin{array}{c|c} a_0 & \\ \hline & a_1 \end{array}\right), \qquad 0 \leq a_0 \leq I_0 \quad \text{and} \quad 0 \leq a_1 \leq I_1,$$

namely, the preparations and effects are represented as block matrices on the even and odd subspaces $\mathcal{F}_0$, $\mathcal{F}_1$.

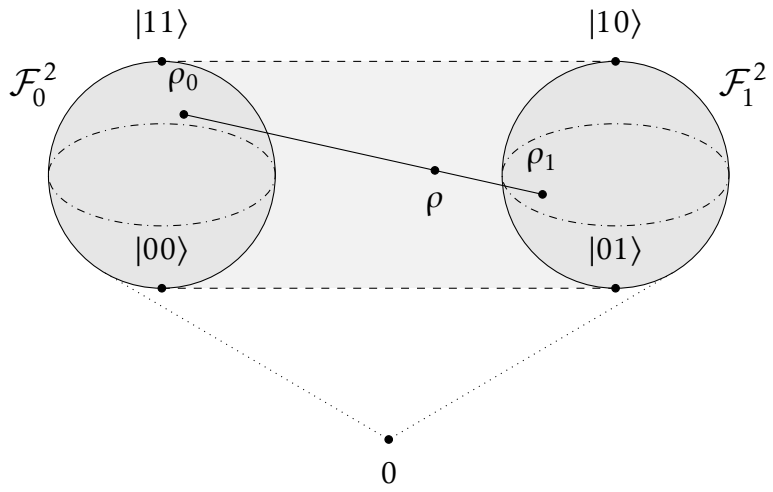


Figure 1.1: A pictorial representation of the state set for two local Fermionic modes is shown. The shaded surface depicts the set of deterministic states, whereas the underlying area delimited by the dotted lines converging to the zero state refers to the conic structure of sub-deterministic preparations. The represented states satisfy $\mathrm{Supp}\,\rho_s \subseteq \mathcal{F}_s^2$ for $s = 0, 1$, while $\rho = p\rho_0 + (1 - p)\rho_1$, $p \in [0, 1]$ is any convex combination of the previous two.

1.2.3 The Jordan-Wigner transformation

We further understand the locality and entanglement features of the FQT only once we introduce the Jordan-Wigner transformation between local Fermionic modes and quantum qubits, firstly proposed in ref. [JW28]. The antisymmetric Fock space $\mathcal{F}^n$ is isometric to the complex Hilbert space of n qubits, as we promptly realize by looking at the Fock basis of eq. (1.7). Thus, we define the unitary map

$$\begin{aligned} U\colon \mathcal{F}^n &\to \mathbb{C}^{2^n} \\ |s_1 s_2 \dots s_n\rangle_F &\mapsto |s_1 s_2 \dots s_n\rangle_Q . \end{aligned}$$

between the space of quantum and Fermionic states. Given the Pauli matrices

$$\sigma^x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.8}$$

we could then promote the operators

$$\sigma_i^{\pm} := \frac{\sigma_i^x \pm i\sigma_i^y}{2}$$

to the quantum equivalents of the creation and annihilation Fermionic operators. On the one hand, we have the correct same-site anticommutation relations $\{\sigma_i^+, \sigma_i^-\} = I$ for $i = 1 \dots n$. On the other hand, spins on different sides do commute, i.e. $[\sigma_i^+, \sigma_j^-] = 0$ for $i \neq j$, unlike Fermions which anticommute. We accordingly adjust our operators by adding a phase factor, which is able to keep track of the other excited modes, to attain the Jordan-Wigner transformation

$$\mathcal{J}(\varphi_i) = e^{-i\pi \sum_{j=1}^{i-1} \sigma_j^+ \sigma_j^-} \cdot \sigma_i^- \tag{1.9a}$$

$$\mathcal{J}(\varphi_i^\dagger) = e^{+i\pi \sum_{j=1}^{i-1} \sigma_j^+ \sigma_j^-} \cdot \sigma_i^+ \tag{1.9b}$$

$$\mathcal{J}(\varphi_i^\dagger \varphi_i) = \sigma_i^+ \sigma_i^-. \tag{1.9c}$$

Remark. The phase term can be rewritten for $i > 0$ as

$$S_i := e^{\pm i\pi \sum_{j=1}^{i-1} \sigma_j^+ \sigma_j^-} = \prod_{j=1}^{i-1} e^{\pm i\pi \sigma_j^+ \sigma_j^-} = \prod_{j=1}^{i-1} (1 - 2\sigma_j^+ \sigma_j^-) = \prod_{j=1}^{i-1} (-\sigma_j^z), \tag{1.10}$$

where we observe that it depends on the chosen order of the systems. This trait greatly limits its applicability to cases where the systems are mapped to sites on manifolds with dimension higher than one.

The transformation $\mathcal{J}$ is actually a $*$-algebra isomorphism and let us build a Fermionic algebra $\mathfrak{F}(n)$ on the top of a n qubit system. We may be tempted to translate all Fermionic expressions into quantum ones through the Jordan-Wigner transformation, however many notion of QT will not apply once they are transformed back. For instance, as we can see from eqs. (1.9a) and (1.9b), local Fermionic operators are generally mapped to a many qubits operator. Therefore, the locality properties are preserved only if the expression involves an even number of Fermionic operators for each site, in order to cancel the phase factor as in eq. (1.9c). For an extensive addendum on the Jordan-Wigner transformation see ref. [Nie05].

1.2.4 Self-adjoint Representation of the Canonical Anticommutation Relations

Instead of describing the behavior of transformations in FQT in terms of the creation and annihilation operators, we introduce another representation of the CAR in terms of self-adjoint operators. The framework is developed in ref. [Der06], where the scalar product of real vectors is implemented through the anticommutation of self-adjoint operators. We may recover the

Fermionic algebra only if we group pairs of orthonormal vectors together. The representation will be of use in chapter 4 where the action of a FQCA over observables is handled thereby. We label with $B_h(\mathcal{H})$ the set of bounded self-adjoint operators on Hilbert space $\mathcal{H}$.

Definition. Let V be a real vector space with a positive scalar product π. The linear map $\mathfrak{s} : V \to B_h(\mathcal{H})$ is a representation of the CAR over V in $\mathcal{H}$ if it satisfies

$$\{\mathfrak{s}(v), \mathfrak{s}(w)\} = 2\pi(v, w), \quad \forall v, w \in V.$$

We say that $\mathfrak{s}$ is an *irreducible* representation of the CAR if the only closed sub-spaces of $\mathcal{H}$ preserved by all $K \in \mathfrak{s}(V)$ are $\{0\}$ and $\mathcal{H}$. Let the scalar product π induce the norm $\|\cdot\|$, the representation $\mathfrak{s}$ further respects the following properties for $v \in V$:

- spectrum $\mathfrak{s}(v) = \{-\|v\|, \|v\|\}$.
- $e^{i\,\mathfrak{s}(v)} = \cos\|v\| I + i\frac{\sin\|v\|}{\|v\|}\,\mathfrak{s}(v)$.
- Let $\overline{V}$ be the completion of V in the norm $\|\cdot\|$. Then there exists a unique extension of $\mathfrak{s}$ to a continuous function which is a representation of the CAR.

Thanks to last item, we henceforth assume V being a real Hilbert space.

Given an orthonormal basis $\{v_i\}$ for V, we say that the self-adjoint operators $\{\mathfrak{s}_i\}$ are a representation of the CAR if $\mathfrak{s}_i = \mathfrak{s}(v_i)$. Most notably, the images $\{\mathfrak{s}_i\}$ do respect $\{\mathfrak{s}_i, \mathfrak{s}_j\} = 2\delta_{ij}$. If we group the operators in pairs $\{(\mathfrak{s}_{2i}, \mathfrak{s}_{2i+1})\}$, then we can recombine them to obtain the usual creation and annihilation operators

$$\varphi_i := \frac{\mathfrak{s}_{2i} - i\,\mathfrak{s}_{2i+1}}{2},$$

which satisfy eq. (1.4). As a consequence only even-dimensional real spaces $V = \mathbb{R}^{2n}$ can represent physical systems, specifically they describe n local Fermionic modes. On the other hand, we may say that the single operator $\mathfrak{s}_i$ is associated to a i-th Majorana mode.

The Jordan-Wigner transformation is an effective way to define a particular self-adjoint representation. Indeed, we introduce the Jordan-Wigner bases

$$(\sigma_1^x, \sigma_1^y, S_2\sigma_2^x, S_2\sigma_2^y, \ldots, S_{2n}\sigma_{2n}^x, S_{2n}\sigma_{2n}^y) \quad \text{for} \quad V = \mathbb{R}^{2n}$$

and

$$(\sigma_1^x, \sigma_1^y, S_2\sigma_2^x, S_2\sigma_2^y, \ldots, S_{2n}\sigma_{2n}^x, S_{2n}\sigma_{2n}^y, S_{2n+1}) \quad \text{for} \quad V = \mathbb{R}^{2n+1},$$

where S_i is the sign operator of eq. (1.10). In particular, the operator S_{2n+1} applies the matrix σ^z to all qubits.

Let us see the most basic examples of the self-adjoint representation:

Example. For $\mathfrak{s} : \mathbb{R}^2 \to B_h(\mathbb{C}^2)$ and $\mathfrak{s}(v) = v_x\sigma^x + v_y\sigma^y$, $v \in \mathbb{R}^2$, we have a single local Fermionic mode.

Example. For $\mathfrak{s} : \mathbb{R}^3 \to B_h(\mathbb{C}^2)$ and $\mathfrak{s}(v) = v_x\sigma^x + v_y\sigma^y + v_z\sigma^z$, $v \in \mathbb{R}^3$, we have a non-physical representation of the CAR.

Fermionic Bogoliubov–Valatin transformations

The definition of the self-adjoint representation $\mathfrak{s}$ relies on the scalar product π of the real Hilbert space V. We are then interested in how the operators $\mathfrak{s}(v)$ transform if we apply a linear transformation that preserves the scalar product π to the vectors $v \in V$, i.e. an orthogonal transformation $R \in \mathsf{O}(V)$. The answer is that there exists a unitary transformation $U \in \mathsf{U}(\mathcal{H})$ such that if we conjugate $\mathfrak{s}(v)$ with U, the result still satisfies the CAR. In the physics literature the fact that orthogonal transformations can be unitarily implemented is associated with the name of Bogolubov transformation.

Theorem 2 (Fermionic Bogoliubov–Valatin)**.** *Let $V = \mathbb{R}^{2n}$, for every $R \in \mathsf{O}(V)$ there exists a unique pair of unitary matrices $\{U_R, -U_R\} \subset \mathsf{U}(\mathcal{H})$ such that*

$$\mathfrak{s}(Rv) = U_R \ \mathfrak{s}(r) \ U_R^\dagger,$$

and we have the following group homomorphism

$$\begin{aligned} \phi : \mathsf{O}(V) &\to \mathsf{U}(\mathcal{H})/\{1,-1\} \\ R &\mapsto \pm U_R. \end{aligned}$$

The homomorphism ϕ is the Pin representation of $\mathsf{O}(V)$.

Fermionic Stone-von Neumann theorem

We now show that every other representation is unitarily equivalent to the Jordan-Wigner one. The following theorems can be viewed as a Fermionic analog of the Stone-von Neumann one.

Theorem 3. *Let $\{\mathfrak{s}_i\}$ be a representation of the CAR over $V = \mathbb{R}^{2n}$ in the Hilbert space $\mathcal{H}$. There exists a Hilbert space $\mathcal{K}$ and a unitary operator $U : \left(\mathbb{C}^2\right)^{\otimes n} \otimes \mathcal{K} \to \mathcal{H}$ such that for $i = 1 \dots n$ we have*

$$U\left(S_i\sigma_i^x \otimes I_{\mathcal{K}}\right)U^\dagger = \mathfrak{s}_{2i-1}, \qquad U\left(S_i\sigma_i^y \otimes I_{\mathcal{K}}\right)U^\dagger = \mathfrak{s}_{2i}.$$

The representation is irreducible iff $\mathcal{K} = \mathbb{C}$.

Theorem 4. *Let $\{\mathfrak{s}_i\}$ be a representation of the CAR over $V = \mathbb{R}^{2n+1}$ in the Hilbert space $\mathcal{H}$. There exists Hilbert spaces $\mathcal{K}_+$, $\mathcal{K}_-$ and a unitary operator $U : \left(\mathbb{C}^2\right)^{\otimes n} \otimes (\mathcal{K}_+ \oplus \mathcal{K}_-) \to \mathcal{H}$ such that for $i = 1 \dots n$ it holds*

$$U\left(S_i \sigma_i^x \otimes I_{\mathcal{K}_+ \oplus \mathcal{K}_-}\right) U^\dagger = \mathfrak{s}_{2i-1},$$
$$U\left(S_i \sigma_i^y \otimes I_{\mathcal{K}_+ \oplus \mathcal{K}_-}\right) U^\dagger = \mathfrak{s}_{2i},$$
$$U\left(S_{n+1} \otimes (I_{\mathcal{K}_+} \oplus I_{\mathcal{K}_-})\right) U^\dagger = \mathfrak{s}_{2n+1},$$

where $S_{n+1} = \sigma_0^z \otimes \cdots \otimes \sigma_n^z$.

Theorem (Fermionic Stone-von Neumann)**.** *Let V be an even-dimensional real Hilbert space, and $\mathfrak{s}$, $\mathfrak{s}'$ be two irreducible representation of the CAR. They are unitarily equivalent.*

Theorems 3 and 4 are extensively employed for the classification of FQCA as they allow us to trace back every Fermionic algebra to an irreducible representation of the CAR conjugated by a unitary operator. Moreover, all irreducible representation are unitarily equivalent to the Jordan-Wigner's, thus the dimension of every algebra representing the CAR over $\mathbb{R}^n$ for n Majorana modes is $2^{n/2}$. The mathematical structure that best fits the representations of the CAR is the $\mathbb{Z}_2$-graded algebra, which is presented in the next section.

1.2.5 $\mathbb{Z}_2$-graded algebras

In § 1.2.1, we claimed that the Kraus operator of Fermionic transformation over n local Fermionic modes belong to the Fermionic algebra $\mathfrak{F}^n$. Here we develop the notion of $\mathbb{Z}_2$-graded algebra, also known as superalgebra, of which the Fermionic algebra is a particular case. Most notably, we state that a $\mathbb{Z}_2$-graded algebra is a *sequence*

$$\mathfrak{A} = (\mathfrak{A}_0, \mathfrak{A}_1),$$

where $\mathfrak{A}_0$, $\mathfrak{A}_1$ are the complex spaces of even and odd operators, respectively. The sum of any two elements is defined if they feature the same parity, i.e. $F_p + G_p \in \mathfrak{A}_p$ for F_p, $G_p \in \mathfrak{A}_p$ and $p = 0, 1$. On the other hand, the algebra product is defined between any two operators $F_p \in \mathfrak{A}_p$, $G_q \in \mathfrak{A}_q$ such that $F_p G_q \in \mathfrak{A}_{p \oplus q}$. We presented a definition that is a slight revision of the graded algebra according to ref. [MB99]. That differs from the usual one by means of the direct sum $\mathfrak{A} = \mathfrak{A}_0 \oplus \mathfrak{A}_1$ in that it forbids the sum of

operators with different parity. For two graded algebras, the most important construction is their graded tensor product: given any two $\mathbb{Z}_2$-graded algebra $\mathfrak{A}$, $\mathfrak{B}$, we denote their graded tensor product as $\mathfrak{A} \boxtimes \mathfrak{B}$. It is indeed a $\mathbb{Z}_2$-graded algebra whose n-th term is defined as

$$(\mathfrak{A} \boxtimes \mathfrak{B})_n := \bigoplus_{p \oplus q = n} (\mathfrak{A}_p \otimes \mathfrak{B}_q),$$

that is

$$\begin{aligned}(\mathfrak{A} \boxtimes \mathfrak{B})_0 &:= (\mathfrak{A}_0 \otimes \mathfrak{B}_0) \oplus (\mathfrak{A}_1 \otimes \mathfrak{B}_1),\\ (\mathfrak{A} \boxtimes \mathfrak{B})_1 &:= (\mathfrak{A}_0 \otimes \mathfrak{B}_1) \oplus (\mathfrak{A}_1 \otimes \mathfrak{B}_0).\end{aligned}$$

Let $F \in \mathfrak{A}_p$, $G \in \mathfrak{B}_q$ be two operators of parities p, q, their graded tensor product is $F \boxtimes G \in \mathfrak{A}_p \otimes \mathfrak{B}_q$ and by extension $F \boxtimes G \in (\mathfrak{A} \boxtimes \mathfrak{B})_{p \oplus q}$. The map $\mathfrak{A}_p \times \mathfrak{B}_q \to (\mathfrak{A} \boxtimes \mathfrak{B})_{p \oplus q}$ is bilinear for every p, q and the family of such bilinear products is universal, see ref. [MB99].

In so doing, the parity superselection rule excludes both sums of vectors such as $|0\rangle + |1\rangle$, but also that of operators. For instance, in our setup $\varphi + \varphi^\dagger \varphi$ does not belong to $\mathfrak{F}$. Such a description is especially effective when dealing with $*$-homomorphisms, as they preserve both the parity and the adjointness and all operators are thus granted to be of definite parity.

In chapter 4 we are interested in describing the commutation and anticommutation relation of operators belonging to the Fermionic algebra $\mathfrak{F}$. The natural definition of graded commutator then arises for a $\mathbb{Z}_2$-graded algebra $\mathfrak{A}$ that reads

$$\{\![F_p, G_q]\!\} := F_p G_q + (-1)^{pq} G_q F_p \tag{1.11}$$

for two operators $F_p \in \mathfrak{A}_p$, $G_q \in \mathfrak{A}_q$. In particular, the graded commutator reduces to the anti-commutator if both operators are odd, and to the usual commutator otherwise. Please note that the graded-, anti-, and usual commutator are all well-defined within a $\mathbb{Z}_2$-graded algebra $\mathfrak{A}$ as they all respect the property of $\{\![F_p, G_q]\!\} \in \mathfrak{A}_{p \oplus q}$ for every $F_p \in \mathfrak{A}_p$, $G_q \in \mathfrak{A}_q$.

Finally, we denote by $\mathfrak{M}_n$ the $\mathbb{Z}_2$-graded full matrix algebra, namely the algebra of endomorphisms $End(\mathcal{F}^n)$ over the Fock space $\mathcal{F}^n$.

Chapter 2

Quantum Cellular Automata

With the term cellular automaton (CA) we refer to a class of *algorithms* that are able to process information distributed on a regular grid in a *local* fashion. The original definition consists of a set of discrete sites properly arranged on a lattice, each of them being in a state belonging to a finite set. The CA is then the *rule of evolution* of the cells' configuration, it occurs in discrete time steps, and respects some notion of locality. Locality is indeed the cornerstone of cellular automata and is implemented by introducing the cell neighborhood, namely a finite set of cells whose state *influences* that of the cell at next time step. Thereby, the evolution of a given cell at time $t+1$ depends only on the state at time t of those cells actually being its neighbors, see fig. 2.1.

Stanisław M. Ulam and John von Neumann first introduced the notion of cellular automaton in the early 1950s as a theoretical tool for analyzing and describing natural phenomena. Both of them were working at the Los Alamos National Laboratory, where S. M. Ulam was studying models of crystal growth while J. von Neumanm was working on the problem self-replicating systems, i.e. mechanisms by which a system can produces a copy of itself. Von Neumann, on suggestion of S. Ulam, proved that a cellular automaton is computationally universal and could be used to construct a Turing machine [VB66]. Moreover, its instructions could be the duplication of its own structure, and even of its instructions, thereby functioning as a self-reproducing device.

Cellular automata proved to be valuable models for describing physical phenomena, such as fluid dynamics, molecular interactions, bacteria colonies, traffic jams, and many other, thanks to their full control and clear definition of interaction locality. The subject has been further popularized as the British mathematician John Horton Conway published the "Game of Life" in Martin Gardner's October 1970 column in Scientific

American [Gar70]. Conway's Game of Life is a particular CA describing the evolution of an infinite two-dimensional grid of square cells—each being either alive or dead—that interacts with its eight neighbors, see fig. 2.1. Although the rule of evolution is rather naive, the model is able to exhibits an astonishing variety of behaviors depending on the initial state of the grid. Most notably, from the definition of simple *local rules*, which in principle say nothing whatsoever about the global behavior, the Game of Life let grid configurations evolve that may stay still, oscillate, or move at constant speeds indefinitely.

Cellular automata rose to the status of full-fledged scientific discipline only a decade after, when in the early 1980s the physicist Stephen Wolfram initiated the first serious formalization program, see ref. [Wol83] and later extension of ref. [CY88]. Some CAs have been proven to be computationally universal, see refs. [Tof77; MH89; Wol02], namely they are able to simulate any Turing machine. This last model describes an abstract machine that manipulates symbols on a strip of tape according to a table of rules in a sequatial manner. In spite of it, cellular automata represent a model for *massive parallel computation*, as their evaluation implies the evolution of the whole grid.

The CA features may allow to describe the physical evolution of systems, but their classical nature prevented their diffusion as a models of theoretical physics. The natural way to overtake this limitation is the extension of the automaton notion to the quantum realm as suggested by Feynman in ref. [Fey82]. This resulted in the so called quantum cellular automaton (QCA) where the classical systems are superseded by quantum systems in local unitary interaction. The rigorous framework has been developed in two distinct formulations: the finite configurations of Hilbert space where the QCA is evaluated in the customary Schrödinger picture onto states, or in terms of the quasi-local algebra of observables. The latter case is here introduced and first presented in ref. [SW04].

In the present chapter we shortly review the common notation and concepts of classical CAs, as they laid the foundation for the subsequent development of QCA. We then thoroughly cover the main result of the theory of quantum cellular automata. Namely, we deal with the definition of quasi-local algebra of observables and homomorphism thereof. Some valuable results required for the next chapters 3 and 4 are presented, among which the structure theorem [ANW11] and the index theorem [Gro+12].

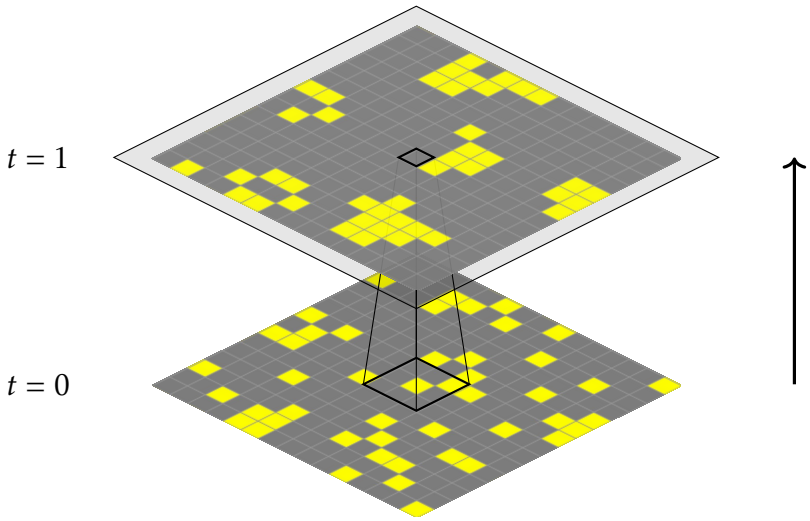


Figure 2.1: Pictorial representation of a CA over a two-dimensional array of cells. The cellular automaton is the rule of evolution of the configuration from time t to time $t + 1$, the state of a given cell is computed from that of their neighboring ones. In particular, the example depicts the evolution of Conway's Game of Life. Each cell—to be considered as a *living* cell—may be either dead or alive and interacts with its eight neighbors according to the following evolutionary rule: i) any live cell with fewer than two live neighbors dies, as if caused by under-population; ii) any live cell with two or three live neighbors lives on to the next generation; iii) live cell with more than three live neighbors dies, as if by overcrowding; iv) any dead cell with exactly three live neighbors becomes a live cell, as if by reproduction.

2.1 Classical Cellular Automata

The present work mostly covers topics pertaining to QCAs and FQCAs. Nonetheless, both frameworks have solid foundations build upon classical cellular automata. For this reason, we hereafter list the principal notions required for dealing with CA, along with some notable results of the field.

Grid Let a grid be a finitely generated group X, namely a group with a finite set of generators $G \subseteq X$ such that $\forall x \in X$, $x = g_1 \cdots g_n$ for some $g_i \in G \cup G^{-1}$. Each element $x \in X$ of the grid is called a site.

Cayley graph Given a grid X and its generators G, we can associate a graph $\Gamma(X, G)$ where the vertices are the elements of the group X and the edges are $\{(n, ng) \mid n \in X, g \in G\}$. A color may be assigned to each generator $g \in G$.

Example. The following grids are all Abelian and regular:

- $X = \mathbb{Z}$, $G = \{g\}$ where $g : \mathbb{Z} \to \mathbb{Z}, z \mapsto z + 1$
- $X = \mathbb{Z}^d$ for $G = \{g_1, \cdots, g_d\}$ where g_i increments the i-th coordinate by one.

Neighborhood We state that any finite subset $N_0 \subseteq X$ is a neighborhood of the identity element $e \in X$. Given a site $x \in X$, $N_x := xN_0$ is the neighborhood of x.

Example. Some well-known neighborhood schemes are:

Von Neumann's $N_x := \{y \in \mathbb{Z}^d \mid \|x - y\|_1 \leq 1\}$, cf. fig. 2.2a.

Moore's $N_x := \{y \in \mathbb{Z}^d \mid \|x - y\|_\infty \leq 1\}$, cf. fig. 2.2b.

Configuration space Let a finite set A accommodate all possible states of a single site $x \in X$, the set A is also known as alphabet. A state or configuration is a function $c : X \to A, x \mapsto c(n) \in A$. We identify with $A^X = \{c : X \to A\}$ the configuration space.

Shift The left-action of X on the configuration space A^X, also known as X-shift, is defined as

$$\begin{aligned} \sigma : X \times A^X &\to A^X \\ (x, c) &\mapsto c' = xc \end{aligned}$$

such that $xc(y) := c(x^{-1}y)$.

(a) Von Neumann's neighborhood. (b) Moore's neighborhood.

Figure 2.2: Graphical representation of two neighborhood schemes in the 2D lattice $\mathbb{Z}^2$. Each box represents a site on the grid, the site x is painted in black whereas the neighborhood N_x in gray.

Local and global rules A local rule is defined over a grid (X, G), a neighborhood N_0, and an alphabet A as the function

$$\tau_0 : A^{N_0} \to A.$$

On the other hand, given a local rule τ_0 we can always evaluate a global rule

$$\tau : A^X \to A^X$$

such that for every $c \in A^X$, $x \in X$

$$\tau(c)(x) \coloneqq \tau_0\left(x^{-1}c\big|_{N_0}\right).$$

Namely, the global rule is computed by firstly shifting the configuration so that x is in the origin e and the neighborhood $N_x \mapsto N_0 = x^{-1}N_x$, then by restricting the configuration to the neihborhood only, where we can safely evaluate the local rule τ_0.

Cellular automaton A CA is a tuple (X, N_0, A, τ_0), where X is a finitely generated group, N_0 is a finite subset of X, A is a finite set of local states, and $\tau_0 : A^{N_0} \to A$ a local function

A defining property of CAs is the concept of locality, which cannot be rigorously stated without the notion of shift. Indeed, it can be shown that the property of commuting with the shifts is structural for CAs.

Theorem (X-equivariance)**.** *Let (X, N_0, A, τ_0) be a cellular automaton and τ its global function. Then τ commutes with all shifts.*

Furthermore, the same property is defining.

Theorem. *Let (X, N_0, A, τ_0) be a cellular automaton. The map $\tau : A^X \to A^X$ is the global rule of (X, N_0, A, τ_0) iff τ commutes with all X-shifts and $\tau(c)(e) = \tau_0(c|_{N_0})$.*

We report here a milestone of the theory of classical cellular automata, i.e. the structure theorem or Curtis–Hedlund–Lyndon theorem, that allows to classify all CA in terms of their global rule. For this purpose, we introduce the topological space $(A, \mathcal{T})$ where we equip the alphabet A with the discrete topology. We can then extend it to the pro-discrete topology for the configuration space by considering $(A^X, \tilde{\mathcal{T}})$ where

$$\tilde{\mathcal{T}} := \{U = \textstyle\prod_{x\in X} U_x | U_x \subset \mathcal{T}, U_x = A \text{ for all but a finite number of indices}\}.$$

Moreover, by defining the Cantor metric on A^X as $d(c_1, c_2) := \frac{1}{k+1}$ if k is finite and 0 otherwise, where $k := \inf\{r : c_1|_{B_r} \neq c_2|_{B_r}\}$ and B_r denotes the ball of radius r around e, one may introduce the Cantor topology on A^X as that induced by the Cantor metric d.

Theorem (Curtis–Hedlund–Lyndon theorem)**.** *Consider a finitely generated group X, a finite alphabet A, and an endomorphism $\tau : A^X \to A^X$, where A^X is equipped with the pro-discrete topology. The map τ is the global rule of a CA iff τ is continuous with respect to the Cantor topology and commutes with the shift operators, i.e. it is X-equivariant.*

2.2 Quantum Cellular Automata

Formalizing cellular automata that evolves grids made of quantum systems is not an easy task. We introduce here the definition of QCA as in ref. [SW04], where the action of the automaton is described as the evolution of the observable algebra in the Heisenberg picture.

Let X be a grid of systems, we indicate with $P(X)$ the set of all subsets of X and with $P_F(X)$ the set of all finite subsets of X. For every site $x \in X$ there is a d-dimensional quantum system, whose observables belong to the full-matrix algebra $\mathfrak{A}_x := \mathfrak{M}_d(\mathbb{C})$. Given $\Lambda \in P_F(X)$ a finite collection of sites, the observable algebra of the corresponding quantum systems is

$$\mathfrak{A}(\Lambda) := \bigotimes_{x\in\Lambda} \mathfrak{A}_x = \bigotimes_{x\in\Lambda} \mathfrak{M}_d(\mathbb{C}). \tag{2.1}$$

Indeed, $\mathfrak{A}(\Lambda)$ is a well-defined C*-algebra generated by all observables acting only on the sites $x \in \Lambda$ and trivially elsewhere. The fact that Λ is a

finite subset of X is here crucial, as it grants the product C*-algebra having a non-divergent operator norm.[1]

The construction of eq. (2.1) provides us with a net of local algebras, which respects the following properties:

- Let $\Lambda_1, \Lambda_2 \in P_F(X)$ be two finite subsets of sites such that $\Lambda_1 \subseteq \Lambda_2$, the algebra $\mathfrak{A}(\Lambda_1) \subseteq \mathfrak{A}(\Lambda_2)$ is a C*-subalgebra. Most notably, we claim that $\mathfrak{A}(\Lambda_1) \otimes I_{\Lambda_2 - \Lambda_1} \cong \mathfrak{A}(\Lambda_2)$.
- For every $A \in \mathfrak{A}(\Lambda_1)$ and $B \in \mathfrak{A}(\Lambda_2)$, the product $AB \in \mathfrak{A}(\Lambda_1 \cup \Lambda_2)$ is well-defined by extending the operators to $A \otimes I_{\Lambda_2}$, $I_{\Lambda_1} \otimes B$, respectively.
- We say that the assigment $\Lambda \mapsto \mathfrak{A}(\Lambda)$ is *local*, namely for every $\Lambda_1, \Lambda_2 \in P_F(X)$ where $\Lambda_1 \cap \Lambda_2 = \emptyset$ it holds

$$[\mathfrak{A}(\Lambda_1), \mathfrak{A}(\Lambda_2)] = 0.$$

If we collect the algebras $\mathfrak{A}(\Lambda)$ altogether, we come to the local or strictly local observables

$$\mathfrak{A}_{\text{local}} := \bigcup_{\Lambda \in P_F(X)} \mathfrak{A}(\Lambda).$$

This is a C*-algebra and its norm is induced by that of each $\mathfrak{A}(\Lambda)$. In terms of this norm we now consider the completion of the local observables.

Definition (Quasi-local algebra)**.** We define the quasi-local algebra of observables as the completion

$$\mathfrak{A} := \overline{\mathfrak{A}_{\text{local}}},$$

with respect to the norm induced by $\mathfrak{A}(\Lambda)$, $\forall \Lambda \in P_F(X)$.

The most natural interpretation of the quasi-local algebra $\mathfrak{A}$ is the collection containing all possible observables that can be arbitrary approximated by local observables $\mathfrak{A}_{\text{local}}$, namely observables defined in finite regions of the grid X. Indeed, if $A \in \mathfrak{A}(\Lambda)$ for some $\Lambda \in P_F(X)$, we say that A is localized in Λ. Coherently, the smallest $\Lambda \in X$ such that $A \in \mathfrak{A}(\Lambda)$ is the support of A and designated as $\text{Supp}(A)$.

[1] In general the tensor product of C*-algebras is a C*-algebra, but the norm is not univocally defined. Nevertheless, for finite dimensional quantum systems the norm is unique, as in case of eq. (2.1). Most notably, for every C*-algebras $\mathfrak{B}(\mathcal{H}_1)$, $\mathfrak{B}(\mathcal{H}_2)$ on spaces $\mathcal{H}_1 := \mathbb{C}^{d_1}$, $\mathcal{H}_2 := \mathbb{C}^{d_2}$, respectively, we have that $\mathfrak{B}(\mathcal{H}_1) \otimes \mathfrak{B}(\mathcal{H}_2) \cong \mathfrak{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.

To rigorously define a quantum cellular automaton, we need to known what kind of maps between observables do not break the algebra structure. Most notably, we say that a function $\alpha : \mathfrak{A} \to \mathfrak{B}$ is a homomorphism between C*-algebras if it is (i) linear, (ii) an algebra homomorphism, i.e. $\alpha(AB) = \alpha(A)\alpha(B)$, $\forall A, B \in \mathfrak{A}$, and (iii) a $*$-homomorphism, namely $\alpha(A^\dagger) = \alpha(A)^\dagger$, $\forall A \in \mathfrak{A}$. Whenever the inverse α^{-1} exists and is a homomorphism, we denote α as an isomorphism; in the same case, if $\mathfrak{A} = \mathfrak{B}$ then α is an automorphism of $\mathfrak{A}$. If $\mathfrak{A}$ and $\mathfrak{B}$ are unital, we call α a unital homomorphism if $\alpha(I_{\mathfrak{A}}) = I_{\mathfrak{B}}$.

The quasi-local algebra plays here the role of the configuration space for classical automata. Indeed, we define the quantum shift of displacement $x \in X$ as the automorphism $\sigma_x : \mathfrak{A}_y \to \mathfrak{A}_{xy}$, $\forall y \in X$, and its extension to whole quasi-local algebra as $\sigma_x : \mathfrak{A}(\Lambda) \to \mathfrak{A}(x\Lambda)$, $\forall \Lambda \subset X$. Within the current framework, see ref. [SW04], we introduce the axiomatic definition of a quantum cellular automaton.

Definition 1 (Quantum cellular automaton)**.** Given a finitely generated group X, the quasi-local algebra of observables $\mathfrak{A}(X)$, where the single site algebra correspond to the full-matrix one $\mathfrak{M}_d(\mathbb{C})$ for some d, and a finite neighborhood $N_0 \subseteq X$, a quantum cellular automaton is a tuple $(X, N_0, \mathfrak{A}, \alpha)$, such that $\alpha : \mathfrak{A}(X) \to \mathfrak{A}(X)$ is (i) a unital $*$-homomorphism of the quasi-local algebra $\mathfrak{A}(X)$, (ii) local, namely $\alpha(\mathfrak{A}(\Lambda)) \subseteq \mathfrak{A}(N_\Lambda)$, $\forall \Lambda \subseteq X$, and (iii) homogeneus, i.e. α commutes with all shifts σ_x, $\forall x \in X$.

We state that α is the *global rule* of the automaton. On the other hand, the *local rule* α_0 is the restriction of the global rule to the site e, namely $\alpha_0 \coloneqq \alpha|_{\mathfrak{A}_0} : \mathfrak{A}_0 \to \mathfrak{A}(N_0)$, see fig. 2.3. As such, the image $\alpha(\mathfrak{A}_0)$ is a C*-algebra isomorphic to $\mathfrak{A}_0$ however embedded in $\mathfrak{A}(N_0)$. By shifting, we obtain the local rule $\alpha_x \coloneqq \sigma_x \circ \alpha_0 \circ \sigma_x^{-1}$ at any site.

Some authors may define a quantum cellular automaton without requiring the homogeneity condition (iii) of definition 1. In that case, the QCA is a local and unital $*$-homomorphism over the quasi-local algebra of observables. Such a condition is even more general then it looks, as one may also drop the constraint of all sites representing the same quantum system, and have the dimension $d(x)$ of the local algebra in eq. (2.1) depending on site $x \in X$. For instance, in § 2.2.2 we will address the index theorem, which has been introduced for inhomogeneous QCAs in ref. [Gro+12].

Unlike classical cellular automata, where we first define the local rule τ_0 and from it compute the global one τ, their quantum counterparts start from the definition of the QCA on the whole grid as a global rule α and then derives the local one α_0 as a restriction. However, there are some criteria to

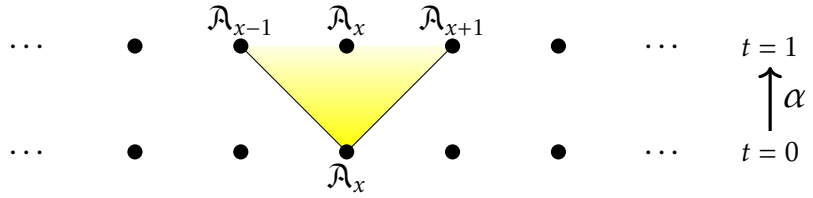


Figure 2.3: Schematic representation of a nearest-neighbors quantum cellular automaton on the one-dimensional lattice $\mathbb{Z}$. The lowest layer of dots represents the sites at $t = 0$. The local rule α_0 then propagates the observable algebra $\mathfrak{A}_x$ of site x to that of its neighbors $N_x = \{x-1, x, x+1\}$ at $t = 1$, represented through the upper layer of dots. The constituent traits of a QCA are homogeneity and locality.

distinguish whether a local rule is really so and represents an admissible automaton.

Theorem 5. *A unital homomorphism $\alpha_0 : \mathfrak{A}_0 \to \mathfrak{A}(N_0)$ is the local rule of a QCA iff*

$$[\alpha(\mathfrak{A}_0), \alpha_x(\mathfrak{A}_x)] = 0, \quad \forall x \in X, x \neq e, \tag{2.2}$$

and with $\alpha_x := \sigma_x \circ \alpha_0 \circ \sigma_x^{-1}$. Moreover, the global rule α is uniquely determined by the local one α_0.

Theorem 5 allows us to check whether an homomorphism is a QCA through checking only a finite number of conditions, i.e. eq. (2.2). A particularly interesting subclass of QCAs on qubits are those that map tensor products of Pauli matrices into tensor products of Pauli matrices. Such automata are called the Clifford QCAs, see refs. [SVW08; Güt+10], whereas in field theory these transformations are also known as quasi-free or Bogolyubov automorphisms, and in phase space quantum mechanics metaplectic transformations. They are an especially simple type of quantum cellular automata that does not allow a quantum computational speedup. Nonetheless, they show complex asymptotics and are basic ingredient for universal quantum computation.

Thanks to theorem 5, we come to the most notable result of QCA theory and its distinct discrepancy to the classical theory of CA, namely that the most relevant QCA are reversible. Before seeing that, we claim that given a QCA $(X, N_0, \mathfrak{A}, \alpha)$ such that α is an automorphism, then $(X, N_0^{-1}, \mathfrak{A}, \alpha^{-1})$ is a QCA as well. Moreover, we know that any unital $*$-homomorphism $\alpha : \mathfrak{A} \to \mathfrak{A}$ is an automorphism if the algebra $\mathfrak{A}$ is finite dimensional and has a trivial center. Hence, we need to find those criteria that let us discern whether a local rule describes a QCA over a finite grid X. We say that

a normal subgroup $\Gamma \triangleleft X$ of the grid X defines a *regular* quotient group $T = X/\Gamma$ with respect to the neighbor N_0 if

$$N_0 \cap N_x \neq \emptyset \Rightarrow N_0 \cap N_{xt} = \emptyset \quad \forall x \in X, t \in T.$$

Namely, if a subgroup T of the grid X is large enough to check the conditions eq. (2.2) without letting them overlap each other, and thus distorting them, we can say that a local rule $\mathfrak{A}_0$ represents a QCAs on T as well. However, in case of finite cardinality T we claim that the QCA is an automorphism.

Theorem 6 (Wrapped QCA)**.** *Given a quantum cellular automaton* $(X, N_0, \mathfrak{A}, \alpha)$ *such that there exists a finite, regular quotient group* T *of the grid* X*. Then we can define a QCA on* T *having the same local rule.*

For an extensive proof see refs. [SW04; Per20]. As a corollary of theorem 6, any QCA defined on a grid X respecting the conditions of theorem 6 is an automorphism. Most notably, QCAs defined on $X = \mathbb{Z}^n$ are automorphisms.

2.2.1 Structure theorem

As for CA, the quantum cellular automata represents a paradigm for massive *parallel* information processing. We may then wonder whether it is possible to conciliate such a description with the more customary one of quantum computation through quantum circuits. It is indeed feasable to implement a QCA through quantum gates, but we need first to introduce the appropriate definition of what is called a finite-depth quantum cellular automaton.

Definition 2. (Finite-depth QCA) A quantum cellular automaton $\alpha : \mathfrak{A} \to \mathfrak{A}$ is a finite-depth QCA if there exists a finite depth quantum circuit that implements it. More specifically, there exists a unitary operator U such that $\alpha : \chi \mapsto U^\dagger \chi U$, and $U = U_d \cdots U_1$ for some U_i. The subscripts denote the quantum circuit depth, and for each them $U_i = \prod_{\Lambda \in P_i} V_\Lambda^i$ such that P_i are some disjoint partitions of X and V_Λ^i are unitaries with support on $\mathfrak{A}_\Lambda$.

Please note that the products of each $U_i = \prod_{\Lambda \in P_i} V_\Lambda^i$ is well-defined, since the operators V_Λ^i commute for every depth i as their supports are disjoint. In the particular case of $X = \mathbb{Z}^n$, we say that a QCA is partitioned if it is implementable through a finite-depth quantum circuit as of definition 2 where the maximum depth $d = 2$. In such a case, we have $U = U_2 U_1$, where

$U_1 = \bigotimes_{2\mathbb{Z}^n} V$, $U_2 = \sigma^{-1} U_1 \sigma$ for a unitary matrix V on 2^n cells and the diagonal shift $\sigma := \sigma_1 \cdots \sigma_n$. The matrix V is also known as the scattering matrix of the partitioned QCA.

In the following, we prove the structure theorem for quantum cellular automata, see ref. [ANW11]. The result tells us that every QCA can be implemented through a localized finite-depth quantum circuit as long as we take advantage of ancillary systems.

Definition. (Ancilla implementation) A finite-depth quantum circuit U implements a unitary operator V through the ancillary system M if there exists a unitary matrix W acting only on ancillas such that $U = V \boxtimes W$. Consequently, a unitary operator U implements a QCA using ancillas if $\alpha \boxtimes \beta : A \mapsto U^\dagger A U$ for some β acting only onto the ancillary system.

In ref. [ANW11], the authors proved that for arbitrary unitary and causal evolution the automaton can be described through local and finite-depth circuits, even in the absence of the requirement of shift-invariance as in item (iii) of definition 1. To prove the claim we make extensive use of ancillas, namely we introduce a whole ancillary grid X so that the QCA is defined on $\tilde{X} := X \sqcup X = X \times \{o, a\}$. We denote by the subscript o the sites of the original grid whilst by a that of the ancillary one. Let s be the generator of $\tilde{X}$ that maps the sites between grids, namely $s : X_o \to X_a$, we then have that the neighborhood scheme $\tilde{N}_0$ for the grid $\tilde{X}$ is N_x itself for $x \in X_o$ and $sN_{s^{-1}x}$ for $x \in X_a$. We promptly see that $\tilde{N}_0$ commutes with s.

Theorem 7 (Structure theorem)**.** *Let α be a reversible QCA on $\mathfrak{A}(X)$ and denote by S_x the swap operator on system $\tilde{\mathfrak{A}}(x) := \mathfrak{A}(x) \otimes \mathfrak{A}(x)$, then there exists some operators*

$$U_x := (I_{\mathfrak{A}(x)} \otimes \alpha)(S_x)$$

that are unitary, commuting, and localized on $N_x \sqcup \{x\}$. Their product then define the QCA $(\tilde{X}, \tilde{N}_0, \tilde{\mathfrak{A}}, \tilde{\alpha})$ where

$$\begin{aligned} \tilde{\alpha} : \tilde{\mathfrak{A}} &\to \tilde{\mathfrak{A}} \\ \chi &\mapsto \left(\prod_x U_x^\dagger \right) \chi \left(\prod_y U_y \right) \end{aligned}$$

such that for every $\chi \in \mathfrak{A}$

$$\tilde{\alpha}(\chi \otimes I) = I \otimes \alpha(\chi), \qquad \tilde{\alpha}(I \otimes \chi) = \alpha^{-1}(\chi) \otimes I.$$

One may wonder what is the maximum depth of the circuit that implements a given QCA. The answer lays in a well result of graph theory,

since the problem is that of "tiling" the grid the partitions so as to wholly cover it, also known as the $L(1,1)$-labeling problem for graphs. Hence, the maximum depth is $\deg^2 \Gamma + 1$, where the graph Γ is that of vertices X and edges $\{(x,y)|x \in X, y \in N_x\}$, whereas the additional layer is due to the swap gates.

Theorem 7 is a specialized version of the general result presented in ref. [ANW11] for QCAs. Quantum cellular automata are *ibidem* a special case of unitary and *causal* operators defined in grids whose element are vertices of an arbitrary graph. More specifically, the grid is a directed graph $\Gamma(X, \mathcal{E})$ where the countable set X contains the nodes of the graph whereas the edges—i.e. a subset of $X \times X$—define the neighborhood scheme as $N_x := \{y|(x,y) \in \mathcal{E}\}$.

Finally, for the sake of completeness we shortly present the problem of universality in the framework of QCA. To truly assert that quantum cellular automata are algorithms for quantum computation we show that any circuit of quantum gates can be implemented through a QCA. Indeed, it has been shown that quantum Turing machines and quantum circuits are polynomially equivalent computational models, see refs. [Chi93; MW19], and that quantum Turing machines are equivalent to QCA with a constant slowdown ref. [Wat95]. A particulary exemplificative model has been introduce in ref. [Rau05a], where were a specific scattering matrix V can be programmed through an ancillary grid to execute any gate belonging to the universal set $\{H, T, C_{\text{NOT}}\}$ of ref. [Boy+00], where $H = 1/\sqrt{2}(X + Z)$ is the Hadamard gate, $T = \sqrt[4]{Z}$, and C_{NOT} is two qubit controlled-NOT. For additional reading see refs. [SFW06; Rau05a; Rau05b]. An analogous problem is that of intrinsic universality, namely the ability of an automaton to implement any other QCAs, see ref. [AG10].

2.2.2 Index theory

Three main perspectives are of particular interest in the task of classification of quantum cellular automata: the group structure, the local circuit structure, and the topological structure of QCAs. Indeed, any two automata defined over a given grid X with the same cell structure can be composed to produce a new QCA, moreover every automaton has an inverse for sufficient hypothesis on the grid X. Surprisingly enough, the group structure is more tricky to define in finite grids. Here, multiple application of a QCA lead to a neighborhood scheme comparable in size to the whole grid, thus rendering the very idea of locality moot. Furthermore, thanks to theorem 7 we showed that every QCA can be implemented through a finite-depth quantum circuit. We may then wonder if it is possible to quantify the minimum amount

of ancillas required to describe the action of the automaton in terms of finite-depth circuits. Lastly, one can define a path equivalence between two QCAs such that they can be continually and locally deformed into each other. That is a classification up to homotopy.

In the simpler case of $X = \mathbb{Z}$ and for an inhomogeneus quantum cellular automaton α without shift invariance, all three structures can be described in term the quantity $\operatorname{ind}\alpha$ known as index of α, see ref. [Gro+12]. The index is a positive rational number $\mathbb{Q}^+$ that can be computed locally, and it is constant on the whole lattice $\mathbb{Z}$ even if the QCAs is not shift invariant. A property is said to be locally computable for an automaton α having neighborhood N if it can be computed by restricting α to any interval region $I \subset \mathbb{Z}$ such that $|I| > |N|$. The set of locally computable invariants is an Abelian group.

The index estimates the amount of ancillary system required by a QCA to be implementable through a finite-depth quantum circuit. Indeed, for $\operatorname{ind}\alpha = 1$ we do not require any ancillary system at all and the automaton α can be continually and locally deformed to the trivial one.

The index and the index theorem describe the action of quantum cellular automata in terms of their support algebras, which we introduce hereafter.

Definition 3 (Support algebra)**.** Let $\mathfrak{B}_1$ and $\mathfrak{B}_2$ be two finite-dimensional C*-algebras and $\mathfrak{A} \subseteq \mathfrak{B}_1 \otimes \mathfrak{B}_2$ a subalgebra. The support algebra $\mathfrak{C} = \mathrm{S}(\mathfrak{A} \text{ on } \mathfrak{B}_1)$ is the smallest subalgebra $\mathfrak{C} \subseteq \mathfrak{B}_1$ such that $\mathfrak{A} \subseteq \mathfrak{C} \otimes \mathfrak{B}_2$.

Theorem 8. *Let $\mathfrak{B}_1$, $\mathfrak{B}_2$, $\mathfrak{B}_3$, and $\mathfrak{A}_1 \subseteq \mathfrak{B}_1 \otimes \mathfrak{B}_2$, $\mathfrak{A}_2 \subseteq \mathfrak{B}_2 \otimes \mathfrak{B}_3$ be C*-algebras. If $\mathfrak{A}_1$ and $\mathfrak{A}_2$ commute in $\mathfrak{B}_1 \otimes \mathfrak{B}_2 \otimes \mathfrak{B}_3$, then so commute $\mathrm{S}(\mathfrak{A}_1$ on $\mathfrak{B}_2)$ and $\mathrm{S}(\mathfrak{A}_2$ on $\mathfrak{B}_2)$ in $\mathfrak{B}_2$.*

Proof. For some bases $\{E_i\}$, $\{F_j\}$ of $\mathfrak{B}_1$, $\mathfrak{B}_3$, respectively, and let $A \in \mathfrak{A}_1$ and $A' \in \mathfrak{A}_2$. The two operators A, A' can be expanded uniquely as

$$A = \sum_i E_i \otimes A_i, \qquad\qquad A' = \sum_j A'_j \otimes F_j.$$

Then by hypothesis

$$[A \otimes I, I \otimes A'] = \sum_{ij} E_i \otimes [A_i, A'_j] \otimes F_j.$$

Since the terms $E_i \otimes F_j$ are a basis of $\mathfrak{B}_1 \otimes \mathfrak{B}_3$ the expansion is unique and $[A_i, A'_j] = 0$ for every i, j. The same applies to the algebras generated by A_i, A'_j, that are the support algebras $\mathrm{S}(\mathfrak{A}_1$ on $\mathfrak{B}_2)$ and $\mathrm{S}(\mathfrak{A}_2$ on $\mathfrak{B}_2)$, respectively. □

Intuitively, the index measures the mean information flux to the left or to the right as a ratio between the dimensions of two support algebras. We now define them as

$$\mathfrak{L}_{2x} \coloneqq \mathrm{S}(\alpha(\mathfrak{A}(\{2x, 2x+1\}) \text{ on } \mathfrak{A}(\{2x-1, 2x\})), \tag{2.3}$$
$$\mathfrak{K}_{2x} \coloneqq \mathrm{S}(\alpha(\mathfrak{A}(\{2x, 2x+1\}) \text{ on } \mathfrak{A}(\{2x+1, 2x+2\})), \tag{2.4}$$

that disassemble the image of $\mathfrak{A}(\{2x, 2x+1\}) = \mathfrak{A}_{2x} \otimes \mathfrak{A}_{2x+1}$, see fig. 2.4.

Theorem 9 (Index theorem)**.** *For every QCA on $X = \mathbb{Z}$ and $\mathfrak{A}_x \coloneqq \mathfrak{M}_{d(x)}$, the support algebras satisfy $\mathfrak{L}_{2x} \cong \mathfrak{M}_{l(2x)}$, $\mathfrak{K}_{2x} \cong \mathfrak{M}_{r(2x)}$. Furthermore, the index of the automaton α is defined as*

$$\operatorname{ind} \alpha \coloneqq \frac{r(2x-1)}{d(2x-1)} = \frac{d(2x)}{l(2x)} = \frac{r(2x+1)}{d(2x+1)} = \dots. \tag{2.5}$$

The quantity is locally computable and everywhere constant, i.e. it is independent of site x.

Proof. We need to prove that

$$\alpha(\mathfrak{A}_{2x} \otimes \mathfrak{A}_{2x+1}) \cong \mathfrak{L}_{2x} \otimes \mathfrak{K}_{2x}. \tag{2.6}$$

and

$$\mathfrak{K}_{2x} \otimes \mathfrak{L}_{2(x+1)} \cong \mathfrak{A}_{2x+1} \otimes \mathfrak{A}_{2(x+1)} \tag{2.7}$$

Starting from the former, we have by definition that $\alpha(\mathfrak{A}_{2x} \otimes \mathfrak{A}_{2x+1}) \subseteq \mathfrak{L}_{2x} \otimes \mathfrak{K}_{2x}$. To show that also the inverse is true we observe that the center of $\mathfrak{L}_{2x} \otimes \mathfrak{K}_{2x}$ is trivial. Indeed, by contradiction, let $W \in Z(\mathfrak{L}_{2x} \otimes \mathfrak{K}_{2x})$ be an element of the center non-proportional to the identity I, i.e. $[W, A] = 0$ for every element $A \in \mathfrak{L}_{2x} \otimes \mathfrak{K}_{2x}$. Nonetheless, W must then commute with $\alpha(\mathfrak{A}_{2x} \otimes \mathfrak{A}_{2x+1})$ and $\alpha(\mathfrak{A}_{2x+1} \otimes \mathfrak{A}_{2(x+1)})$ as well, the latter thanks to theorem 8. By the very same argument, W must commute with all images $\alpha(\mathfrak{A}_{2y} \otimes \mathfrak{A}_{2y+1})$ and $\alpha(\mathfrak{A}_{2y+1} \otimes \mathfrak{A}_{2(y+1)})$ for every $y \in \mathbb{Z}$, that altogether sum to the quasi-local algebra $\alpha(\mathfrak{A})$. Thus, we come to a contradiction since the quasi-local algebra has a trivial center. Thanks to eq. (2.6), we know that

$$d(2x)d(2x+1) = l(2x)r(2x). \tag{2.8}$$

On the other hand, one can prove eq. (2.7) in a similar fashion. As a matter of fact, $\mathfrak{K}_{2x}$ and $\mathfrak{L}_{2(x+1)}$ do have to commute in $\mathfrak{A}_{2x+1} \otimes \mathfrak{A}_{2(x+1)}$, as so do the image under automaton of $\mathfrak{A}_{2x} \otimes \mathfrak{A}_{2x+1}$ and $\mathfrak{A}_{2(x+1)} \otimes \mathfrak{A}_{2(x+1)+1}$ and theorem 8 holds. However, $\mathfrak{K}_{2x}$ and $\mathfrak{L}_{2(x+1)}$ are the only support algebras of

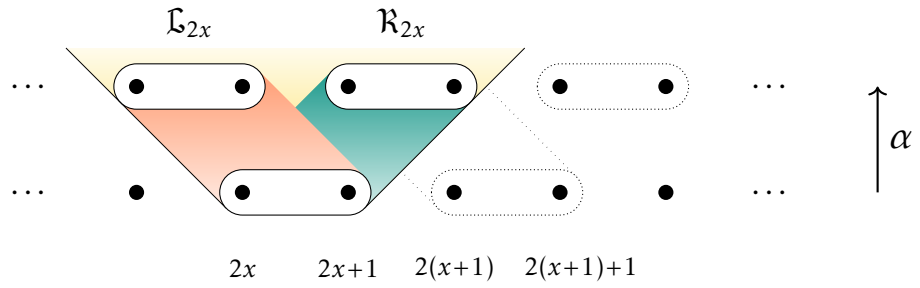


Figure 2.4: The one-dimensional grid $\mathbb{Z}$ is represented in the picture as a layer of dots, the lower one being that at time t whereas the upper one at time $t+1$ after applying the automaton α. For discussing the index theorem, see theorem 9, the automaton acts on the obsevables of site pairs $(2x, 2x+1)$. The images are then split into the support algebras $\mathfrak{L}_{2x} \otimes \mathfrak{R}_{2x}$.

the image of α localized in $\mathfrak{A}_{2x+1} \otimes \mathfrak{A}_{2(x+1)}$, and the last must be included in the image α since the automaton is an automorphism. As a consequence, we have here as well that

$$r(2x)l(2(x+1) = d(2x+1)d(2(x+1)). \tag{2.9}$$

Combining eqs. (2.8) and (2.9) toghether we have the thesis eq. (2.5). □

Example. The d-shift σ_d has $d(x) = d$, $r(2x) = d^2$ and $l(2x) = 1$, $\forall x \in \mathbb{Z}$, thus index $\operatorname{ind} \sigma_p = d^2/d = d$.

The index allows us to classify quantum cellular automata modulo translations. It is indeed an group homomorphism between QCAs $\{\alpha, \circ\}$ with composition and the positive rational number $\{\mathbb{Q}^+, \cdot\}$ with multiplication. At the same time, the index of the tensor product of two QCAs $\alpha \otimes \beta$, which is still a quantum cellular automaton on the joint grid, is the product of the two indices, i.e. $\operatorname{ind}(\alpha \otimes \beta) = \operatorname{ind} \alpha \ \operatorname{ind} \beta$. The most striking result notwithstanding, is that QCAs featuring ind = 1 are implementable through finite-depth quantum circuits *without ancillary systems*. This can be seen from eqs. (2.6) and (2.7), which allows for some automorphisms to be defined in case of equipartite dimensions. Such automorphisms are unitary matrices for the two layer block decomposition.

Many attempts to generalize the result of theorem 9 in ref. [Gro+12] to other grids have been proposed, see refs. [FH20; Haa21; FHH22; HFH22].

Chapter 3

The T-process

Quantum cellular automata are rigorous and effective theoretical tools for describing massive parallel quantum information processing. Indeed, the model is able to give meaning to statements such as computation over a possibly infinite number of systems concurrently, and homogeneous—i.e. translation invariant—interactions. Such results are in fact essential for simulating and describing physical phenomena that evolve under those circumstances. Nevertheless, the treatment of such models is not always as straightforward as it gets. Due to its constitutional delocalization on the grid, QCAs are usually handled through the description of their local rule or the block decomposition when available. In the following, we present the T-operator—whose name is due to its domain being T-shaped—which represents the equivalent of the Choi operator for a QCA, cf. § 1.1.1. The operator bears all valuable information of the QCA evolution in a *local* fashion. Moreover, all T-operators are in one-to-one relationship with the quantum cellular automata, namely we provide the necessary and sufficient condition for a given T-operator to represent a valid QCA.

The T-operator and the T-process have been introduced in refs. [Per20; Per21] as mean for probing the causal influence of a given automaton. The result extends the construction of theorem 7, see ref. [ANW11], where we proved that for every automaton α the automorphism $\alpha \otimes \alpha^{-1}$ is implementable through a finite-depth quantum circuit. Such a result is corroborated in the simpler case of $X = \mathbb{Z}$ by the index theorem 9 of ref. [Gro+12], which confirms us the same thesis since $\mathrm{ind}(\alpha \otimes \alpha^{-1}) = 1$. The results of the following chapter do not require the QCAs being homogeneous, as assumed in definition 1 instead.

3.1 A new definition of QCA

The dissertation of quantum cellular automata in chapter 2 rests on the rigorous notions of quasi-local algebra and its homomorphisms. A QCA is then required to preserve observables from one step to the next one. Nevertheless, the main property of an algebra homomorphism, i.e. $\alpha(AB) = \alpha(A)\alpha(B)$, has no operational interpretation in terms of effects, as neither a product nor a composition thereof is somehow meaningful.[1] The same does not apply for quantum operations, which are thoroughly defined through the Kraus theorem. Indeed, the composition of quantum operations leads to the multiplication of their Kraus operators. In turn, the Kraus operators of transformations live in an appropriate C*-algebra. A unital $*$-automorphism α then naturally induces a supermap $\mathscr{A}$ that preserves both the composition and conic structure of transformations over a grid X, by mapping the Kraus operators $\{C_i\}$ of any transformation $\mathcal{C}$ to $C_i' = \alpha(C_i)$ of a new map $\mathcal{C}' := \mathscr{A}(\mathcal{C})$. Such a definition of QCA is rigorously given in the present section.

Henceforth, we assume the automaton being an *automorphism* α of the quasi-local algebra, i.e. there exists an inverse homomorphism α^{-1}. We may then implement the supermap $\mathscr{A}$ by conjugating every transformation $\mathcal{C}$ with the automorphism α. Indeed, one can extend the definition of every automaton α to describe a quantum operation through its action onto effects in the Heisenberg picture, namely $\alpha : \mathrm{Eff}(\Lambda) \to \mathrm{Eff}(N_\Lambda)$. Then the meaning of conjugating $\mathcal{C}$ by α is easily understood if we evaluate the probability of the closed circuit

$$(E|\alpha^{-1}\mathcal{C}\alpha|\rho) = \mathrm{Tr}[\rho\ \alpha(C^\dagger\ \alpha^{-1}(E)\ C)] = \mathrm{Tr}[\rho\ \alpha(C)^\dagger\ E\ \alpha(C)] = (E|\mathscr{A}(\mathcal{C})|\rho)$$

for some state ρ, effect E, and transformation $\mathcal{C}$ with Kraus operator C. We have here defined with the same symbol α the automorphism and the quantum operation. The nature of the map is however clear from context.

An introductory example is the (right) shift σ. Most notably, let $x \in X$ and $\Lambda \subseteq X$, the shift σ_x is an automorphism of the quasi-local algebra as defined in chapter 2 such that $\sigma_x : \mathfrak{A}(\Lambda) \to \mathfrak{A}(\Lambda x)$. The shift supermap Σ_x instead conjugates any given transformation with the shift operation σ_x, i.e.

$$\begin{aligned} \Sigma_x : \mathrm{Transf}(\Lambda \to \Lambda) &\longrightarrow \mathrm{Transf}(\Lambda x \to \Lambda x) \\ \mathcal{B} &\mapsto \sigma_x^{-1}\mathcal{B}\sigma_x. \end{aligned}$$

[1] There is no product of effects E, E' such that $\Pr(\alpha(EE')|\rho) = \mathrm{Tr}[\alpha(EE')\rho] = \mathrm{Tr}[\alpha(E)\alpha(E')\rho]$ has sense for some density matrix ρ.

It is worth noting that both the transformation σ_x and the supermap Σ_x are well-defined in case of extension. Namely, let C be a quantum system, we can define the shift $\sigma_x \in \mathrm{Transf}(\Lambda C \to (\Lambda x)C)$ by applying the automaton $\sigma_x \otimes I$ to $\mathrm{Eff}(\Lambda C)$. Equivalently, the supermap $\Sigma_x : \mathrm{Transf}(\Lambda C \to \Lambda C) \longrightarrow \mathrm{Transf}((\Lambda x)C \to (\Lambda x)C)$ then conjugates any given transformation with the extended channel σ_x. We are now ready to provide an extensive and general definition of QCA in terms of supermap, which also includes the shift Σ_x.

Definition 4 (Quantum cellular automaton)**.** A QCA is a tuple $(X, N_0, \mathfrak{A}, \mathscr{A})$, where X is a finitely generated group, $N_0 \subseteq X$ a finite subset of the grid defining the neighborhood scheme, $\mathfrak{A}$ the quasi-local algebra over X, and the local rule $\mathscr{A}$ is a supermap that satisfies for $\Lambda \subset X$:

1. *Locality:* $\mathscr{A}$ is local and maps local transformation to local transformations according to the neighborhood scheme N of the grid, i.e.

$$\mathscr{A}_\Lambda : \mathrm{Transf}(\Lambda \to \Lambda) \longrightarrow \mathrm{Transf}(N_\Lambda \to N_\Lambda). \tag{3.1}$$

   Moreover, for $\mathcal{C} \in \mathrm{Transf}(\Lambda \to \Lambda)$ and $\Lambda' \subset X$ it satisfies

$$\mathscr{A}_{\Lambda\cup\Lambda'}(\mathcal{C} \otimes \mathcal{I}_{\Lambda'-\Lambda}) = \mathscr{A}_\Lambda(\mathcal{C}) \otimes \mathcal{I}_{N(\Lambda'-\Lambda)}. \tag{3.2}$$

2. *Homomorphism:* $\mathscr{A}$ is a homomorphism of quantum operations, i.e. it preserves both its conic and multiplicative monoid structure. In particular, $\mathscr{A}$ is (a) linear, (b) maps atomic transformation to atomic transformation, and (c) for $\mathcal{B}, \mathcal{C} \in \mathrm{Transf}(\Lambda \to \Lambda)$

$$\mathscr{A}(\mathcal{B} \circ \mathcal{C}) = \mathscr{A}(\mathcal{B}) \circ \mathscr{A}(\mathcal{C}). \tag{3.3}$$

3. (Optional) *Homogeneity:* $\mathscr{A}$ is homogeneous, i.e. it commutes with all left shifts

$$\mathscr{S}_x : \mathrm{Transf}(\Lambda \to \Lambda) \longrightarrow \mathrm{Transf}(x\Lambda \to x\Lambda) \quad \forall x \in X.$$

All aforementioned properties must hold for any external quantum system C as well, namely $\mathscr{A}_\Lambda$ satisfies $\mathscr{A}_\Lambda : \mathrm{Transf}(\Lambda C \to \Lambda C) \longrightarrow \mathrm{Transf}(N_\Lambda C \to N_\Lambda C)$ and eqs. (3.2) and (3.3).

Remark. The definition of $\mathscr{A}$ onto only $\mathrm{Transf}(\Lambda \to \Lambda)$ is no particular restriction. Actually, any transformation between a different number of sites can always be viewed as an operations on more sites such that the site number at input equals that at output, where some of them are left untouched. Moreover, in the special case of effects $\mathrm{Eff}(\Lambda) = \mathrm{Transf}(\Lambda \to I)$

the action of the automaton according to the two definitions is manifestly the same. Let $E \in \mathrm{Eff}(\Lambda)$ and the transformation $\mathcal{E} \in \mathrm{Transf}(\Lambda \to \Lambda)$ with Kraus operators $\{E_i\}$ such that $E = \sum_i E_i^\dagger E_i$, then $(E|\alpha = (I|\mathcal{E}\alpha = (I|\alpha\alpha^{-1}\mathcal{E}\alpha = (I|\mathscr{A}(\mathcal{E})$.

We now show that the definitions 1 and 4 describe the very same class of QCA and are thus equivalent. However, we first need the following lemma that applies a well-known result of abstract algebra to our case.

Theorem 10. *Let A, B be two quantum systems, $\mathscr{A}$ be a homomorphism of quantum operations, i.e. it is a quantum supermap*

$$\mathscr{A} : \mathrm{Transf}(A \to A) \longrightarrow \mathrm{Transf}(B \to B)$$

such that it preserves atomicity and the composition of quantum operations

$$\mathscr{A}(\mathcal{B}\mathcal{C}) = \mathscr{A}(\mathcal{B})\mathscr{A}(\mathcal{C})$$

for $\mathcal{B}, \mathcal{C} \in \mathrm{Transf}(A \to A)$. Then there exists a unique unital $*$-isomorphism

$$\alpha : \mathfrak{A}_A \to \mathfrak{A}_B$$

between the C-algebras of Kraus operators on systems A, B, specifically $\mathfrak{A}_A \coloneqq \mathrm{Eff}_{\mathbb{R}}(A)$ and $\mathfrak{A}_B \coloneqq \mathrm{Eff}_{\mathbb{R}}(B)$. Moreover, such isomorphism is spatial, namely there exits a unitary matrix $U : \mathcal{H}_B \to \mathcal{H}_A$ such that*

$$\alpha : A \to U^\dagger A U.$$

Proof. The action α of a supermap onto the Kraus operators that preserves atomicity is linear as stated in theorem 1. Moreover, the Kraus map $\mathfrak{K}$ of § 1.1.1 is here a monoidal isomorphism since transformations $\mathrm{Transf}(A \to A)$, $\mathrm{Transf}(B \to B)$ act from a system onto itself. We infer that $\alpha \coloneqq \mathfrak{K}\mathscr{A}\mathfrak{K}^{-1}$ is an algebra homomorphism over the Kraus operators. However, every homomorphism over the full matrix algebra is an isomorphism. Furthermore, all isomorphisms between standard operator algebras on normed spaces are *spatial*. This is a well established result of abstract algebra, see refs. [Che73; Šem95]. □

Remark. Since the isomorphism α is spatial as a consequence of theorem 10, every quantum cellular automaton $\mathscr{A}$ preserves the *group* structure of reversible quantum operations.

Theorem. *The two definitions 1 and 4 are equivalent.*

Proof. Let $(X, N_0, \mathfrak{A}, \alpha)$ be a QCA according to definition 1 and $(X, N_0, \mathfrak{A}, \mathscr{A})$ one as of definition 4. We then have that α is an automorphism of the quasi-local algebra of observables whereas $\mathscr{A}$ is a supermap between quantum transformations onto the grid X.

($\Rightarrow$) Given an automorphism α we build our supermap as follows. For every transformation $\mathcal{C} \in \mathrm{Transf}(\mathfrak{A}_\Lambda \to \mathfrak{A}_\Lambda)$ we consider its minimal decomposition[2] in Kraus operators $\{C_i\}$ such that $\mathcal{C} : \rho \mapsto \sum_i C_i \rho C_i^\dagger$. The image of the automaton is then the transformation $\mathcal{C}' := \mathscr{A}(\mathcal{C})$ having Kraus operators $C_i' := \alpha(C_i)$, namely

$$\mathscr{A} : \left(\rho \mapsto \sum_i C_i \rho C_i^\dagger \right) \longmapsto \left(\rho \mapsto \sum_i \alpha(C_i)\ \rho\ \alpha(C_i^\dagger) \right).$$

Thereby, the image transformation $\mathcal{C}'$ is in fact linear and completely-positive thanks to the Kraus theorem. Moreover, the quantum operation $\mathcal{C}'$ preserves the trace of states the same way $\mathcal{C}$ does. Indeed, let $\mathcal{D}$ be an atomic and deterministic quantum operation and D its only Kraus operator, then for $\mathcal{D}' := \mathscr{A}(\mathcal{D})$ we have that

$$(\mathcal{D}')^\dagger(I) = \alpha(D^\dagger) I \alpha(D) = \alpha(D^\dagger D) = \alpha(I) = I,$$

since the automaton is unital, and thus $\mathrm{Tr}[\mathcal{D}'(\rho)] = \mathrm{Tr}[\mathcal{D}(\rho)] = \mathrm{Tr}[\rho]$ for every density matrix ρ. Namely $\mathcal{D}'$ is trace-preserving too. If $\mathcal{D}$ is atomic but trace-non-increasing, only $\mathrm{Tr}[\mathcal{D}'(\rho)] = \mathrm{Tr}[\mathcal{D}(\rho)]$ holds. The set of transformation is a cone and every quantum operation $\mathcal{C}$ can be decomposed into a conical combination of atomic transformations $\mathcal{D}_i$ such that $\mathcal{C} = \sum_i \mathcal{D}_i$. This way we observe that $\mathrm{Tr}[\mathscr{A}(\mathcal{C})(\rho)] = \sum_i \mathrm{Tr}[\mathscr{A}(\mathcal{D}_i)(\rho)] = \sum_i \mathrm{Tr}[\mathcal{D}_i(\rho)] = \mathrm{Tr}[\mathcal{C}(\rho)]$ for every transformation $\mathcal{C}$.

The supermap $\mathscr{A}$ is indeed linear and granted to preserve the atomicity of transformations and adjointess. Thanks to the map α being an automorphism, the composition of transformations is preserved as well: given any two quantum operations $\mathcal{C}, \mathcal{D} \in \mathrm{Transf}(\mathfrak{A}_\Lambda \to \mathfrak{A}_\Lambda)$ with Kraus decompositions $\{C_i\}$, $\{D_j\}$, respectively, we have

$$\begin{aligned} \mathscr{A}(\mathcal{C} \circ \mathcal{D})(\rho) &= \sum_{ij} \alpha(C_i D_j)\ \rho\ \alpha(D_j^\dagger C_i^\dagger) \\ &= \sum_{ij} \alpha(C_i)\alpha(D_j)\ \rho\ \alpha(D_j)^\dagger \alpha(C_i)^\dagger = (\mathscr{A}(\mathcal{C}) \circ \mathscr{A}(\mathcal{D}))(\rho) \end{aligned}$$

[2]The Kraus decomposition is said to be minimal if all $\{C_i\}$ are linearly independent. In such a case, given any two Kraus sets $\{C_i\}$, $\{C_j\}$ of the same transformation $\mathcal{C}$, there always exists an isometry V such that $V^\dagger V = I$ and $C_i = \sum_j V_{ij} C_j$. The action of the supermap $\mathscr{A}$ is thus well-defined as the automorphism α is linear.

for every preparation $\rho \in \mathrm{St}(\Lambda)$. This concludes the proof of item 2 of definition 4, viz. the supermap $\mathscr{A}$ is a automorphism of quantum operations.

Thanks to the locality of the automaton α, the image transformation $\mathcal{C}'$ only acts on sites in the neighborhood of the original transformation $\mathcal{C}$. Namely, $\mathcal{C}' \in \mathrm{Transf}(\mathfrak{A}_{N(\Lambda)} \to \mathfrak{A}_{N(\Lambda)})$ since $C_i \in \mathfrak{A}_\Lambda$ and thus $\alpha(C_i) \in \mathfrak{A}_{N(\Lambda)}$. On the other hand, the automorphism α commutes with all shifts σ_x by definition, thus the same does $\mathscr{A}$.

($\Leftarrow$) To univocally derive an automorphism of the observable algebra from the automaton $\mathscr{A}$ we focus on its action upon atomic transformations $\mathrm{Transf}_A(x \to x)$ on single sites. The quantum operations $\mathrm{Transf}_A(x \to x)$ span altogether the entire set of transformations on the whole grid X through conic combinations, and at the same time their Kraus operators make up the quasi-local algebra of observables according to construction of § 2.2. We take here advantage of theorem 10. Let $\Lambda \subset X$ be a finite subset of sites,

$$\mathfrak{Q}_\Lambda := \mathrm{Span}_{\mathbb{R}}(\mathrm{Transf}(\Lambda \to \Lambda))$$

the algebra of quantum operations upon sites Λ and $\mathscr{A} : \mathfrak{Q}_\Lambda \to \mathscr{A}(\mathfrak{Q}_\Lambda)$ the restriction of $\mathscr{A}$ onto $\mathfrak{Q}_\Lambda$, where $\mathscr{A}(\mathfrak{Q}_\Lambda) \subset \mathfrak{Q}_{N(\Lambda)}$. We then have a bijection between $\mathscr{A}$ and the isomorphism $\alpha_\Lambda : \mathfrak{A}_\Lambda \to \mathfrak{A}_{N(\Lambda)}$ for all Λ. Since the isomorphism α_x is spatial, we have that $\alpha_x(I_x) = I_{N(x)}$ and

$$[\alpha_{xy}(\mathfrak{A}_x), \alpha_{xy}(\mathfrak{A}_y)] = 0 \quad \forall x \neq y.$$

The two last expressions imply that α_x is the local rule of the automaton α thanks to theorem 5. The locality and homogeneity properties of α directly derive from properties 1, 3 of definition 4, respectively. □

3.2 The T-operator

The automaton $\mathscr{A}$ according to definition 4 must handle any system extension C to the grid X. In particular, if we consider an ancillary grid X as extension $C = X$, see fig. 3.1a, we can evaluate the action of the automaton onto transformations between the two grids. Such a property is of vital relevance for the definition of the T-operator.

We define the swap operator $\mathcal{S} \in \mathrm{Transf}(AA \to AA)$ for every quantum system A through its action onto atomic and factorized states $\rho \otimes \sigma$ as simply $\mathcal{S} : \rho \otimes \sigma \mapsto \sigma \otimes \rho$, then the definition can be extended to any state $\mathrm{St}(AA)$ by linearity. Henceforth we denote by $\mathcal{S}$ the swap between the original and ancillary grid, whereas we say that $\mathcal{S}_x$ swaps the site $x \in X$ between the

two grids, see fig. 3.1b. We have then the two following straightforward identities:

$$\mathcal{S} = \prod_{x\in X} \mathcal{S}_x, \qquad \alpha \otimes \alpha^{-1} = \mathcal{S}(\alpha^{-1} \otimes \mathcal{I})\mathcal{S}(\alpha \otimes \mathcal{I}).$$

We are then ready to give a more suitable definition for the protocol of ref. [ANW11]. Namely, we introduce a procedure for locally implementing a QCA in terms of definition 4.

Definition 5 (T-operator)**.** Let $\mathscr{A}$ be a quantum cellular automaton, we define the T-operator as

$$\mathcal{T}_x := \mathscr{A}(\mathcal{S}_x) = (\alpha^{-1} \otimes \mathcal{I})\mathcal{S}_x(\alpha \otimes \mathcal{I}), \tag{3.4}$$

for $x \in X$, and α being the automaton automorphism of the quasi-local algebra.

The T-operator of the QCA is the conjugation of the swap operator on a given site x with the automaton, cf. fig. 3.1c. The result is an atomic transformation due to atomicity of composition. For the sake of clarity, we shall denote the transformation with the symbol $\mathcal{T}_x$ in calligraphy font whereas its only Kraus operator with the capital letter T_x.

By definition of neighborhood, the transformation $\mathcal{T}_x$ acts only on sites $N_x \sqcup x$, namely on the neighborhood N_x on the original grid and on x on the ancillary one, and is thus localized. Since $\mathscr{A}$ is a homomorphism of quantum operations and the swap transformation satisfies both $\mathcal{S}_x^2 = \mathcal{I}$ and $[\mathcal{S}_x, \mathcal{S}_y] = 0$ for every x, y, we obtain

$$\mathcal{T}_x^2 = \mathcal{I} \tag{3.5}$$

$$[\mathcal{T}_x, \mathcal{T}_y] = 0, \tag{3.6}$$

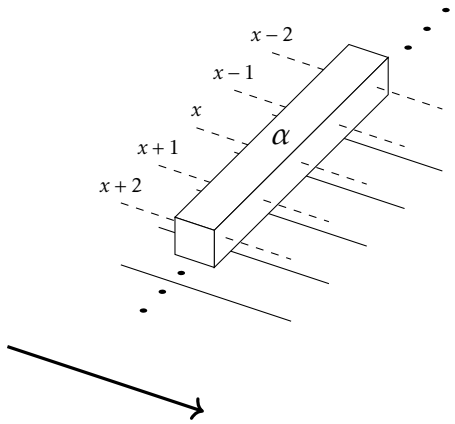
for all x, y. Equations (3.5) and (3.6) are distinctive features of the T-operators and, as we shall see later, embed the commutation relations of the automaton local rule. In general, thanks to eq. (3.6) the product

$$\mathcal{T}_\Lambda := \prod_{x\in\Lambda} \mathcal{T}_x$$

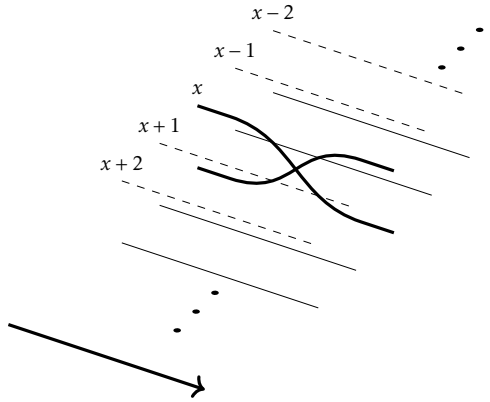
is well-defined for $\Lambda \subseteq X$, and $\mathcal{T}_X = \mathcal{S}(\alpha^{-1} \otimes \alpha)$.

There are then two more characteristic properties of the T-operator that allows us to uniquely define its class among other transformations. Namely, for every transformation $\mathcal{C} \in \mathrm{Transf}(x \to x)$ for $x \in X$ we have

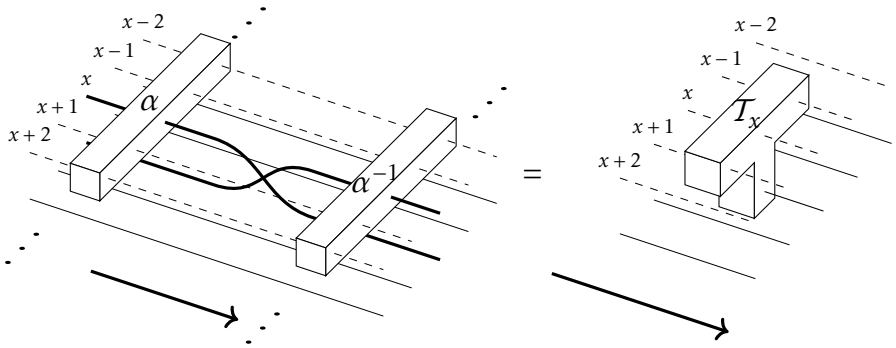
$$\begin{aligned}\mathcal{T}_x(\mathcal{I} \otimes \mathcal{C})\mathcal{T}_x &= (\alpha^{-1} \otimes \mathcal{I})\mathcal{S}_x(\alpha \otimes \mathcal{I})(\mathcal{I} \otimes \mathcal{C})(\alpha^{-1} \otimes \mathcal{I})\mathcal{S}_x(\alpha \otimes \mathcal{I}) \\ &= (\alpha^{-1} \otimes \mathcal{I})\mathcal{S}_x(\mathcal{I} \otimes \mathcal{C})\mathcal{S}_x(\alpha \otimes \mathcal{I}) = (\alpha^{-1} \otimes \mathcal{I})(\mathcal{C} \otimes \mathcal{I})(\alpha \otimes \mathcal{I}) = \mathscr{A}(\mathcal{C}) \otimes \mathcal{I}, \end{aligned} \tag{3.7}$$



(a) The automorphism α of the observable quasi-local algebra over the grid $X = \mathbb{Z}$ describes a quantum operation. In particular, the transformation can be extended to neglect any other quantum system C, here $C = \mathbb{Z}$ is an ancillary grid, which has been depicted as a one-dimensional lattice at the lower level.



(b) The operator $\mathcal{S}_x$ swaps two sites at position x in the main grid $X = \mathbb{Z}$ and in the ancillary one.



(c) The T-operator $\mathcal{T}_x = \mathscr{A}(\mathcal{S}_x)$ is defined as the image of the swap $\mathcal{S}_x$ under the action of the automaton $\mathscr{A}$ of definition 4. The automaton conjugates the swap with the automorphism α. The domain and image of the transformation is then the neighborhood N_x in the original grid and the input site x in the ancillary one. In picture, for simplicity the neighborhood of α is $N_x = x-1, x, x+1$.

Figure 3.1: The automorphism α of the observable quasi-local algebra depicted in fig. (a) naturally defines a quantum transformation $\alpha^\dagger : \mathrm{Eff}(\Lambda) \to \mathrm{Eff}(N_\Lambda), E \mapsto \alpha(E)$ in the Heisenberg picture for $\Lambda \subseteq X$, and N_0 the neighborhood. Thereby, we conjugate the swap operator $\mathcal{S}_x$ at site $x \in X$ of fig. (b) to obtain the T-operator in fig. (c).

and

$$\begin{aligned}\mathcal{T}_{N(x)}(\mathcal{C}\otimes\mathcal{I})\mathcal{T}_{N(x)} &= (\alpha^{-1}\otimes\mathcal{I})\mathcal{S}_{N(x)}(\alpha\otimes\mathcal{I})(\mathcal{C}\otimes\mathcal{I})(\alpha^{-1}\otimes\mathcal{I})\mathcal{S}_{N(x)}(\alpha\otimes\mathcal{I})\\ &\quad(\alpha^{-1}\otimes\mathcal{I})\mathcal{S}_{N(x)}(\mathscr{A}^{-1}(\mathcal{C})\otimes\mathcal{I})\mathcal{S}_{N(x)}(\alpha\otimes\mathcal{I})\\ &= (\alpha^{-1}\otimes\mathcal{I})(\mathcal{I}\otimes\mathscr{A}^{-1}(\mathcal{C}))(\alpha\otimes\mathcal{I}) = (\mathcal{I}\otimes\mathscr{A}^{-1}(\mathcal{C})).\end{aligned} \tag{3.8}$$

By accordingly conjugating any transformation $\mathcal{C}$ with the T-operators $\mathcal{T}_x$ we obtain the image of the automaton $\mathscr{A}$ on the other grid. Therefore, the T-operator accommodates all the required information to describe the QCA.

Theorem 11. *Let the transformations $\mathcal{T}_x$ act onto sites $N_x \sqcup x$, then the quantum operation $\mathcal{T}_x$ is the T-operator of a QCA $\mathscr{A}$ according to definition 5 iff $\mathcal{T}_x$ satisfies:*

1. $\mathcal{T}_x^2 = \mathcal{I}$.
2. $[\mathcal{T}_x, \mathcal{T}_y] = 0\ \forall x, y$.
3. *Given any transformation $\mathcal{C} \in \mathrm{Transf}(\Lambda \to \Lambda)$ for $\Lambda \subseteq X$, the conjugation with the operator $\mathcal{T}_x$ is*

$$\mathcal{T}_\Lambda(\mathcal{I}\otimes\mathcal{C})\mathcal{T}_\Lambda = \mathcal{C}'\otimes\mathcal{I}, \tag{3.9}$$

such that $\mathcal{C}' \in \mathrm{Transf}(N_\Lambda \to N_\Lambda)$.

Proof. Given an automaton $\mathscr{A}$, we introduce the operator $\mathcal{T}_x$ as in definition 5, then it satisfies properties 1, 2, and 2 as shown in eqs. (3.5), (3.6), and (3.7), respectively.

To prove the opposite we show that the map from $\mathcal{C}$ to $\mathcal{C}'$ in eq. (3.9) is indeed an automaton as of definition 4. We define for every $\Lambda \subseteq X$ the following supermaps

$$\begin{aligned}\mathscr{E} : \mathrm{Transf}(\Lambda \to \Lambda) &\longrightarrow \mathrm{Transf}(X\Lambda \to X\Lambda)\\ \mathcal{C} &\mapsto \mathcal{I}\otimes\mathcal{C},\end{aligned}$$

and

$$\begin{aligned}\mathscr{D}_\rho : \mathrm{Transf}(N_\Lambda X \to N_\Lambda X) &\longrightarrow \mathrm{Transf}(N_\Lambda \to N_\Lambda)\\ \mathcal{G} &\mapsto (e_X|\mathcal{G}|\rho_X),\end{aligned} \tag{3.10}$$

as encoder and decoder, respectively, where $e_X \in \mathrm{Eff}_1(X)$ represents the deterministic effect and $\rho \in \mathrm{St}_1(X)$ a deterministic state of the the ancillary grid. Please note that $\mathscr{D}_\rho$ represents an effect in the higher-order quantum

theory that discards the ancillary grid, namely $(e_X|\mathcal{G}|\rho_X)|\tau_{N(\Lambda)}) = \mathrm{Tr}_X[\mathcal{G}(\rho_X \otimes \tau)] \in \mathrm{St}(N_\Lambda)$ for every $\tau \in \mathrm{St}(N_\Lambda)$. We now want to prove that

$$\mathscr{A} := \mathscr{D}_\rho \, \mathscr{T} \, \mathscr{E} \tag{3.11}$$

is a QCA according to definition 4 and generates the $\mathcal{T}_x$ operator, where $\rho \in \mathrm{St}(X)$ and $\mathscr{T}$ is the supermap that conjugates with the operator $\mathcal{T}_x$ everywhere on the grid, i.e.

$$\mathscr{T} : \mathcal{D} \mapsto \mathcal{T}_X \mathcal{D} \mathcal{T}_X.$$

The map $\mathscr{A}$ is indeed linear and maps atomic transformations to atomic transformations thanks to atomicity of composition. The supermap $\mathscr{A}$ preserves the composition of quantum operation. Indeed, we know that $\mathcal{T}_x$ is the inverse of itself thanks to item 1. Hence, for $\Lambda \subset X$ and any two transformations $\mathcal{B}, \mathcal{C} \in \mathrm{Transf}(\Lambda \to \Lambda)$ we have

$$\mathscr{T}(\mathcal{B} \circ \mathcal{C}) = \mathcal{T}_X \, \mathcal{B} \, \mathcal{C} \, \mathcal{T}_X = \mathcal{T}_X \, \mathcal{B} \, \mathcal{T}_X \mathcal{T}_X \, \mathcal{C} \, \mathcal{T}_X = \mathscr{T}(\mathcal{B}) \circ \mathscr{T}(\mathcal{C}).$$

Please note that the product $\mathcal{T}_X = \prod_{x \in X} \mathcal{T}_x$ is well-defined thanks to property 2 of definition 5. Moreover, the supermap $\mathscr{A}$ of eq. (3.11) is local according to the neighborhood scheme thanks to property 3 of definition 5 since transformation on sites $\Lambda \subset X$ are mapped to transformation over N_Λ. The homogeneity of the automaton α is provided if $\mathcal{T}_x = \mathcal{T}_y$ for all x, y. Finally, we observe that thanks to the right hand side of eq. (3.9) being factorized, the choice of ρ in eq. (3.10) is irrelevant as long as it is deterministic, i.e. $(e|\rho) = \mathrm{Tr}[\rho] = 1$. □

In the particular case of a homogeneous automaton $\mathscr{A}$, i.e. it satisfies property 3 of definition 5, we may drop the x subscript of $\mathcal{T}_x$ altogether, as we have $\mathcal{T}_x = \mathcal{T}_y$ for every x, y. In such case, the automaton is uniquely defined by the operator $\mathcal{T}$ and condition 2 of theorem 11 must only be checked for $[\mathcal{T}, \mathcal{T}_x] = 0$ where $\mathcal{T}_x = \sigma_x \circ \mathcal{T} \circ \sigma_x^{-1}$ and $\forall x$ such that $N_0 \cap N_x \neq \emptyset$.

3.3 Decomposition

In the previous section we analyzed thoroughly the properties that define the T-operator. Here we observe that the choice of the swap transformation $\mathcal{S}_x$ in definition 5 of $\mathcal{T}_x$ is due to its particular role in the higher-order quantum theory. In this framework, we have that quantum operations represent system states instead, and supermaps are the true transformations. Among

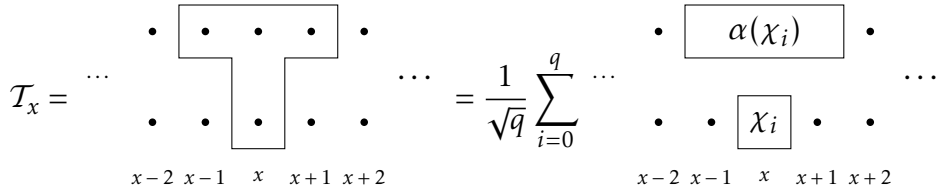


Figure 3.2: A pictorial representation of the T-operator decomposition. The grid on which acts the automaton is a one-dimensional lattice $X = \mathbb{Z}$ depicted as the upper layer, wheras the lower one is the ancillary grid. The T-operator bears both the input and the output of the quantum cellular automaton.

others, the swap $\mathcal{S}$ between two systems stands here for the maximally entangled state, being a transformation in the usual quantum theory.

Indeed, given a system A and its Hilbert space $\mathcal{H}_A$, we may define the swap operator $\mathcal{S} \in \mathrm{Transf}(AA \to AA)$ between two copies of A through its Kraus operator over $\mathfrak{A}_A \otimes \mathfrak{A}_A$ as

$$S = \frac{1}{\sqrt{q}} \sum_{i=0}^{q} \chi_i \otimes \chi_i,$$

where $\{\chi_i\}$ is an orthonormal basis of the C*-algebra $\mathfrak{A}_A$ and $q := \dim(\mathfrak{A}_A)$. Thus, computing the action of the automaton on $\mathcal{S}_x$ is straightforward and its Kraus operator reads

$$T_x = \frac{1}{\sqrt{q}} \sum_{i=0}^{q} \alpha(\chi_i) \otimes \chi_i, \tag{3.12}$$

acting over $\mathfrak{A}_{N(x)} \otimes \mathfrak{A}_x$. The T-operator is defined over $N_x \sqcup x$ and can then be decomposed into the basis of the input algebra over site x in the ancillary grid, and the output of the QCA on N_x in the original grid. Thereby, the operator $\mathcal{T}_x$ accommodates both the input and the output of the quantum cellular automaton, see fig. 3.2. Following the same construction, we can extend the decomposition of eq. (3.12) for T_Λ and any subset $\Lambda \subseteq X$.

A clear analogy can be drawn by comparing the T-operator to the Choi operator of quantum theory defined in § 1.1.1. Indeed, the swap transformation plays here the role of the maximally entangled state $|I\rangle\!\rangle\langle\!\langle I|$ in the Choi-Jamiołkowski isomorphism. Please note that in the higher-order quantum theory inputs are quantum operations and transformations

	Quantum operation $\mathcal{C}$	Quantum cellular automaton $\mathscr{A}$
Probe	Max. entangled state $\|I\rangle\!\rangle\langle\!\langle I\|$	Swap operator $\mathcal{S}_x$
	$\|I\rangle\!\rangle = \sum_i \|i\rangle \otimes \|i\rangle$	$S_x = \sum_i \chi_i \otimes \chi_i$
Choi	$\rho_{\mathcal{C}} = (\mathcal{C} \otimes \mathcal{I})(\|I\rangle\!\rangle\langle\!\langle I\|)$	$\mathcal{T}_x = (\mathscr{A} \otimes \mathcal{I})(\mathcal{S}_x)$
	$= \|C\rangle\!\rangle\langle\!\langle C\|$	$\mathcal{T}_x(\rho) = T_x \rho T_x^\dagger$
	$\|C\rangle\!\rangle = \sum_{ij} \|i\rangle \otimes (C_{ij}\|j\rangle)$	$T_x = \sum_i \alpha(\chi_i) \otimes \chi_i$

Table 3.1: Comparison between the Choi operator of a transformation $\mathcal{C} \in \mathrm{Transf}(A \to A)$ and the T-operator $\mathcal{T}_x$ of a QCA $\mathscr{A}$. For simplicity of exposition, the transformation $\mathcal{C}$ is assumed to be atomic and C is its only Kraus operator. The operators $\{\chi_i\}$ are a valid basis of the single-site observable algebra. It should be noted that the T-operator is the Choi operator of the QCA *local rule* $\mathscr{A}_0$.

thereof are a supermaps. Hence, the maximally entangled state $|I\rangle\!\rangle\langle\!\langle I|$ becomes the swap transformation $\mathcal{S}_x$, the quantum operation $\mathcal{C}$ turns into the supermap $\mathscr{A}$, which applied to $|I\rangle\!\rangle\langle\!\langle I|$ and $\mathcal{S}_x$ return the Choi operator $\rho_{\mathcal{C}}$ and the T-operator $\mathcal{T}_x$, respectively. The former is a state whereas the latter is a quantum channel, i.e. the input of a supermap. A side-by-side comparison is provided in table 3.1.

Remark. It is worth noting that the T-operator represents the Choi of the *local rule* $\mathscr{A}_0$ of the automaton. To be precise, the Choi of the whole QCA $\mathscr{A}$ is

$$\mathcal{T} := \mathscr{A}(\mathcal{S}) = \prod_{x \in X} \mathscr{A}(\mathcal{S}_x) = \prod_{x \in X} \mathcal{T}_x.$$

3.4 No classification through T-operators

Thanks to theorem 11 we can rigorously define the class of T-operators. It actually provides the necessary and sufficient conditions for an operator $\mathcal{T}_x$ to faithfully represent a quantum cellular automaton. One may then try to classify all possible T-operators so as to describe the set of QCAs. However, such a procedure does not provides any valuable insight for checking the commutation relations of local rules, i.e. through theorem 5. As we will show, the requirements of theorem 11 directly translate to that of theorem 5, thus denying us any real advantage in the classification task.

The T-operator must satisfy the condition 2 of theorem 11, i.e. $[\mathcal{T}_x, \mathcal{T}_y] = 0$ for every $x, y \in X$, which in turn is inherited from the automaton being a

homomorphism. We can solve the equation through the decomposition of eq. (3.12) for $x \neq y$ to attain

$$[\mathcal{T}_x, \mathcal{T}_y] = \sum_{ij} [\alpha(\chi_i), \alpha(\chi_j)] \otimes \chi_i \otimes \chi_j = 0 \tag{3.13}$$

where for $\chi_i \in \mathfrak{A}_x$, $\chi_j \in \mathfrak{A}_y$, $\alpha(\chi_i) \in \mathfrak{A}_{N(x)}$, and $\alpha(\chi_j) \in \mathfrak{A}_{N(y)}$. Equation (3.13) is then satisfied only for

$$[\alpha(\chi_i), \alpha(\chi_j)] = 0, \quad \forall i, j.$$

The condition is clearly equivalent to that of theorem 5, we are then directly checking the commutation relations of the QCA local rule.

3.5 Estimating the index

The T-operator allows us to easily compute the index of a QCA. Indeed, we show hereafter that such task is a linear problem, once we are given the operator $\mathcal{T}_x$. We henceforth assume the grid be the one-dimensional lattice, i.e. $X = \mathbb{Z}$, and the automaton be homogeneous. The site on which the $\mathcal{T}$ operator acts are labeled with the numbers 0 to 3 starting from the site e on the ancillary lattice and carry on on the original grid as depicted in fig. 3.3, such that $T : \mathcal{H}_0 \otimes \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \to \mathcal{H}_0 \otimes \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$. To estimate the index of α, we need to calculate the dimension of the algebra

$$\mathfrak{K}_{2x} = \mathrm{S}(\alpha(\mathfrak{A}(2x, 2x+1)) \text{ on } \mathfrak{A}(2x+1, 2(x+1))). \tag{2.4}$$

From the construction of fig. 2.4 we promptly observe that $\mathfrak{K}_{2x}$ commutes with both $\alpha(\mathfrak{A}_{2(x+1)})$ and $\alpha(\mathfrak{A}_{2(x+1)+1})$. These are all the commutation relations required to define the algebra and its basis. Thanks to decomposition of eq. (3.12), we know that the image of the automaton completely resides in the T-operator. We are then able to obtain the bases

$$F_{i,j} \coloneqq \mathrm{Tr}_{0,3}[T\ (X_i \otimes I_{1,2} \otimes X_j)],$$
$$G_{k,l,m} \coloneqq \mathrm{Tr}_{0,2,3}[T\ (X_k \otimes I_1 \otimes X_l \otimes X_m)] \otimes I_2,$$

for $\mathrm{S}(T \text{ on } \mathfrak{A}_{1,2})$ and $\mathrm{S}(T \text{ on } \mathfrak{A}_1) \otimes I_2$, respectively. The algebra $\mathfrak{K}_{2x}$ is the commutant

$$\mathfrak{K}_{2x} = [\mathrm{S}(T \text{ on } \mathfrak{A}_{1,2}) \cup \mathrm{S}(T \text{ on } \mathfrak{A}_1) \otimes I_2]',$$

so by defining

$$\Phi_{i,j} \coloneqq (F_{i,j} \otimes I - I \otimes F_{i,j}^T),$$
$$\Gamma_{i,j,k} \coloneqq (G_{k,l,m} \otimes I - I \otimes G_{k,l,m}^T),$$

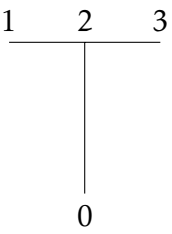


Figure 3.3: Domain labeling for the T-operator $\mathcal{T}$ of a homogeneous automaton.

the operator $Y \in \mathfrak{A}_{12}$ then satisfies

$$[Y, \mathrm{S}(T \text{ on } \mathfrak{A}_{1,2})] = 0 \qquad \Leftrightarrow \qquad \Phi_{i,j}|Y\rangle\rangle = 0 \qquad \forall i, j$$

and

$$[Y, \mathrm{S}(T \text{ on } \mathfrak{A}_1) \otimes I_2] = 0 \qquad \Leftrightarrow \qquad \Gamma_{i,j,k}|Y\rangle\rangle = 0 \qquad \forall k, l, m.$$

Finally, one can find all solutions Y of both the above equations by evaluating the kernel of

$$\Xi := \sum_{i,j} \Phi_{i,j}^{\dagger} \Phi_{i,j} + \sum_{k,l,m} \Gamma_{k,l,m}^{\dagger} \Gamma_{k,l,m}.$$

Indeed, one has

$$\mathfrak{K}_L = \mathrm{Ker}\, \Xi. \tag{3.14}$$

Chapter 4

Fermionic Quantum Cellular Automata

One may be be tempted to transpose the result of QCAs to automata dealing with local Fermionic modes instead of qubits, hoping that they all apply unaffected. Indeed, Fermions have been proved to be computationally equivalent to qubits [BK02] and the Jordan-Wigner lets us directly map quantum operators to Fermionic ones through a $*$-isomorphism. However, we prove here that FQCAs are substantially different from their quantum counterparts as they presents a class of automata that are genuinely Fermionic.

In particular, in the present chapter we classify all nearest-neighbors Fermionic quantum cellular automata over the one-dimensional lattice $X = \mathbb{Z}$ where at each site we find a single local Fermionic mode. In such class we firstly separate the shifts from the locally implementable ones, and then further divide the rest into two subsets depending on the properties of image support algebra over the nearest sites. In particular, there we find some FQCAs that are equivalent to the quantum ones and some that are unique to the Fermionic realm.

The definition of Fermionic quantum cellular automaton requires equivalent notions to those of QCAs. Indeed, let $X = \mathbb{Z}$ be the grid and F_x the $\mathbb{Z}^2$-graded algebra of observables for a single local Fermionic mode at site $x \in X$. We define the quasi-local algebra F of observables and the homomorphism α thereof. For every pair of self-adjoint, odd, local operators ξ, $\upsilon \in \mathsf{F}_x$ such that $\{\xi, \upsilon\} = 0$, then the homomorphism must preserve the CAR, i.e. $\{\alpha(\xi), \alpha(\upsilon)\} = 0$, and be local $\alpha(\mathsf{F}_x) \subset \mathsf{F}_{x-1,x,x+1}$. Moreover, we require the automaton α to be homogeneous and thus commute with all shifts σ_x.

Fermionic Pauli matrices For sake of simplicity we denote the Pauli matrices In terms of the annihilation and creation operators φ_k, $\varphi_k^\dagger$:

$$X_k = \varphi_k + \varphi_k^\dagger, \qquad Y_k = i\varphi_k - i\varphi_k^\dagger, \qquad Z_k = \varphi_j^\dagger \varphi_k - \varphi_k.$$

Thereby, we represent the CAR of Fermionic modes on the lattice $\mathbb{Z}$ by assigning to each site x the pair (X_x, Y_x). All operators X_x, Y_x must then anticommute $\forall x$. However, the same does not apply if we consider the local self-adjoint operators $\xi_x \in \{X_x, Y_x, Z_x\}$, $\upsilon_y \in \{X_y, Y_y, Z_y\}$: in fact, they anticommute $\{\xi_x, \upsilon_y\} = 2\delta_{\xi\upsilon}$ if $x = y$ whereas graded-commute $\{\!\{\xi_x, \upsilon_y\}\!\} = 0$ otherwise.

4.1 Index theory for Fermionic quantum cellular automata

Before proceeding to the classification we first briefly summarize the result of the index theory for Fermionic quantum cellular automata. In refs. [Fid+19; Far20], the subject has been thoroughly covered and it has been shown that the index of a Fermionic automaton can have irrational values as well, whereas the index spectrum for QCAs belongs to $\mathbb{Q}^+$ only. We define the $\mathbb{Z}_2$-graded support algebra as the equivalent of definition 3 for the Fermionic quantum theory, namely

Definition ($\mathbb{Z}_2$-graded support algebra)**.** Let $\mathfrak{B}_1$ and $\mathfrak{B}_2$ be two finite-dimensional $\mathbb{Z}_2$-graded algebras and $\mathfrak{A} \subseteq \mathfrak{B}_1 \boxtimes \mathfrak{B}_2$ a subalgebra. The $\mathbb{Z}_2$-graded support algebra $\mathfrak{C} := \mathrm{S}(\mathfrak{A} \text{ on } \mathfrak{B}_1)$ is the smallest subalgebra $\mathfrak{C} \subseteq \mathfrak{B}_1$ such that $\mathfrak{A} \subseteq \mathfrak{C} \boxtimes \mathfrak{B}_2$.

By means of the definition of support algebra for the Fermionic algebra, we can now prove the equivalent of theorem 8 in the Fermionic case as well.

Theorem 12. *Let $\mathfrak{B}_1$, $\mathfrak{B}_2$, $\mathfrak{B}_3$, and $\mathfrak{A} \subseteq \mathfrak{B}_1 \boxtimes \mathfrak{B}_2$, $\mathfrak{A}' \subseteq \mathfrak{B}_2 \boxtimes \mathfrak{B}_3$ be $\mathbb{Z}_2$-graded algebras. If $\mathfrak{A}$ and $\mathfrak{A}'$ graded-commute in $\mathfrak{B}_1 \boxtimes \mathfrak{B}_2 \boxtimes \mathfrak{B}_3$, then so graded-commute $\mathrm{S}(\mathfrak{A}$ on $\mathfrak{B}_2)$ and $\mathrm{S}(\mathfrak{A}'$ on $\mathfrak{B}_2)$ in $\mathfrak{B}_2$.*

Proof. We directly check that

$$\{\!\{E \boxtimes A \boxtimes I, I \boxtimes A' \boxtimes F\}\!\} = E \boxtimes \{\!\{A, A'\}\!\} \boxtimes F \tag{4.1}$$

for elements of definite parity. Indeed, thanks to our definition of $\mathbb{Z}_2$-graded algebra of § 1.2.5, the linear combinations of elements with different

parity are forbidden. If we pick the bases $\{E_i\}$ for $\mathfrak{B}_1$ and $\{F_j\}$ for $\mathfrak{B}_3$ with elements of definite parity, we can expand every operator of $\mathfrak{A}$, $\mathfrak{A}'$ as

$$A = \sum_i E_i \boxtimes A_i, \qquad A' = \sum_j A'_j \boxtimes F_j \tag{4.2}$$

respectively, for some $A_i \in \mathrm{S}(\mathfrak{A} \text{ on } \mathfrak{B}_2)$ and $A'_j \in \mathrm{S}(\mathfrak{A}' \text{ on } \mathfrak{B}_2)$. By hypothesis, and thanks to eq. (4.1), we have that in $\mathfrak{B}_1 \boxtimes \mathfrak{B}_2 \boxtimes \mathfrak{B}_3$

$$\{\![A, A']\!\} = \sum_{ij} E_i \boxtimes \{\![A_i, A'_j]\!\} \boxtimes F_j = 0. \tag{4.3}$$

The linear independency of bases $\{E_i\}$, $\{F_j\}$ leads us to $\{\![A_i, A'_j]\!\}$ in $\mathfrak{B}_2$, $\forall ij$. The thesis then follows. □

The above result is the starting point for proving the validity of theorem 9 in the Fermionic realm as well. Indeed, an index can be accordingly defined for FQCAs with the same properties, see refs. [Fid+19; Far20]. In particular, the observables of two sites belongs to a $\mathbb{Z}_2$-graded full matrix algebra $\mathfrak{M}$ that features a trivial center as well. Therefore, the setting of fig. 2.4 and eqs. (2.6) and (2.7) also hold in the Fermionic case.

The index is the square root of $\dim(\mathfrak{A}_{2x})/\dim(\mathfrak{L}_{2x})$ of eqs. (2.3) and (2.4), see fig. 2.4. However, the proof of ref. [SW04] does not hold for the Fermionic case and $\mathfrak{L}_{2x}$, $\mathfrak{R}_{2x}$ must not be $\mathbb{Z}_2$-graded full matrix algebras. Thus, the quantum and Fermionic indexes do differ by the spectrum of values they can assume: instead of rational numbers, the index of a FQCA belongs to the multiplicative group of $2^{n/2}$ for $n \in \mathbb{Z}$. Indeed, on the one hand the elementary system that can be moved by a QCA shift is the qudit, i.e. the support algebras $\mathfrak{L}_{2x}$, $\mathfrak{R}_{2x}$ are full matrix. On the other, a Fermionic automaton is free to move around Majorana modes, that are odd self-adjoint operators representing a single vector in the real space $\mathbb{R}^n$. Since all irreducible representation of the CAR are unitarly equivalent to the Jordan-Wigner thanks to theorems 3 and 4, we can compute the algebra dimension from that generated by either $(X_0, Y_0, X_1, Y_1, \ldots, X_n, Y_n)$, that is 2^{2n}, or $(X_0, Y_0, X_1, Y_1, \ldots, X_n, Y_n, Z_1 Z_2 \cdots Z_n)$, namely 2^{2n+1}. The index is then the square root of ratios between such values. In fact, the generator of the shift group for the one-dimensional FQCAs is the Majorana shift:

$$\begin{aligned} \sigma_M : X_n &\mapsto Y_n, \\ Y_n &\mapsto X_{n+1}. \end{aligned} \tag{4.4}$$

It is straightforward to see that the shift automaton $\sigma = \sigma_M^2$, see fig. 4.1, hence $\mathrm{ind}(\sigma_M) = \sqrt{2}$.

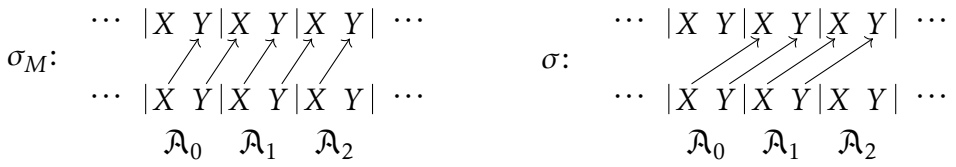


Figure 4.1: Graphical representation of the Majorana automaton σ_M, which features an irrational index equal to $\mathrm{ind}(\sigma_M) = \sqrt{2}$, and of the shift automaton σ of index one.

4.2 Classification of one-dimensional, nearest-neighbors Fermionic Quantum Cellular Automata

The defining trait of a FQCA is being a homomorphism of the Kraus algebra, here in particular the Fermionic one. We begin by requiring the graded-commutation of the image of the two farthest algebras, namely $\{\![\alpha(\mathfrak{A}_1), \alpha(\mathfrak{A}_3)]\!\} \in \mathfrak{A}_0 \boxtimes \mathfrak{A}_1 \boxtimes \mathfrak{A}_2 \boxtimes \mathfrak{A}_3 \boxtimes \mathfrak{A}_4$, where in general $\alpha(\mathfrak{A}_1) \in \mathfrak{A}_0 \boxtimes \mathfrak{A}_1 \boxtimes \mathfrak{A}_2$ and $\alpha(\mathfrak{A}_3) \in \mathfrak{A}_1 \boxtimes \mathfrak{A}_2 \boxtimes \mathfrak{A}_3$. Let

$$\mathfrak{E}_L \coloneqq \mathrm{S}(\alpha(\mathfrak{A}_3) \text{ on } \mathfrak{A}_2) \quad \text{and} \quad \mathfrak{E}_R \coloneqq \mathrm{S}(\alpha(\mathfrak{A}_1) \text{ on } \mathfrak{A}_2), \tag{4.5}$$

thanks to theorem 12 we know that $\{\![\mathfrak{E}_L, \mathfrak{E}_R]\!\} = 0$. So we proceed by scrutinizing all available cases of subalgebras $\mathfrak{E}_L, \mathfrak{E}_R \subseteq \mathfrak{A}_2$, in particular we have:

1. One support algebra is the $\mathbb{Z}_2$-graded full matrix algebra, whereas the other cannot but be the trivial one consisting of the identity element I only.

2. Both support algebras are generated by a single operator each, which graded-commute. In particular, we have: (a) both support algebras are generated by the even operator Z and are therefore Abelian, (b) each support algebra is generated by an odd operator, say G_L for $\mathfrak{E}_L$ and G_R for $\mathfrak{E}_R$, such that the two anti-commute, i.e. $\{G_L, G_R\} = 0$.

3. One support algebra is trivial, while the other is either the full $\mathbb{Z}_2$-graded matrix one as in case 1, (a) generated by a single operator, or (b) trivial as well.

It is straightforward to see that case 3b reduces to a local automaton implementable as a unitary transformation, namely an automorphism of the

Fermionic algebra for a single local Fermionic mode. On the other hand, we now prove that cases 1 and 3a belong to the class of shift and Majorana automata, respectively, whereas cases 2a and 2b are the locally-implementable ones.

Remark. The self-adjoint representation of the CAR introduced in § 1.2.4 proves to be a valuable theoretical tool for describing support algebras for cellular automata in FQT. In particular, that allowed us to verify the graded-commutation of two algebras $\mathfrak{A}_1$, $\mathfrak{A}_2$ by checking only one condition. Indeed, had we instead considered the creation operators $\phi \in \mathfrak{A}_1$, $\psi \in \mathfrak{A}_2$, such that $\{\phi, \phi^\dagger\} = \{\psi, \psi^\dagger\} = 2I$, we would have had to check both the anti-commutation of the operators themselves, namely $\{\phi, \psi\} = 0$, and that of their adjoints as well, i.e. $\{\phi, \psi^\dagger\} = 0$. Thereby, we check two condition instead of the single one for the self-adjoint representation.

Cases 1 and 3a Assume without loss of generality that $\mathfrak{E}_L = \mathfrak{M}$, i.e. the $\mathbb{Z}_2$-graded full matrix algebra for a single local Fermionic mode, and $\mathfrak{E}_R = \{I\}$. In such a case, the image $\alpha(\mathfrak{A}_1) \in \mathfrak{A}_0 \boxtimes \mathfrak{A}_1$ lays on two sites only. We can then apply theorem 12 as before and evaluate $\{\!\![\alpha(\mathfrak{A}_1), \alpha(\mathfrak{A}_2)]\!\!\} \in \mathfrak{A}_0 \boxtimes \mathfrak{A}_1 \boxtimes \mathfrak{A}_2$, which is zero iff $\{\!\![\mathfrak{E}_C, \mathfrak{E}_L]\!\!\} = 0$ for $\mathfrak{E}_C = \mathrm{S}(\alpha(\mathfrak{A}_1)$ on $\mathfrak{A}_1)$ and $\mathfrak{E}_L = \mathrm{S}(\alpha(\mathfrak{A}_2)$ on $\mathfrak{A}_1)$. However, since $\mathfrak{E}_L$ is the $\mathbb{Z}_2$-graded full matrix algebra, $\mathfrak{E}_C$ cannot but be the trivial one. Thus, every automaton of case 1 must be a automorphism between the algebra of a site and that of its previous, namely a backward shift. For case 3a, we instead assume $\mathfrak{E}_L$ being generated by a single operator E. We follow the same steps as before and attain that $\mathfrak{E}_C$ is generated by a single operator F as well, where $\{\!\![E, F]\!\!\} = 0$. For every two self-adjoint, odd operators ξ, $\upsilon \in \mathfrak{A}_1$ such that $\{\xi, \upsilon\} = 0$, the automaton maps them to

$$(\xi, \upsilon) \mapsto (E \boxtimes I, I \boxtimes F) \in \mathfrak{A}_{01}.$$

One can prove with ease that such a homomorphism is indeed the local rule of an automaton, and that it can be implemented through a combination of the Majorana shift σ_M and local automorphisms $\mathcal{U}$, see fig. 4.2b.

4.2.1 Commuting support algebras

In case 2a, both algebras $\mathfrak{E}_L$, $\mathfrak{E}_R$ are generated by the even operator Z and thus *commute*, namely $[\mathfrak{E}_L, \mathfrak{E}_R] = 0$. We may decompose the image of any odd operator $\xi \in \mathfrak{A}_2$ over the basis $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$, or $I \pm Z$, in $\mathfrak{A}_0$, $\mathfrak{A}_2$ as

$$\alpha(\xi) = \sum_{ij} |i\rangle\langle i| \boxtimes A_{ij}(\xi) \boxtimes |j\rangle\langle j|, \tag{4.6}$$

where $i, j \in \{0,1\}$ and for some $A_{ij}(\xi) \in \mathfrak{A}_1$. The above condition strongly resemble that of the QCA of ref. [SW04], indeed we obtain the same result of A_{ij} being themselves automata $\forall i, j$. In particular, for every pair of odd operators $\xi, \upsilon \in \mathfrak{A}_1$ such that $\{\xi, \upsilon\} = 0$ we have

$$\{\alpha(\xi), \alpha(\upsilon)\} = \sum_{ij} |i\rangle\langle i| \boxtimes \{A_{ij}(\xi), A_{ij}(\upsilon)\} \boxtimes |j\rangle\langle j| = 0, \tag{4.7}$$

which is equivalent to

$$\{A_{ij}(\xi), A_{ij}(\upsilon)\} = 0, \quad \forall i, j. \tag{4.8}$$

Equation (4.8) let us define A_{ij} as automorphisms thanks to theorems 3 and 4, and write $A_{ij}(\xi) = U_{ij} \xi U_{ij}^\dagger$ for some unitary matrices $U_{ij} \in U(2)$.

Remark. Due to the automaton α being parity preserving, the set of unitary matrices is constrained to those of definite parity, namely the two multiplicative subgroups

$$SU_0(2) \coloneqq \{\exp(i\theta Z)\}, \quad SU_1(2) \coloneqq \left\{\exp\left(i\frac{\pi}{2}(\cos(\eta)X + \sin(\eta)Y)\right)\right\}, \tag{4.9}$$

for some angles θ, η.

Finally, we require the graded-commutation of the images of nearest-site algebras, namely $\{\![\alpha(\mathfrak{A}_1), \alpha(\mathfrak{A}_2)]\!\} = 0$. Given some odd operators $\xi \in \mathfrak{A}_1$, $\upsilon \in \mathfrak{A}_2$, let us consider

$$\{\alpha(\xi) \boxtimes I, I \boxtimes \alpha(\upsilon)\} = 0. \tag{4.10}$$

We can substitute the decomposition of the automaton of eq. (4.6) in eq. (4.10) and attain

$$\sum_{ijkl} \left\{ |i\rangle\langle i| \boxtimes A_{ij}(\xi) \boxtimes |j\rangle\langle j| \boxtimes I, I \boxtimes |k\rangle\langle k| \boxtimes A_{kl}(\upsilon) \boxtimes |l\rangle\langle l| \right\} = 0, \tag{4.11}$$

which is equivalent to

$$\sum_{jk} \left\{ A_{ij}(\xi) \boxtimes |j\rangle\langle j|, |k\rangle\langle k| \boxtimes A_{kl}(\upsilon) \right\} = 0, \tag{4.12}$$

for all i, l. To complete the classification we need to derive some further properties of the four matrices U_{ij} describing the operators $A_{ij}(\xi)$ of the center algebra $\mathfrak{E}_C = \mathrm{S}(\alpha(\mathfrak{A}_1)$ on $\mathfrak{A}_1)$. For this reason, we prove the Fermionic variant to the lemma 9 of ref. [SW04] by accordingly taking into account the parity of the operators under analysis.

Theorem 13. *Let $\mu, \nu \in \{0,1\}$, and U_μ, V_ν be 2×2 unitary matrices such that*

$$\sum_{\mu,\nu}\left\{U_\mu \xi U_\mu^\dagger \boxtimes |\mu\rangle\langle\mu|, |\nu\rangle\langle\nu| \boxtimes V_\nu \upsilon V_\nu^\dagger\right\} = 0 \tag{4.13}$$

for all ξ, υ odd operators. Then the operators $U_\alpha U_\beta^\dagger$ and $V_\gamma V_\delta^\dagger$ are all diagonal to the computational basis $\forall \alpha, \beta, \gamma, \delta \in \{0,1\}$.

Proof. Let $E_\mu = U_\mu \xi U_\mu^\dagger$, $F_\nu = V_\nu \upsilon V_\nu^\dagger$, and observe that eq. (4.13) is in fact a difference of the exchanged terms, i.e.

$$\sum_{\nu\mu}\left(E_\mu|\nu\rangle\langle\nu| \boxtimes |\mu\rangle\langle\mu|F_\nu - |\nu\rangle\langle\nu|E_\mu \boxtimes F_\nu|\mu\rangle\langle\mu|\right) = 0 \tag{4.14}$$

due to the operators E_μ, F_ν being odd. To simplify the sum, we multiply both sides of eq. (4.14) by $|\alpha\rangle\langle\alpha| \boxtimes |\gamma\rangle\langle\gamma|$ on the left and by $|\beta\rangle\langle\beta| \boxtimes |\delta\rangle\langle\delta|$ on the right. It is worth noting that the operators are even and thus freely commute. The anti-commutator then reads

$$|\alpha\rangle\langle\alpha|E_\gamma|\beta\rangle\langle\beta| \boxtimes |\gamma\rangle\langle\gamma|F_\beta|\delta\rangle\langle\delta| = |\alpha\rangle\langle\alpha|E_\delta|\beta\rangle\langle\beta| \boxtimes |\gamma\rangle\langle\gamma|F_\alpha|\delta\rangle\langle\delta|. \tag{4.15}$$

We are then free to choose υ such that $\langle\gamma|F_\alpha|\delta\rangle = 0$, as a result of which the right hand side of eq. (4.15) vanishes. For this purpuse, let $\upsilon = V_\alpha^\dagger|\gamma'\rangle\langle\delta'|V_\alpha$ for some $\gamma', \delta' \in \{0,1\}$, $\delta' \neq \delta$, so that

$$|\alpha\rangle\langle\alpha|E_\mu|\beta\rangle\langle\beta| \boxtimes |\gamma\rangle\langle\gamma|V_\beta V_\alpha^\dagger|\gamma'\rangle\langle\delta'|V_\alpha V_\beta^\dagger|\delta\rangle\langle\delta| = 0. \tag{4.16}$$

Both factors $\langle\alpha|E_\mu|\beta\rangle$ and $\langle\gamma|V_\beta V_\alpha^\dagger|\gamma'\rangle$ of eq. (4.16) can be made non-zero by an appropriate choice of values ξ, γ', respectively. Hence, $\langle\delta'|V_\alpha V_\beta^\dagger|\delta\rangle = 0$ and $V_\alpha V_\beta^\dagger$ must be diagonal to the computational basis $\forall\alpha,\beta$. The whole procedure can be repeated by choosing an appropriate value for ξ, and obtain that $U_\alpha U_\beta^\dagger$ are also diagonal $\forall\alpha,\beta$ *to the same basis*. □

Theorem 13 tells us that we can diagonalize all U_{ij} of the A_{ij} operators. To do so, we properly choose a local automaton $\mathcal{U}(\xi) := U\xi U^\dagger$, where U is any of the matrices U_{ij}, and prepend it the automaton under analysis, i.e. $\alpha \mapsto \alpha\mathcal{U}$. All U_{ij} of the new automaton are then even and simultaneously diagonalizable to the computational basis of the Fock space $\mathcal{F}_1$. Since we are interested in classifying all automata modulo local ones, we are still free to apply a second local automaton $\mathcal{V}(\xi) := V\xi V^\dagger$ such that $VU_{00} = I$.

We summarize the steps taken so far: the operators U_{ij} of the automaton $\mathcal{V}\alpha\mathcal{U}$ are all even and diagonal to the computational basis, plus $U_{00} = I$. Let

us refer with the symbol $\oplus$ the sum modulo two and say $\xi = |a\rangle\langle a\oplus 1|$, $v = |b\rangle\langle b\oplus 1|$ for some $a,b\in\{0,1\}$. Furthermore, let $U_{ij} = e^{i\phi_{ij}}|0\rangle\langle 0| + e^{-i\phi_{ij}}|1\rangle\langle 1|$, so that we have

$$A_{ij}(\xi) = U_{ij}\xi U_{ij}^\dagger = e^{2i(-1)^a\phi_{ij}}|a\rangle\langle a\oplus 1|, \tag{4.17}$$

and so by substituting eq. (4.17) for both ξ and v in eq. (4.12)—which has been further developed in eq. (4.14)—we obtain

$$(-1)^a(\phi_{i,b} - \phi_{i,b\oplus 1}) = (-1)^b(\phi_{a,l} - \phi_{a\oplus 1,l}) \mod 2\pi, \tag{4.18}$$

for all $i,l,a,b\in\{0,1\}$. Since we have $\phi_{00} = 0$ thanks to our choice of pre-multiplying the automaton by $\mathcal{V}$, we evaluate eq. (4.18) for $i = l = 0$ and for $i = l\oplus 1$ to observe that $\phi_{10} = \phi_{01}$, and $\phi_{11} = 2\phi_{01} = 2\phi_{10}$, respectively. Therefore, let $\phi\in[0,2\pi)$ be the only parameter left, we can write $U_{ij} = Q_\phi^i Q_\phi^j$ where

$$Q_\phi = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi}\end{pmatrix}.$$

With such a definition of U_{ij}, we observe from eq. (4.6) that the action of the automaton can be described through a two-mode dephasing operator D_ϕ defined in $U(4)$ as

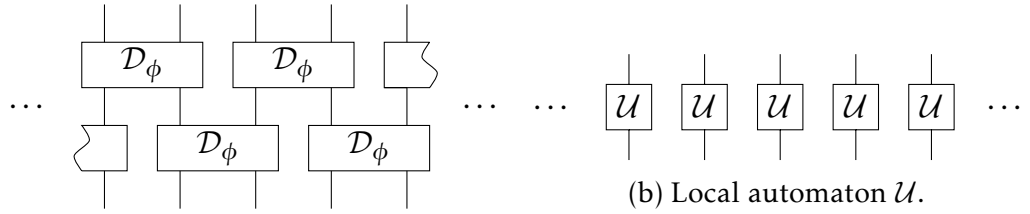
$$D_\phi = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi}\end{pmatrix}, \tag{4.19}$$

such that

$$\alpha(\xi) = (D_\phi\boxtimes I)(I\boxtimes D_\phi)(I\boxtimes\xi\boxtimes I)(I\boxtimes D_\phi)^\dagger(D_\phi\boxtimes I)^\dagger.$$

The Fermionic automata of case 2a are then the composition of the group of dephasing automata of fig. 4.2a, namely a partitioned FQCA with scattering matrix D_ϕ, and completely automorphisms fig. 4.2b. The action of the automaton can be evalueted from the image of the two orthogonal operators X, Y as well. Indeed, we have

$$\begin{aligned}
\alpha(X) = {} & \frac{\cos\phi+1}{2}\, I\boxtimes(\cos(\phi)X - \sin(\phi)Y)\boxtimes I \\
& + \frac{\sin\phi}{2}\, I\boxtimes(\sin(\phi)X + \cos(\phi)Y)\boxtimes Z \\
& + \frac{\sin\phi}{2}\, Z\boxtimes(\sin(\phi)X + \cos(\phi)Y)\boxtimes I \\
& + \frac{\cos\phi-1}{2}\, F\boxtimes(\cos(\phi)\sigma_x - \sin(\phi)Y)\boxtimes Z \\
\alpha(Z) = {} & I\boxtimes Z\boxtimes I
\end{aligned}$$



(a) Dephasing automaton $\mathcal{D}_\phi$.

(b) Local automaton $\mathcal{U}$.

Figure 4.2: Caption

In summary, this class of Fermionic quantum cellular automata is equivalent to the quantum case of QCAs with Abelian support algebras $\mathfrak{E}_L = \mathrm{S}(\alpha(\mathfrak{A}_1)$ on $\mathfrak{A}_0)$, $\mathfrak{E}_R = \mathrm{S}(\alpha(\mathfrak{A}_1)$ on $\mathfrak{A}_2)$ generated by the operator Z, see section IV.G of ref. [SW04]. However, the major difference is here that the algebras $\mathfrak{E}_L$, $\mathfrak{E}_R$ can only be generated by the even operator Z, whereas in QCAs any vector $\hat{\mathbf{v}} \cdot \boldsymbol{\sigma}$ is allowed.

4.2.2 Anti-commuting support algebras

In case 2b, we have that $\mathfrak{E}_L$, $\mathfrak{E}_R$ are generated by two odd operators G_L, G_R, respectively, such that they anti-commute, i.e. $\{G_L, G_R\} = 0$. In spite of case 2b, where we can derive some notable properties of the central support algebra $\mathfrak{E}_C$, here we can not draw the same conclusions from the CAR of two operators belonging to the same site. In particular, the results derived in § 4.2.1 for FQCA and in section IV.E of ref. [SW04] for QCA are not applicable here. The reason is that we may not decompose the members of algebras $\mathfrak{E}_L$, $\mathfrak{E}_R$ in terms of projectors onto the generator eigenspaces, as they have non-definite parity and are therefore forbidden by the parity superselection rule.

Remark. We are interested in classifying FQCA modulo local ones. We are then free to select some $\mathcal{U}(\xi) = U\xi U^\dagger$ such that $\mathcal{U}(G_L) = X$, $\mathcal{U}(G_R) = Y$. Henceforth, we will focus on $\alpha \mapsto \mathcal{U}\alpha$ where the algebras $\mathfrak{E}_L$, $\mathfrak{E}_R$ are generated by the operators X, Y, respectively.

We begin by decomposing the image of a self-adjoint, odd operator $\xi \in \mathfrak{A}_1$ over the sites $\mathfrak{A}_0 \boxtimes \mathfrak{A}_1 \boxtimes \mathfrak{A}_2$. Most notably,

$$\alpha(\xi) = X \boxtimes A_\xi \boxtimes Y + X \boxtimes B_\xi \boxtimes I + I \boxtimes C_\xi \boxtimes Y + I \boxtimes D_\xi \boxtimes I, \tag{4.20}$$

for some operators A_ξ, B_ξ, C_ξ, and D_ξ. Thanks to the automaton being parity preserving, we know that B_ξ, C_ξ are even operators, whereas A_ξ and D_ξ are odd. Moreover, the automaton is a $*$-homomorphism and preserves

adjunction as well. Hence, we observe that A_ξ is *anti-Hermitian* whilst B_ξ, C_ξ, and D_ξ are all Hermitean.

We proceed by evaluating the anti-commutation of nearest-site algrabras, namely $\{\![\alpha(\mathfrak{A}_1), \alpha(\mathfrak{A}_2)]\!\} = 0$. Hence, let us consider two self-adjoint, odd operators ξ, υ, such that they anti-commute, i.e. $\{\xi, \upsilon\} = 0$. Their image under the action of the automaton then reads

$$\{\![\alpha(\xi) \boxtimes I, I \boxtimes \alpha(\upsilon)]\!\} = X \boxtimes E \boxtimes Y + X \boxtimes F \boxtimes I + I \boxtimes P \boxtimes Y + I \boxtimes Q \boxtimes I = 0 \quad (4.21)$$

where

$$E = [A_\xi \boxtimes Y, X \boxtimes A_\upsilon] + A_\xi \boxtimes [Y, C_\upsilon] + [B_\xi, X] \boxtimes A_\upsilon, \quad (4.22a)$$
$$F = [A_\xi \boxtimes Y, X \boxtimes B_\upsilon] + A_\xi \boxtimes \{Y, D_\upsilon\} + [B_\xi, X] \boxtimes B_\upsilon, \quad (4.22b)$$
$$P = [C_\xi \boxtimes Y, X \boxtimes A_\upsilon] + C_\xi \boxtimes [Y, C_\upsilon] + \{D_\xi, X\} \boxtimes A_\upsilon, \quad (4.22c)$$
$$Q = \{C_\xi \boxtimes Y, X \boxtimes B_\upsilon\} + \{D_\xi, X\} \boxtimes B_\upsilon + C_\xi \boxtimes \{Y, D_\upsilon\}. \quad (4.22d)$$

The operators of eqs. (4.22a) to (4.22d) act on two local Fermionic modes and must vanish altogether. We use here a notable property of the algebra $\mathcal{F}^2$ of two local Fermionic modes, namely that the even operators $\mathcal{F}_0^2 = (\mathcal{F}_0 \boxtimes \mathcal{F}_0) \oplus (\mathcal{F}_1 \boxtimes \mathcal{F}_1)$ are the direct sum of operators either even or odd in both sites. Equivalently, the odd operators $\mathcal{F}_1^2 = (\mathcal{F}_0 \boxtimes \mathcal{F}_1) \oplus (\mathcal{F}_1 \boxtimes \mathcal{F}_0)$ are the direct sum of operators with alternate parity in the two sites. Therefore, we may write eq. (4.22a) as $E = E_{00} + E_{11}$, where

$$E_{00} \coloneqq [A_\xi \boxtimes Y, X \boxtimes A_\upsilon], \qquad E_{11} \coloneqq A_\xi \boxtimes [Y, C_\upsilon] + [B_\xi, X] \boxtimes A_\upsilon, \quad (4.23)$$

and they must be null separately. Particularly, for $\xi = \upsilon = \mathbf{p} \cdot \boldsymbol{\sigma}$, $\mathbf{p} \in \mathbb{R}^3$, and $\mathbf{p} \perp \hat{\mathbf{z}}$, we have

$$E_{00} = 2\mathbf{p}_x(\mathbf{p} \times \hat{\mathbf{y}})_z \, I \boxtimes Z + 2\mathbf{p}_y(\hat{\mathbf{x}} \times \mathbf{p})_z \, Z \boxtimes I = 0, \quad (4.24)$$

which is true iff $\mathbf{p} = 0$. Namely, for every ξ we have that

$$A_\xi = 0, \quad (4.25)$$

and most of the terms in eqs. (4.22a) to (4.22d) vanish as well. Equations (4.22b) and (4.22c) reduce to

$$F = [B_\xi, X] \boxtimes B_\upsilon = 0, \qquad P = C_\xi \boxtimes [Y, C_\upsilon] = 0,$$

respectively, and deal with operators B_ξ, C_ξ that must be even, i.e. a linear combination of I and Z. Thus, for $\xi = \upsilon$ the operators F, P are null iff

$$B_\xi, C_\xi \propto I. \quad (4.26)$$

As a consequence of eqs. (4.25) and (4.26), all terms of eqs. (4.22a) to (4.22d) are zero but Q_{00}.

Thus far, we checked the anticommutation relations of algebras that are one or two sites apart. We are then left with the requirement that the images of two anticommuting operators $\xi, \upsilon \in \mathfrak{A}_1$ must anticommute in $\mathfrak{A}_0 \boxtimes \mathfrak{A}_1 \boxtimes \mathfrak{A}_2$, i.e. $\{\alpha(\xi), \alpha(\upsilon)\} = 0$. By substituting therein the decomposition of eq. (4.20) we obtain

$$\{\alpha(\xi), \alpha(\upsilon)\} = I \boxtimes M_{II} \boxtimes I + X \boxtimes M_{XI} \boxtimes I + I \boxtimes M_{IY} \boxtimes Y - X \boxtimes M_{XY} \boxtimes Y = 2\delta_{\xi\upsilon}, \quad (4.27)$$

where the operators

$$\begin{aligned} M_{II} &= -\{A_\xi, A_\upsilon\} + \{B_\xi, B_\upsilon\} + \{C_\xi, C_\upsilon\} + \{D_\xi, D_\upsilon\}, \\ M_{XI} &= \{A_\xi, C_\upsilon\} + \{C_\xi, A_\upsilon\} + [B_\xi, D_\upsilon] - [D_\xi, B_\upsilon], \\ M_{IY} &= \{A_\xi, B_\upsilon\} + \{B_\xi, A_\upsilon\} + [D_\xi, C_\upsilon] - [C_\xi, D_\upsilon], \end{aligned}$$

and

$$M_{XY} = \{A_\xi, D_\upsilon\} + \{D_\xi, A_\upsilon\} + [B_\xi, C_\upsilon] + [C_\xi, B_\upsilon]$$

are all null due to eqs. (4.25) and (4.26) but M_{II}.

We have left to check both eqs. (4.21) and (4.27), which eventually read

$$(\{B_\xi, B_\upsilon\} + \{C_\xi, C_\upsilon\} + \{D_\xi, D_\upsilon\}) = \delta_{\xi\upsilon} I, \quad (4.28)$$

$$(\{D_\xi, X\} \boxtimes B_\upsilon + C_\xi \boxtimes \{Y, D_\upsilon\}) = 0, \quad (4.29)$$

respectively. To solve eq. (4.29) we introduce the following parametrization

$$B_\xi := b_\xi I, \qquad C_\xi := c_\xi I, \qquad D_\xi := \mathbf{v}_\xi \cdot (X, Y), \quad (4.30)$$

for some $b_\xi, c_\xi \in \mathbb{R}$, $\mathbf{v}_\xi \in \mathbb{R}^2$, that allows us to compute the term Q_{00} and reduce eq. (4.29) to a scalar one, i.e.

$$(\mathbf{v}_\xi)_x b_\upsilon + c_\xi (\mathbf{v}_\upsilon)_y = 0. \quad (4.31)$$

Please note that the term Q_{00} is not symmetric for the exchange of operators ξ, υ. For $\xi = \upsilon$, we find that

$$Q_{00} = (b_\xi, c_\xi) \cdot \mathbf{v}_\xi = 0,$$

that can be easily satisfied by defining the following polar coordinates

$$b_\xi := \rho_\xi \cos\theta_\xi, \qquad c_\xi := \rho_\xi \sin\theta_\xi, \qquad \mathbf{v}_\xi = \kappa_\xi(-\sin\theta_\xi, \cos\theta_\xi), \quad (4.32)$$

for some $\rho_\xi \geq 0$, $\kappa_\xi \in \mathbb{R}$, and some angle θ_ξ. Thereby, eq. (4.28) is the Euclidean norm of the vector $(\rho_\xi \cos\theta_\xi, \rho_\xi \sin\theta_\xi, -\kappa_\upsilon \sin\theta_\upsilon, \kappa_\upsilon \cos\theta_\upsilon) \in \mathbb{R}^4$, and for $\xi = \upsilon$ reads $\rho_\xi^2 + \kappa_\xi^2 = 1$. The equation can once more be satisfied through introducing some polar coordinates

$$\rho_\xi := \cos\eta_\xi, \qquad \kappa_\xi := \sin\eta_\xi, \tag{4.33}$$

for some angle η_ξ. Hence, the image of every self-adjoint, odd operator ξ is embedded in a torus (η_ξ, θ_ξ). In particular, as a consequence of eqs. (4.30), (4.32) and (4.33) every such operator is is mapped by the FQCA to

$$\begin{aligned}\xi \mapsto \cos(\eta_\xi)\Big(\cos(\theta_\xi)\, X\boxtimes I\boxtimes I + \sin(\theta_\xi)\, I\boxtimes I\boxtimes Y\Big)\\ + \sin(\eta_\xi)\Big(-\sin(\theta_\xi)\, I\boxtimes X\boxtimes I + \cos(\theta_\xi)\, I\boxtimes Y\boxtimes I\Big).\end{aligned}$$

Finally, we have to require both eqs. (4.28) and (4.31) when $\xi \neq \upsilon$. To do so, we introduce the vectors

$$\hat{\mathbf{e}}_\xi := (\cos\eta_\xi, \sin\eta_\xi), \qquad \hat{\mathbf{t}}_\xi := (\cos\theta_\xi, \sin\theta_\xi) \tag{4.34}$$

of unit norm, and do the same for $\hat{\mathbf{e}}_\upsilon$, $\hat{\mathbf{t}}_\upsilon$. In this manner, the operators Q for $\{\![\alpha(\xi)\boxtimes I, I\boxtimes\alpha(\upsilon)]\!\}$ and $\{\![\alpha(\upsilon)\boxtimes I, I\boxtimes\alpha(\xi)]\!\}$ read

$$(\hat{\mathbf{e}}_\upsilon \times \hat{\mathbf{e}}_\xi)_z (\hat{\mathbf{t}}_\xi)_y (\hat{\mathbf{t}}_\upsilon)_x = 0, \tag{4.35}$$

whereas eq. (4.28) becomes

$$(\hat{\mathbf{e}}_\xi \cdot \hat{\mathbf{e}}_\upsilon)(\hat{\mathbf{t}}_\xi \cdot \hat{\mathbf{t}}_\upsilon) = 0. \tag{4.36}$$

We distinguish two cases that satisfy eqs. (4.35) and (4.36):

(i) $\hat{\mathbf{e}}_\xi \nparallel \hat{\mathbf{e}}_\upsilon$, hence $\hat{\mathbf{t}}_\xi$, $\hat{\mathbf{t}}_\upsilon$ are parallel to either $\hat{\mathbf{x}}$ or $\hat{\mathbf{y}}$ and $\hat{\mathbf{e}}_\xi \perp \hat{\mathbf{e}}_\upsilon$. In terms of angles (η_ξ, θ_ξ) we have $\eta_\xi = \eta_\upsilon + \pi/2 + \pi\mathbb{Z}$ and either $\theta_\xi = \theta_\upsilon = \pi\mathbb{Z}$ or $\theta_\xi = \theta_\upsilon = \pi/2 + \pi\mathbb{Z}$.

(ii) $\hat{\mathbf{e}}_\xi \parallel \hat{\mathbf{e}}_\upsilon$, and thus $\hat{\mathbf{t}}_\xi \perp \hat{\mathbf{t}}_\upsilon$. The polar coordinates then read $\eta_\xi = \eta_\upsilon + 2\pi\mathbb{Z}$ and $\theta_\xi = \theta_\upsilon + \pi/2 + \pi\mathbb{Z}$.

From the above classification we observe that case (i) reduces to the Majorana shift σ_M. Indeed, the operators ξ, υ are mapped to either

$$(\xi, \upsilon) \mapsto (X\boxtimes I\boxtimes I, I\boxtimes Y\boxtimes I) \quad \text{or} \quad (\xi, \upsilon) \mapsto (I\boxtimes I\boxtimes Y, I\boxtimes X\boxtimes I)$$

that are the same bases of case 3a.

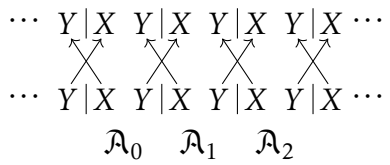


Figure 4.3: Graphical representation of the forking automaton that shifts one Majorana mode to left and the other to the right.

The novel result of this classification is represented by case (ii). In fact, this class describes a linear combination tuned by $\eta = \eta_\xi = \eta_\upsilon$ between a completely-local automaton, which simply rotates the basis (ξ, υ) locally, and the forking automaton that maps the basis

$$(\xi, \upsilon) \mapsto (X \boxtimes I \boxtimes I, I \boxtimes I \boxtimes Y),$$

see fig. 4.3. The latter FQCA has no quantum analogue as it would visibly violate the commutation rules of the quasi-bosonic algebra.

Chapter 5

Quantum Simulation of *Zitterbewegung* effect

Quantum cellular automata are a valuable theoretical tool for describing a vast plethora of physical phenomena. Indeed, in addition to being powerful tools for quantum information protocols ranging from computation to simulations, a QCA is especially suitable to reproduce genuine phenomena of quantum field theory and relativistic quantum mechanics. For this reason, we are interested in devising and developing hardware platform able to simulate the evolution of a QCA.

Although local, the non-linear interactions of a quantum cellular automaton are challenging to reproduce in a controlled fashion. The same does not apply to quantum walks (QWs), a the particular case of QCAs whose action is linear in the field operators. First introduced in ref. [ADZ93], the quantum version of a random walk was modeled through measurements along the Z-component of a spin-½ particle over a one-dimensional lattice, which decide whether the particle moves to the right or to the left. The measurement was then replaced by a unitary operator on the spin-½ quantum system, also denoted internal degree of freedom or *coin system*, with the QW representing a discrete unitary evolution of a particle state with the internal degree of freedom given by the spin. The formal definition of QW can be found in refs. [Amb+01; NV00] for the one-dimensional case, and in ref. [Aha+01] for graphs of any dimension. See also ref. [Kem03] for a complete review.

A direct relation between the time evolution produced by the one-dimensional Dirac Hamiltonian and the QW dynamics can be obtained [Str06], introducing the so-called Dirac Cellular Automaton. We focus on the experimental realization of a QW simulating the *Zitterbewegung* effect in a photonic platform based on the scheme proposed in ref. [BDT13]. We

use the OAM of light to encode the *walker* system that is directly linked to the position of the Dirac particle, while the *coin* is codified in the polarization degree of freedom. The structured wavefront characterizing OAM states and their high-dimensionality motivate the wide applications that these states have found both in the classical regime, regarding microscopy [Für+05; Tam+06], optical trapping [Zha04] and communication [Wil+15; Boz+13; Wan16], and in quantum information processing for the development of protocols in quantum communication [Wan+15; Coz+19a; Coz+19b], computation [Lan+08; RRG07], metrology [Fic+12; DAm+13; Cim+21] and cryptography [Mir+15; Bou+18b]. Moreover, OAM-based platforms offer the possibility to produce a QW dynamics on a line without an exponential increase of the number of optical elements with respect to the length of the walk [Car+15; Gio+18].

Here, we move beyond the present status of experimental OAM-based quantum walk platforms, implementing 8 steps of a QW with a controllable initial state and an arbitrary projective measurement stage at the output. Employing this platform we reproduced the one-dimensional Dirac QW and we were able to efficiently simulate the *Zitterbewegung* effect. Our work demonstrates the capability of photonic platforms of simulating relativistic behaviour difficult to observe in real case scenarios, paving the way for further experimental implementations of QCA.

5.1 Linear Quantum Cellular Automaton: the Quantum Walk

As we introduced in § 2.2, quantum cellular automata describe the unitary evolution of a lattice of cells, each representing a quantum system. The evolution occurs in discrete steps and it is *local*, namely the state of a cell after a certain step $t+1$ depends only on the state of finitely many neighboring cells after the preceding step t, see fig. 2.3. Let us consider the one-dimensional nearest-neighbor lattice $\mathbb{Z}$ and a local Bosonic (Fermionic) mode per cell. We associate every site $x \in \mathbb{Z}$ with an algebra of field operators $\psi_{x,a}$ where the index $a \in S$ belongs to a finite set S and denotes some internal degree of freedom (e.g. polarization, spin, helicity, etc). The field operators fulfill either the canonical commutation relations (CCR)

$$[\psi_{x,a}, \psi^\dagger_{y,b}] = \delta_{x,y}\delta_{a,b} \qquad [\psi_{x,a}, \psi_{y,b}] = [\psi^\dagger_{x,a}, \psi^\dagger_{y,b}] = 0,$$

or the CAR as in eq. (1.4) and § 1.2.1

$$\{\psi_{x,a}, \psi^\dagger_{y,b}\} = \delta_{x,y}\delta_{a,b} \qquad \{\psi_{x,a}, \psi_{y,b}\} = \{\psi^\dagger_{x,a}, \psi^\dagger_{y,b}\} = 0,$$

for $x, y \in \mathbb{Z}$ and $a, b \in S$. A quantum cellular automaton α is then a local and translation invariant automorphism in the representation of the CCR (CAR) algebra which is a one-step evolution of the lattice. We give a Fock space representation of the CCR (CAR) algebra by introducing the N-excitations (particles) states

$$|(x_1, a_1), \ldots, (x_N, a_N)\rangle := \psi^\dagger_{x_1,a_1} \cdots \psi^\dagger_{x_N,a_N} |\Omega\rangle$$

where $|\Omega\rangle$ is the vacuum state. If we consider the particular case of a free, i.e. non-interacting, evolution, the QCA action is linear in the field operators, namely

$$\alpha(\psi_{x,a}) = \sum_{y\in\mathbb{Z}} \sum_{b\in S} U^*_{y,b;x,a} \psi_{y,b},$$

where the coefficients $U_{y,b;x,a}$ turn out to be matrix elements of a unitary operator on the subspace spanned by single-particle states.

Thus, the dynamics is completely determined by the quantum walk (QW) U on the single-particle Hilbert space $\mathbb{C}^S \otimes l_2(\mathbb{Z})$, namely

$$|\psi(t+1)\rangle = U|\psi(t)\rangle, \tag{5.1}$$

$$U|a\rangle|x\rangle = \sum_{y\in\mathbb{Z}} \sum_{b\in S} U_{y,b;x,a} |b\rangle\big|y\big\rangle, \tag{5.2}$$

$$|a\rangle|x\rangle := |(x,a)\rangle. \tag{5.3}$$

We will now focus on the case where S is associated to a two-dimensional space, in particular the polarization of the system described by the circular basis, i.e. $S = \{L, R\}$. Because the evolution is translation invariant it is convenient to represent the unitary operator U in eqs. (5.1) and (5.2) through the momentum representation:

$$U = \int_{-\pi}^{\pi} \mathrm{d}k\, U(k) \otimes |k\rangle\langle k|, \qquad U(k)|\pm\rangle_k = e^{\mp i\omega(k)}|\pm\rangle_k \tag{5.4}$$

where we introduced the plane waves

$$|k\rangle := \sum_x \frac{e^{ikx}}{\sqrt{2\pi}} |x\rangle,$$

and $U(k) \in \mathsf{SU}(2)$ is a unitary matrix with eigenvectors $|+\rangle_k$ and $|-\rangle_k$. In general, $U(k)$ can have determinant which depends on k. However, one can prove that every QW can be decomposed in terms of left or right shifts on the lattice and QW such that $U(k) \in \mathsf{SU}(2)$ for all k, thanks to the index theorem for QW [Gro+12].

For instance, the QW corresponding to the one particle sector of the Dirac Cellular Automaton [BDT13; BDT15] reads as follows:

$$U(k) = \begin{pmatrix} ne^{-ik} & -im \\ -im & ne^{ik} \end{pmatrix}, \qquad \omega(k) = \arccos(n\cos(k)) \tag{5.5}$$

for some real numbers n, m such that $n^2 + m^2 = 1$.

For a given quantum walk U, it is useful to introduce an *effective Hamiltonian* H which obeys $U = e^{-iH}$. The Hamiltonian H generates a continuous time evolution which interpolates the evolution of the quantum walk. We refer to the support $\mathcal{H}_+$, resp. $\mathcal{H}_-$, of the projector

$$P_\pm := \int_{-\pi}^{\pi} \mathrm{d}k \, |\pm_k\rangle\langle\pm_k| \otimes |k\rangle\langle k|$$

as the subspace of *positive*, resp. *negative*, energy states.

In particular, for the QW of eq. (5.5) we have

$$H = \int_{-\pi}^{\pi} \mathrm{d}k \, H(k) \otimes |k\rangle\langle k|, \tag{5.6}$$

$$H(k) = \frac{\omega(k)}{\sin\omega(k)} \begin{pmatrix} n\sin(k) & m \\ m & -n\sin(k) \end{pmatrix} \tag{5.7}$$

and one can easily verify that for small k and m the one dimensional Dirac equation

$$i\partial_t \psi(k,t) = (k\sigma_z + m\sigma_x)\psi(k,t)$$

is recovered. The above considerations show that the QW in eq. (5.5) provides a quantum simulation of the one dimensional Dirac free field and can be used to observe relativistic quantum effects pertaining regimes that are difficult to access experimentally.

5.2 *Zitterbewegung*

One of the main predictions of the Dirac equation is the existence of antiparticles. As first noticed by Schrödinger [Sch30], interference of a Dirac particle with its antiparticle is responsible for the so-called *Zitterbewegung* effect, namely the oscillation of the expected value of the position operator X [Tha92]. Direct observation of this phenomenon in particle physics would be prohibitive since it requires preparing a coherent superposition of particle and antiparticle states for which the oscillation amplitude is of the order of the Compton wavelength (10^{-12} m for an electron).

Since this phenomenon ultimately depends only on the presence of positive and negative energy states, it can be observed also in QW [BDT13]. For the case of a quantum walk on a one-dimensional lattice—see eq. (5.4)—the position operator is $X := \sum_{x\in\mathbb{Z}} x I \otimes |x\rangle\langle x|$ and its time evolution $X(t) = U^{-t} X U^t$ can be computed by integrating the differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} X(t) = -[H,[H,X]],$$

where H is the effective Hamiltonian. We obtain

$$X(t) = X(0) + Vt + \frac{1}{2iH}\left(e^{2iHt} - I\right)F,$$

for

$$V := \int_{-\pi}^{\pi} \mathrm{d}k \, \frac{\omega'(k)}{\omega(k)} H(k) \otimes |k\rangle\langle k|, \quad F := [H,X] - V,$$

where V is the velocity operator and F is responsible for the oscillating motion. Since $FP_\pm = P_\mp F$, we have that the *Zitterbewegung* occurs only for states which are a superposition of positive energy (particle) and negative energy (antiparticle) states. Indeed by taking the expectation value of $X(t)$ with respect to a state $|\psi\rangle = |\psi_+\rangle + |\psi_-\rangle$, where $|\psi_\pm\rangle \in \mathcal{H}_\pm$, we have

$$\langle X(t)\rangle = x_+(t) + x_-(t) + x_0 + z(t)$$

where

$$\begin{aligned} x_\pm(t) &:= \langle \psi_\pm | X(0) + Vt | \psi_\pm \rangle \\ x_0 &:= 2\,\mathrm{Re}\,\langle \psi_+ | X(0) - (2iH)^{-1} F | \psi_- \rangle \\ z(t) &:= 2\,\mathrm{Re}\,\langle \psi_+ | (2iH)^{-1} e^{2iHt} F | \psi_- \rangle. \end{aligned}$$

We see that interference between positive and negative energy states causes a shift x_0 of the mean value of the position plus an oscillating term $z(t)$. Let us now consider states whose particle and antiparticle components are both smoothly peaked around some momentum eigenstate, i.e.

$$c_+ |\psi_+\rangle + c_- |\psi_-\rangle \quad \text{for} \quad |\psi_\pm\rangle = \int \frac{\mathrm{d}k}{\sqrt{2\pi}} g(k) |\pm\rangle_k |k\rangle,$$

where $|c_+|^2 + |c_-|^2 = 1$ and $|g(k)|^2$ is peaked around k_0. Therefore, for small value of t, the oscillating terms can be approximated as follows:

$$z(t) = |c_+||c_-||f(k_0)| \cos(2\omega(k_0)t + \phi_0) \tag{5.8}$$

where we defined $f(k) := \langle +_k | F | -_k \rangle / (2i\omega(k))$ and ϕ_0 is some suitable phase.

5.3 Simulation and results

To experimentally realize the Dirac cellular automaton, we employ the two components of photons angular momentum, the spin and the orbital angular momentum, to encode coin and walker states of a quantum walk, respectively. The position states $\{|x\rangle, x \in \mathbb{Z}\}$ are represented by eingenstates of the OAM, in particular henceforth we consider its expression in the eigenstates basis of Laguerre-Gaussian modes, see ref. [All+92]. While, as internal degree of freedom we chose the orthonormal basis $\{|R\rangle, |L\rangle\}$ corresponding to right and left circularly polarization, respectively.

In our platform, the polarization can be controlled by a set of waveplates. In the circularly polarized basis, the action of a quarter-waveplate (QWP) followed by a half-waveplate (HWP) can be described by the following unitary matrix:

$$C = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{2i(\alpha-\beta)} & ie^{2i\alpha} \\ ie^{-2i\alpha} & e^{-2i(\alpha-\beta)} \end{pmatrix}$$

where α, β are the angles of the fast-axes with respect to the horizontal axis.

A conditional shift in OAM degree of freedom is implemented using a device called q-plate, see ref. [MMP06], which is a thin plate made of a birefringent material with a direction for the optical axis that is not uniform over the device. The angle between the optical axis and the horizontal axis of the device follows the relation $\gamma = \alpha_0 + q\phi$, where α_0 is the initial angle, q is the topological charge of the device and ϕ is the azimuthal angle on the device plane. The delay introduced on the propagation by such arrangement of the optical axis produces a modulation of the wavefront, the q-plate action, in the momentum representation, can be described by the following unitary operator:

$$Q(k) = \begin{pmatrix} \cos\frac{\delta}{2} & ie^{i2\alpha_0} \sin\frac{\delta}{2}\, e^{ik} \\ ie^{-i2\alpha_0} \sin\frac{\delta}{2}\, e^{-ik} & \cos\frac{\delta}{2} \end{pmatrix},$$

where $k = 2q\phi$ and $\delta \in [0, \pi]$ is the q-plate tuning. The latter is directly linked to the effect of the device in the manipulation of the angular momentum of light. This parameter can be electrically tuned between the switch-on value ($\delta = \pi$) and the switch-off one ($\delta = 0$), corresponding to no change at all. We realize a 8-steps QW on a line, where each step is composed of a q-plate and a set of quarter-waveplate and half-waveplate. Then, the single step is given by the composition:

$$U(k) = Q(k)C. \tag{5.9}$$

To control both input OAM modes and the projective measurement apparatus used to reconstruct the output distribution, the entire setup is enclosed between two spatial light modulators (SLMs) as shown in fig. 5.1. This configuration has been already proved suitable for the implementation of the QW dynamics in prior experiments, where shorter dynamics or fixed initial states were employed [Gio+18; Car+15]. The inputs of the setup are triggered single-photon states produced via spontaneous parametric down conversion in a periodically poled potassium titanyl phosphate (ppKTP) nonlinear crystal. These are coupled to a single-mode fiber (SMF) and then sent to the first SLM. The latter is used to modulate the spatial profile of photons in order to obtain the desired initial state at the entrance of the quantum walk. Therefore the input states of the setup are of the following factorised form:

$$|\psi\rangle_{\text{in}} := \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle) \otimes \sum_{x\in\mathbb{Z}} g(x)\,|x\rangle,$$

where $g : \mathbb{Z} \to \mathbb{R}$ and $\sum_x |g(x)|^2 = 1$.

A second SLM instead is employed in the measurement stage along with a SMF to project the output state onto the computational basis and extract the occupation probability of each OAM mode [Mai+01; Bol+13; Qas+14; Bou+18a; Sup+21]. Before doing that, the polarization degree of freedom is traced out using a series composed of a QWP, a HWP and a PBS. In this way, we are able to measure only the OAM components of the walker state at the end of the QW. The discrete size of SLM pixels determines the modulation efficiency of the device especially for high OAM values [Bol+13; Qas+14], while the divergence of the OAM modes [Sup+21; Car+15] needs to be engineered and accounted depending on the number of steps. In particular, our setup gives us full control over OAM states $|x\rangle$ such that $|x| \leq 5$, and we choose a wavepacket which stays confined therin for the whole evolution. Moreover, since the platform performs up to eight evolution steps, it is convinient that the *Zitterbewegung* period $T = 2\pi/2\omega_0$, see eq. (5.8), be of the order of four, so as to observe two complete oscillations.

Let us consider the quantum walk step

$$U(k) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{ik} & e^{ik} \\ -e^{-ik} & e^{-ik} \end{pmatrix}, \tag{5.10}$$

that can be experimentally implemented by choosing the following parameters $\delta = \pi$, $\alpha_0 = \pi/4$, $\alpha = -\pi/4$ and $\beta = \pi/4$ in eq. (5.9). One can show that the dispersion relation $\omega(k)$ of $U(k)$ is that of the walk of eq. (5.5)

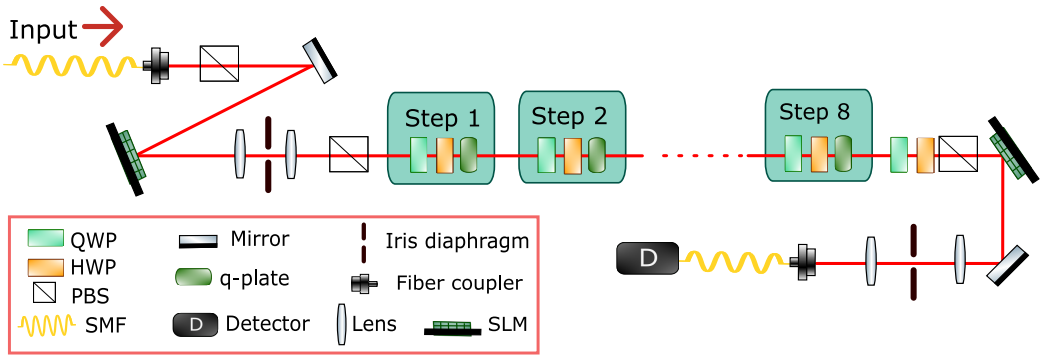


Figure 5.1: The Dirac Cellular Automaton evolution is implemented through an eight-steps discrete-time quantum walk (QW) in the OAM of light. First of all, single photon states are generated through spontaneous parametric down-conversion in a periodically poled potassium titanyl phosphate (ppKTP) nonlinear crystal. After projecting the polarization of single-photons on the horizontal one through a polarizing beam splitter (PBS), the desired input state is produced via a spatial light modulator (SLM) and, after a spatial filtering performed with an iris diaphragm, is sent to the QW. Each step of the latter consist in a coin operator, implemented by a quarter-waveplate (QWP) and a half-waveplate (HWP), and a shift operator performed using a q-plate. Then, the polarization is traced out using a series of QWP, HWP and PBS. The output state probability distribution is measured with a projective measurement executed via a further SLM followed by a single-mode fiber (SMF), the resulting coupled signal is detected by an avalanche photodiode detector.

for $m = n = \sqrt{2}/2$. We are then interested in those states that are superposition of positive and negative energy eigenstates, and at the peak angular wavenumber k_0 features: (i) zero group velocity $\omega'(k_0) = \partial_k \omega(k_0) = 0$, (ii) angular frequency equal to $\pi/4$, and (iii) appreciable *Zitterbewegung* amplitude given by $|c_+| = |c_-| = 1/\sqrt{2}$ and $|f(k_0)| = 1$, see eq. (5.8). We selected the initial state

$$|\psi\rangle_{\text{in}} := \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle) \otimes \sum_{x\in\mathbb{Z}} G_{x_0,\sigma}(x)\,|x\rangle,$$

where $G_{x_0,\sigma}(x)$ is the truncated normal distribution between -5 and 5, centered in $x_0 = 0$, and with standard deviation $\sigma = 3.0$. For such a spatial distribution, the wavefunction in momentum representation resembles a normal distribution peaked at $k_0 = 0$ and with standard deviation $1/\sigma = 1/3$.

This setup allows us to have a precise control having direct access to the different evolution parameters and, thus, reproduce the Dirac evolution step-by-step simply turning on the right number of q-plates.

Exploiting the QW dynamics implemented with the setup, we experimentally study the *Zitterbewegung* effect of the Dirac relativistic evolution in the space of single-photon OAM. To this aim, we use q-plates with topological charge $q = 1/2$ and select the angles of the waveplates in order to reproduce the evolution operator reported in eq. (5.10). Notably, we realized a state-of-the-art platform able to reach 8 steps of the Dirac QW evolution for arbitrary initial states in dimension 11.

We simulated the oscillatory behavior of the position of a one dimensional relativistic particle encoding this degree of freedom in the OAM of photons. Making thus the relation $|x\rangle = |m\rangle$, where x is the position ad m is the value of the OAM. This encoding is explicitly reported in fig. 5.2. We considered as input a Gaussian state localized around the position $|0\rangle$, generated using the first SLM in fig. 5.1, and observed its evolution step by step. In particular, for each step we turned on the relative q-plate setting $\delta = \pi$, traced out the information stored in the polarization and measured via the second SLM and the SMF the walker state distribution over the computational basis $\{|i\rangle\}_{i=-5}^{5}$, opportunely taking into account for the efficiencies of the measurement holograms [Bol+13; Qas+14]. From the measurements, we extracted the occupation probabilities of each site and derived the evolution of the mean position. Most notably, from a theoretical prospective, we expect a Gaussian distribution that oscillates around the position $x = 0$ during the evolution. The oscillation of the Gaussian peak follows the sinusoidal expression in eq. (5.8) with frequency

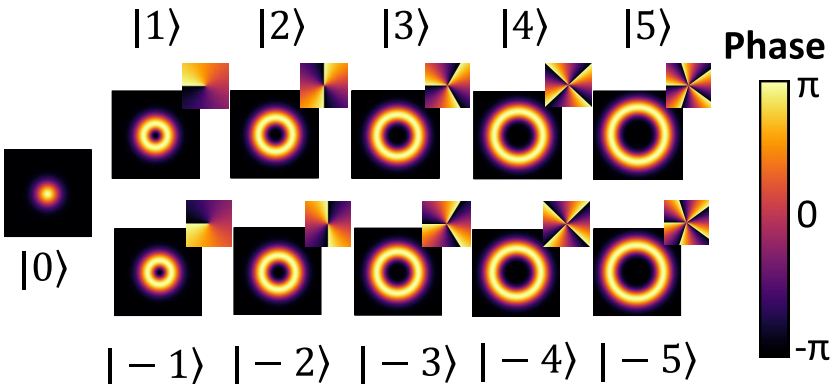
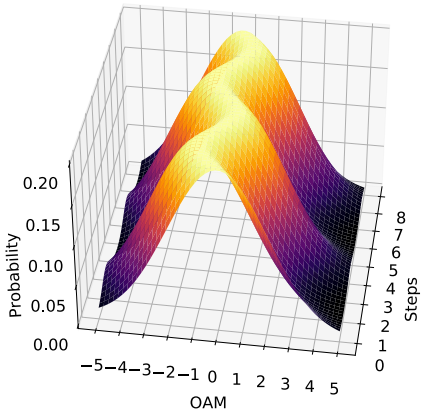


Figure 5.2: Mapping between the OAM space and the position space. In particular, each position of the Dirac particle is identified with a different OAM eingenstate. For the latter, we report both the intensity and the phase of the wave function as expressed in the Laguerre-Gaussian modes basis.

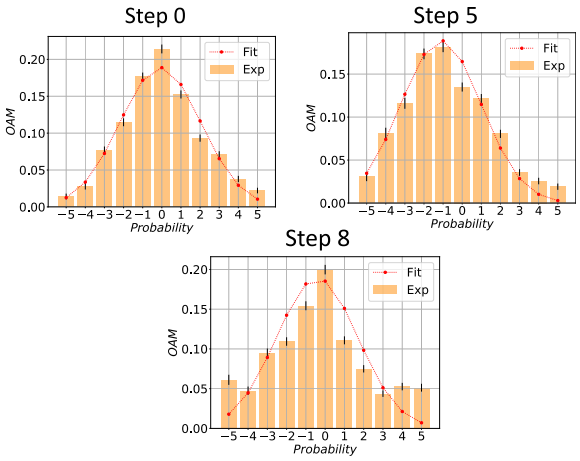
$\omega = 2\omega(k_0) = \pi/2$ and amplitude $A = |c_+||c_-||f(k_0)| = 0.5$. Since in the experiment we only have access to the portion of the distribution between $x = -5$ and $x = 5$, the reference values for ω and A are different. Therefore, at each step, we performed a fit over the distributions in a truncated interval of the position space spanned by $x \in [-5, 5]$ with Gaussian functions whose mean values oscillate along the evolution direction

$$f(t, y) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y - \mu_0 - A\cos(\omega t + \phi))^2}{2\sigma^2}\right), \tag{5.11}$$

where t represents the step of the QW, y the values of probability distributions over the OAM basis, μ_0 the mean of the Gaussian distribution and σ its standard deviation. This fitting procedure is used to derive the oscillation parameters for both theoretical and experimental distributions. The results in the experimental case are shown in fig. 5.3a, where the 3d plot reports the time evolution of the fitted Gaussian envelopes. Moreover, in panel b of § 5.3 we reported the comparison between the experimental distribution and the fitted one obtained following eq. (5.11) for three different steps of the evolution $t = 0, 5, 8$. A slight discrepancy which increases with the number of steps can be observed mainly due to experimental imperfections. Indeed comparing step-by-step the experimental distribution with the one simulated by taking into account such imperfections, we reached a mean fidelity of $\mathcal{F} = 0.990 \pm 0.004$.

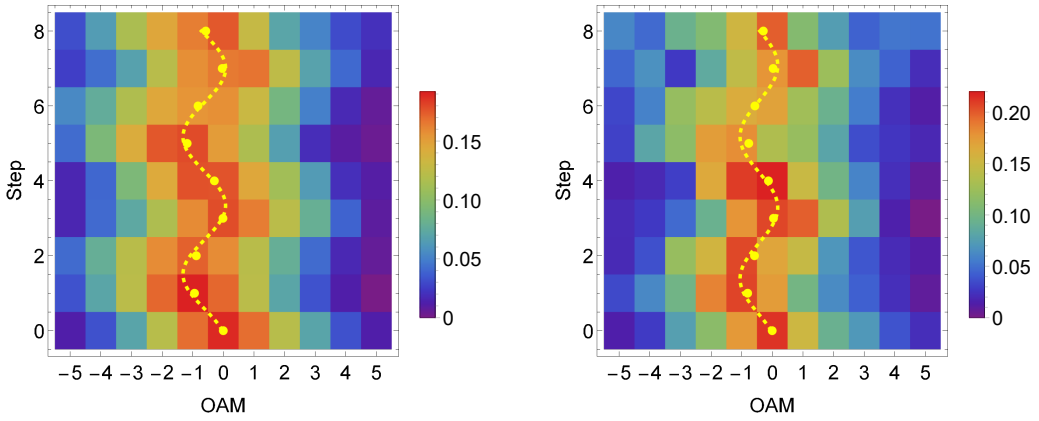


(a) Representation of the Gaussian fit performed on experimental data. The 3d function shown is obtained by fitting the experimental data with the function in eq. (5.11), where the assumed theoretical model is characterized by a Gaussian distribution that oscillates around the initial position during the evolution.



(b) Comparison between the experimental distribution and the fitted function for three different steps of the evolution. Here 0 represents the input state.

Figure 5.3: Data fit and analysis. Although satisfactory similarities can be observed, the difference between histograms and plotted curves increases with the step evolution and this is mainly due to experimental imperfections. The reported errors on experimental data are due to the Poissonian statistics of the measured counts.



(a) Ideal distribution: we report the evolution obtained following the ideal noiseless model of the quantum walk.

(b) Experimental distribution: experimental data is shown.

Figure 5.4: The plots show the output state distribution over the OAM computational basis for each time step considered, we indicate with 0 the initial input state. Yellow points represent the behavior of the mean position during the steps of the evolution.

Discussion

The main result of the experiment consists in the successful simulation of the *Zitterbewegung* oscillations through a photonic platform. The data is reported in § 5.3 together with the theoretical ideal noiseless distribution. The yellow dashed lines represent the oscillations of the mean values of the fitted Gaussian functions. For the theoretical distribution the sinusoidal curve in fig. 5.4a is characterized by values equal to $\omega = 1.714 \pm 0.017$ and $A = 0.695 \pm 0.032$. Experimentally, we obtained an oscillation very similar to the expected one with values that correspond to $\omega = 1.655 \pm 0.009$ and $A = 0.615 \pm 0.017$, the measured behavior is reported in fig. 5.4b. From both the numerical results and the plots shown in § 5.3 it can be seen how the implemented platform is capable of simulating the dynamics of a free relativistic particle, reproducing its typical *Zitterbewegung* trembling motion.

Chapter 6

Conclusions and Future Perspectives

The main subject of the thesis is cellular automata in quantum and Fermionic theories. In particular, its aim is to contribute to the long-term goal of developing a rich and well-grounded framework of CA in different theories. Such an effort is motivated by the belief that physical phenomena can be described through rules of information processing. Moreover, the informational approach to physics provides for a replacement of the mechanical laws to purely informational first principles, from which the mechanics would be an emergent phenomenon.

Quantum cellular automata are promising models for describing fundamental quantum fields, as they allow for the evolution of infinitely many systems. This is possible thanks to its defining notion of locality. In chapter 3, we introduced a new definition of QCA as a super-map between transformations onto the grid instead of the canonical homomorphism of the observable algebra. The two definitions have been proved to be equivalent. The reason for this lies in the peculiar property of quantum theory where the C*-algebra defines both the effects and the transformations. Notwithstanding, QCAs defined in terms of super-maps allows for some revisions to the key principles behind it. Indeed, the real innovation lies here in the new concept of locality. Transformations onto the grid have to be interpreted as interactions of the field with external systems, e.g., another field, and the automaton can then be applied thereto. We conjugate the QCA with the transformation $\mathcal{C}$ to obtain

$$\mathcal{C}' = \alpha^{-1}\mathcal{C}\alpha,$$

that is well-defined if we require α to be an automorphism. We may then

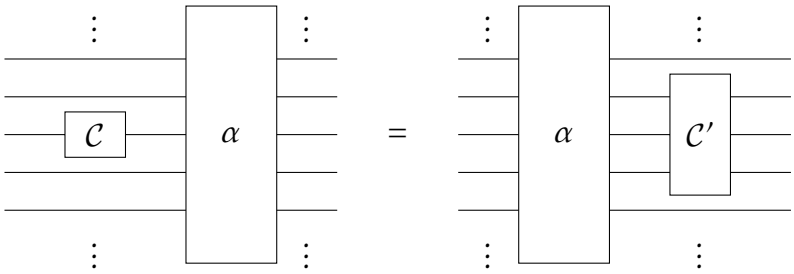


Figure 6.1: Circuit describing the action of the automaton α onto a local transformation $\mathcal{C}$. The quantum operation can be interpreted as local perturbation to the grid, such a perturbation may be scattered by the automaton at most onto the neighborhood.

rewrite it as

$$\mathcal{C}\alpha = \alpha\mathcal{C}', \tag{6.1}$$

see fig. 6.1. Namely, we apply a perturbation to the grid and then evolve it through the automaton. We then may obtain the same result as first evolving the grid by means of the QCA, and only then apply an accordingly revisited transformation $\mathcal{C}'$ onto the neighborhood. The automaton is so required to "spread" the perturbation at most onto the neighborhood. On the contrary, if the transformed operation would need to act onto larger areas, or even the whole grid, that would have meant that the QCA manipulates the grid non-locally. The fact that both notions of locality, namely in terms of effects and transformations, define the same class of QCAs is a very special property of quantum theory, see ref. [Per21].

Furthermore, through the definition of QCAs in terms of automorphism of quantum operation, instead of observables, we may give a clear interpretation to the property of homomorphism of the C*-algebra. On the one hand, no operational interpretation can be given to the product of two observables. On the other hand, the product of two Kraus operators is straightaway related to the composition of two quantum operations. If we consider the setup of eq. (6.1), the transformation $\mathcal{C}$ may then be whatever complex quantum circuit acting on the grid, the automaton must then preserve the structure of the circuit. In particular, all quantum operations making up the circuit must then transform accordingly, but their causal structure must be left invariant since

$$\mathscr{A}(\mathcal{B}\mathcal{C}) = \mathscr{A}(\mathcal{B})\mathscr{A}(\mathcal{C}).$$

More formally, a QCA is required to preserve the algebra and conic structures of quantum operations.

By means of this new definition, we introduced the T-operator $\mathcal{T}_x$ as a local operator onto sites $N_x \sqcup \{x\}$, where N_x denotes the neighborhood of x, that contains all the information to uniquely define a QCA. The T-operator plays here the role of the Choi operator for quantum operations, indeed the T-operator is the Choi of the QCA local rule. Indeed, by decomposing the operator $\mathcal{T}_x$ we observed that it contains both the input and the output of the local rule α_0. Consistently, the T perfectly encodes all information about the QCA, and therefore the index can be computed from it. Moreover, some properties have been derived in theorem 11 that are necessary and sufficient for defining a QCA. One may then be tempted to classify all T-operators so as to classify the QCAs. However, the decomposition of § 3.3 directly translates conditions 2 of theorem 11, i.e. $[\mathcal{T}_x, \mathcal{T}_y] = 0$ for all x, y, into the commutation relation of the local rule, thus vanishing any kind of theoretical advantage. If we continue our analogy to the Choi operator, in the case of quantum operations every operator $\rho_{\mathcal{C}}$ represents an admissible transformation iff $0 \leq \mathrm{Tr}_0[\rho_{\mathcal{C}}] \leq I$. Here, the condition for the T-operator to describe a valid QCA are indeed more complex to resolve. However, the T-operators preserve the conic structure of QCAs and are then valid candidates for studying irreversible QCAs. Indeed, the uncoherent combination of QCAs reduces to the linear combination of its T-operators, since

$$(\mathscr{A} + \mathscr{B})(\mathcal{S}_x) = \mathcal{T}_x + \mathcal{T}'_x.$$

We then proceeded into classifying all nearest-neighbor Fermionic quantum cellular automata on the one-dimensional lattice with one local Fermionic mode per site. We briefly introduced the index theory for FQCA, where we observed that the index can assume irrational values as well, more specifically $\mathrm{ind}\,\alpha = 2^{n/s}$. On the contrary, the spectrum of quantum cellular automata is the set of rational index values only. This feature of FQCAs becomes more clear as soon as we describe their action in terms of the self-adjoint representation of the CAR. Under this hypothesis, the creation, and annihilation operator are defined starting from a pair of Majorana modes. The Fermionic automaton is then free to move around single Majorana modes within the neighborhood. The particular case of a shift of index $\sqrt{2}$ is that of the Majorana shift, which shifts forwards only one Majorana mode and switches the other in-place. Such a behavior is in stark contrast with QCAs, where the minimum system that can be freely placed around is the qudit.

By requiring the anti-commuation relation of the local rule, we successfully classified all such Fermionic cellular automata. In particular, the set can be divided into two classes, based on the kind of support alge-

bras of the image on the nearest neighbors. Since these support algebras must graded-commute, they can either commute or anti-commute. On the one hand, those FQCA having an Abelian support algebra onto the nearest neighbors are in one to one correspondence with a particular class of QCA. On the other hand, the other class has anticommuting support algebras. This is a novel class of automata that strictly pertains to the Fermionic case with no quantum counterparts. In the latter class, a generator of non-local interaction actually forks the Majorana modes, shifting one to the left and the other to the right, see fig. 4.3. From what we have seen so far, the self-adjoint representation of the CAR is more suitable for describing FQCA. In particular, they might be elevated as the fundamental system on which the Fermionic quantum cellular automaton acts. As a future perspective, one may evaluate if it is appropriate to define FQCAs over Majorana modes. In particular, this would require the assessment of whether a well-defined and full-fledged theory can ever exist thereof. Since all representations of the CAR are unitarily equivalent to the Jordan-Wigner's one, any theory describing Majorana modes would inevitably be non-quantum. Namely, states and transformations cannot be represented onto Hilbert spaces. On the other hand, a further development of FQCAs may proceed with classifying automata over higher dimensional lattices and with more than one local Fermionic mode per site.

Finally, in chapter 5 we reported the results of a collaboration for an experiment where we successfully simulated a relativistic phenomenon over a photonic platform. In particular, we observed the *Zitterbewegung* of a particle, i.e. trembling motion, that is a well-known effect of relativistic quantum mechanics experienced by a wave-function in a coherent superposition of particle and antiparticle states. We contributed by providing the theoretical background, evaluating preparatory numerical simulations and optimizing the parameter space for attaining the best visibility. The next experiment in this line of research may try to introduce some inhomogeneity in the quantum walk evolution, so as to represent potentials. In so doing, we could simulate phenomena such as scattering from potential and observing bound states. Of course, the long-term goal of this kind of experiments are the ability of implementing interacting evolution in order to simulate full-fledged quantum cellular automata, both for simulating physical phenomena and for harnessing its computational advantage.

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