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INTERAZIONE LOCALE ISOTROPA NUMBER PRESERVING IN AUTOMI CELLULARI DI DIRAC A TEMPO DISCRETO

LOCAL ISOTROPIC NUMBER PRESERVING INTERACTION IN DISCRETE TIME DIRAC QUANTUM CELLULAR AUTOMATA

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Abstract

Ci si propone di studiare delle interazioni locali isotrope che preservino il numero di eccitazioni nell'ambito degli automi cellulari quantistici (QCA) di Dirac evoluti a tempo discreto. Un QCA è un reticolo di celle contenenti sistemi quantistici che interagiscono con un numero finito di primi vicini in modo tale che la loro evoluzione sia unitaria.
Come punto di inizio si è considerata l'evoluzione libera del QCA. Nel caso di interesse, i sistemi quantistici presi in esame sono composti da fermioni, in particolare è stata considerata l'evoluzione lineare di vettori di generatori dell'algebra dei fermioni (ossia operatori di creazione e distruzione fermionici). Le ipotesi fatte al fine di descrivere tale evoluzione libera sono: linearità, località, unitarietà, omogeneità (quest'ultima considerata come invarianza per traslazioni sul reticolo visto come un grafo di Cayley) e isotropia discreta.
Nel caso di due gradi di libertà interni, i generatori dell'algebra dei fermioni sono rappresentati come vettori della forma (a_u, a_d), interpretati come spinori, ed è possibile derivare da questo formalismo l'equazione di Weyl. Riguardo al Dirac QCA, l'evoluzione si ottiene accoppiando due automi di Weyl e l'equazione di Dirac può essere derivata dall'evoluzione libera di vettori della forma $(a_{u_1}, a_{d_1}, a_{u_2}, a_{d_2})$, interpretabili come bispinori.
Data l'evoluzione libera, è stata introdotta un'interazione locale, descritta da un operatore unitario che rappresenta il più generale disallineamento tra le basi locali nell'algebra fermionica locale a differenti istanti (discreti) di tempo. Tale operatore deve essere posto invariante sotto lo stesso gruppo di isotropia dell'evoluzione lineare. È stata imposta inoltre la conservazione del numero di eccitazioni.
L'interazione è descritta da un operatore unitario della forma $\prod_x e^{iH_x}$, dove x indica la cella sulla quale sta agendo e H_x sono polinomi di operatori fermionici nelle ipotesi descritte.
Al fine di rispettare la conservazione del numero di eccitazioni, ogni H_x sarà composto di monomi aventi un uguale numero di operatori di creazione e distruzione, in particolare da 2 a 8 operatori (termini di ordine maggiore si annullano a causa del principio di esclusione di Pauli). Si è quindi passati a studiare i termini 4-lineari della forma $f_i f_j f_k f_l$, dove f_i è un operatore fermionico che può essere del tipo a o $a^\dagger$, con i citati vincoli di conservazione del numero di eccitazioni e isotropia (per esempio, $a^\dagger_{u_1} a_{u_1} a^\dagger_{d_1} a_{d_1}$). Si è inoltre studiato un modo di rappresentare tali operatori usando forme bilineari di matrici gamma di Dirac o prodotti delle stesse.
È stata inoltre studiata un'interazione particolare nel caso di due particelle, sfruttando la composizione di $J := e^{iH_x}$ con l'operatore unitario $D \otimes D$ che descrive lo step di evoluzione lineare dell'automa di Dirac per due particelle. In particolare sono stati ricavati gli stati che risolvono l'equazione agli autovalori

$J(D \otimes D)|\psi\rangle = e^{-i\omega}|\psi\rangle$. Per semplificare i calcoli riguardanti l'algebra dei fermioni, è stato impiegato un modulo Python dedicato alla manipolazione di espressioni matematiche, Sympy. Sfruttando questo strumento, sono stati scritti algoritmi utili a determinare la forma di H_x.

Abstract

In this thesis, we study a local isotropic number preserving interaction following discrete-time evolution of the Dirac Quantum Cellular Automata (QCA).
A QCA consists of a lattice of cells of quantum systems interacting with a finite number of neighbours in such a way that their evolution is unitary.
We started using as a background the free evolution of the QCA. In our case the quantum systems are composed of fermions, in particular it has been considered the free evolution of vectors of the generator of the fermions algebra (i.e. Fermionic raising and lowering operators).
The hypothesis made in order to describe this free evolution are: linearity, unitarity, locality, homogeneity (in this scenario the latter is intended as invariance under translations on the lattice conceived as a Cayley graph) and discrete isotropy.
In the 2-dimensional case, the Fermionic algebra generators are represented as vectors of the form (a_u, a_d), interpreted as spinors, and it is possible to recover the Weyl equation. The Dirac case is obtained by coupling two Weyl automata and the Dirac equation can be recovered from the free evolution of vectors of the form $(a_{u1}, a_{d1}, a_{u2}, a_{d2})$ intended as bispinors.
Given the free evolution, we introduce a local interaction, described by a unitary operator which represents the most general misalignment between the local bases in the local Fermionic algebra at different time steps.
This operator needs to be invariant under the same isotropy group of the linear automaton. We also imposed number preservation, which means that the excitation number is conserved.
The interaction is described by a unitary operator of the form $\prod_x e^{iH_x}$, where x indicates the cell on which it is acting and the H_x are suitable polynomials of Fermionic operators.
In order to provide number preservation, each H_x will have monomials composed of an equal numbers of Fermionic creation and annihilation operators, in particular from 2 to 8 operators (higher order terms vanish because of the Pauli exclusion principle). We studied then the 4-linear terms of the form $f_i f_j f_k f_l$, where f_i is a Fermionic operator, which can be either a or $a^\dagger$, and with the obvious constraints of number preservation and isotropy (e.g. $a^\dagger_{u1} a_{u1} a^\dagger_{d1} a_{d1}$). We also studied a way to represent them using bilinear forms of Dirac gamma matrices or products of them.
Moreover, we studied a special interaction in the two particle sector, exploiting the composition of $J := e^{iH_x}$ with the unitary operator $D \otimes D$ describing the linear evolution step of the Dirac automaton for two particles. In particular, we derived the states solving the eigenvalue equation $J(D \otimes D)|\psi\rangle = e^{i\omega}|\psi\rangle$.
The cumbersome characterization of the most general form of the polynomial H_x has been automatized through some calculations using the symbolic mathemat-

ics module for Python, sympy. With this tool, we wrote algorithms capable of handling calculations taking into account the algebra of the Fermionic operators.

Contents

INTRODUCTION

The idea of simulating physics exploiting an informational paradigm has been seen as an achievable objective in the last four decades. The fatherhood of the idea of using a computation based on an intrinsecally probabilistic system, such as a quantum system in order to imitate the behaviour of other quantum systems is traditionally attributed to R. P. Feynman, who in [Fey82] also pointed out the need for having a suitable criterion for discretizing space, time and fields since we cannot have infinite precision in describing (and consequently imitating) the objects of our observation.
However, the relationship between algorithms, intended as simple rules manipulating a certain amount of *information*, and the physical laws they are meant to simulate or the physics that we observe was guessed a few years before by Zuse [Zus70] and was based on the notion of Cellular Automaton (CA), looking at the Universe as the emergent phenomenon of these rules.
Cellular Automata are d-dimensional lattices of bits or d-its that update over discrete timesteps. The update rule is based uniquely on the state of the updating bit and its neighbours (usually its *nearest* neighbours) [Far20].
CA are usually defined over infinite lattices or on finite lattices with periodic boundary conditions. Furthermore, they are called *reversible* if for each current configuration there is exactly one previous configuration and viceversa [Wie08].
Cellular Automata alone are of course an extremely interesting tool: one can think for example of Conway's *Game of Life* [Gam70] or Wolfram's classification of one-dimensional CA [Wol83] and the huge amount of unpredictability they generate which is often addressed to as *complexity*. However, classical CA cannot be the answer to the Feynman's problem of simulation. They lack of intrinsic probabilistic properties useful to describe for example quantum phenomena, and even if probabilistic CA were proposed [ENJ10], they are not enough to reproduce the behaviour of quantum systems. Only a "quantum" CA, intended as a CA endowed with quantum properties [1] can be suitable to reproduce all the physical systems

[1] I am in particular referring to the ability of exploiting or simulating entanglement, which is a crucial quantum property.

studied so far.
All these ideas are formalized in the notion of Quantum Cellular Automata (QCA). They are a generalization of (classical) cellular automata (CA) and in particular of reversible CA.
QCA were introduced by Grössing and Zeilinger who worked on the first model of QCA [GZ88], other names involved in the first papers on this topic are Watrous [Wat95], Margolus [Mar90] and Arrighi [AFW08]. The most famous and complete mathematical formalization of QCA was elaborated by Schumacher and Werner [SW04].
In all these works a QCA is conceived as a d-dimensional lattice of non distinguishable finite-dimensional quantum systems, a finite set of states, a finite neighbourhood scheme and a set of local unitary transition rules [Wie08].
The quantum systems in each cell can also be represented by Fermionic or Bosonic creation and annihilation operators, i.e. quantum fields [2]. Their evolution exploiting the Heisenberg picture is useful to link QCA to Quantum Field Theory (QFT), a theory of systems but also a theory which recovers mechanical notions through quantization rules and equations evolving physical systems.
In this way QCA become very powerful tools for recovering physics from informational principles and simple algebraic rules: space and time can be eventually recovered as emergent phenomena [DP14] as well as Weyl, Dirac and Maxwell equations [BB94, BDT15, BDP16a].
This work inherits the spirit and the purposes discussed so far and has the intent of expanding the theory of Weyl and Dirac Fermionic QCA by introducing interaction operators after a free (linear) evolution step. The main hypotesis on the interaction terms are locality, – i.e. each of them acts on a precise site on the lattice – number preservation – namely they do not create or destroy modes – and isotropy – that is the fact that they respect invariance under the isotropy group in tridimensional lattices.
The next chapters are organized as follows: in Chapter 1 the theory of QCA is detailed in order to review some useful results and we analyze the relationship between QCA and Quantum Walks (QW), namely their "first quantization" version, in Chapter 2 we review our two Fermionic QCA of interest: Weyl and Dirac QCA and we describe the free evolution, in Chapter 3 we classify all the local isotropic number preserving interactions for Weyl and Dirac QCA, while in Chapter 4 we provide the analytical solution of a particular interesting interaction out of the ones classified. Since we have met some cumbersome calculations in our work, expecially during the classification part, we have coded a python module dedicated to handle the Fermionic algebra ehich is based on *Sympy*. In Appendix A it is presented and commented in some of its parts.

[2] Also referred to as Fermionic (Bosonic) modes.

CHAPTER 1

A SHORT REVIEW OF QUANTUM CELLULAR AUTOMATA

Quantum Mechanics was surely revolutionary when it was discovered in the early twentieth century. Alongside with Einstein's relativity it is one of the greatest achievements of the human mind ever reached. A change in paradigm, like it happened for the Copernican revolution, is certainly important to see things from a different perspective, but it is just a seed for the upcoming discoveries, which require time and effort in order to be made. In this sense Quantum Mechanics has gone through many formulations and has been studied widely, even if it is not yet fully understood by the community of physicists, still reminiscent of Feynman's motto *Shut up and calculate*.

Nowadays Quantum Mechanics has been deeply discussed in its fundations and it has been put beside the idea of thinking physical phenomena as algorithms and information processing. In this sense it is possible to reformulate Quantum Mechanics starting from an information processing theory as a subset of the wider Quantum Information Theory. In [DCP17] starting from the framework of operational probabilistic theories (OPTs), equipped with a structure for composition of systems and processes, a Quantum Theory (QT) is derived, intended as the general theory of physical systems that lies at the core of Quantum Mechanics, which can be conceived instead as the quantum generalization of classical Hamiltonian mechanics.

This means that in a sense, we have a low-level theory of physical systems and an high-level language of mechanics which emerges from the former [Per20b].

In order to complete the program of providing a description of physical laws through *exact* algorithms based on this low -level language a viable path is the one of Quantum Cellular Automata (QCA). As we will review in the first part of this work, they have been successful in recovering free fields dynamics, such as

Weyl, Dirac and Maxwell equations.
Having a general, but precise idea on these automata is crucial in order to have the full picture of the problem we will face.

1. CLASSICAL CELLULAR AUTOMATA

Quantum Cellular Automata, as the name suggests, are the quantum counterpart of Cellular Automata (CA). What "Quantum" means in this context will be clear at the end of the chapter. At the moment we will focus on the idea at the basis of classical CA.
CA were introduced by S. Ulam and J. von Neumann in the '40s. Von Neuman was working on self-replicating systems, while Ulam on growth of crystals on discrete lattices. They conceived the idea of creating a self-replication model with a discrete system [vN51].
In its first talk on the topic, von Neumann starts from the idea of *Turing's Theory of Computing Automata* and describes an automaton as a *black box* which possesses a finite number of states and a description on how its state is changed formalized in a set of rules. This "primitive" model of CA is still influenced (in a sense the example provided by von Neumann is equivalent) by the common representation given for the Turing's machine and the local update rule for each state is sequential and based on a "moving tape" with markable fields inspected by a machine which can mark and unmark sequentially each of them in order to change their state. In the same occasion, von Neumann also described a self-replicating system based on a composition of different automata and studied the complexity of the resulting automaton.
This idea was furtherly developed by von Neumann and Ulam (who was interested in finding applications in discrete fluidodynamics) and applied also on two dimensional automata and formalized in *von Neumann's universal constructor* with 29 states on a two-dimensional grid.
Another remarkable historical result is *Greenberger- Hastings* CA, which was desigend to model excitable media and has inspired papers on the mathematical study of cardiac arrythmia [GH78, MDZ19].
In the subsequent years a huge effort was made in order to formalize the idea of CA. A definition specialized to the monodimensional case is [IG06]

Definition 1.1.1. *A Cellular Automaton is a triple* $(a(t), \{S_A\}, f_A)$ *composed by a lattice* $a(t)$ *of cells, an alphabet* $\{S_A\}$ *of states in which each can be and* f_A *an update rule.*
In the monodimensional case f_A *is a function* $f_A : \{S_A\}^3 \longrightarrow \{S_A\}$.

Calling $a_x(t)$ an individual lattice cell, with x index depending on the geometry and the dimensionality of the lattice and t time parameter depending on the number of evolution steps, in the mondimensional case we have $a_n(t+1) = f_A[a_{n-1}(t), a_n(t), a_{n+1}(t)]$.

We are focusing our attention on monodimensional CA because the wider effort in classification of CA was made by Wolfram in [Wol83] for monodimensional CA. For this class of automata it is particularly intuitive to understand how the evolution rule works: given a cell $a_n(t)$ at time step t, its monodimensional neighbourhood is composed of $a_n(t)$ and its prime neighbours, i.e. the cell on the left and the cell on the right of $a_n(t)$.
With this definition of neighbourhood, Wolfram formalized his *256 Rules*. This is the complete classification of monodimensional CA with 3-cells neighbour. To provide an example, let us consider the most unpredictable rule, *Rule 110*.
Following the definition, the alphabet for each cell is $S_A := \{0, 1\}$ the local update rule is a function $f_A := \{0, 1\}^3 \longrightarrow \{0, 1\}$ defined in this way:

$a_{n-1}(t), a_n(t), a_{n+1}(t)$	$a_n(t+1)$
(0,0,0)	0
(0,0,1)	1
(0,1,0)	1
(0,1,1)	0
(1,0,0)	1
(1,0,1)	1
(1,1,0)	1
(1,1,1)	0

From top to bottom the second column of the table, we read 110 in binary (01101110). Each update rule of this classification can be built exploiting the binary translation of its name substituted to the second column of the previous table. Other formulations have been proposed, one based on matrices as a representation for the update rule can be found in [ENJ10].
It is not difficult to generalize these ideas to further dimensions [Wie08].

Definition 1.1.2. *Given d dimension of the lattice and $\mathcal{N} \subset \mathbb{Z}^d$ a finite neighbourhood scheme, the local transition function for $d - dimensional$ CA is defined as a function $f_A : \{S_A\}^{\mathcal{N}} \longrightarrow \{S_A\}$.*

A very famous example of bidimensional CA which is also an extremely interesting toy model is *Conway's Game of Life*. The Game of Life is an automaton

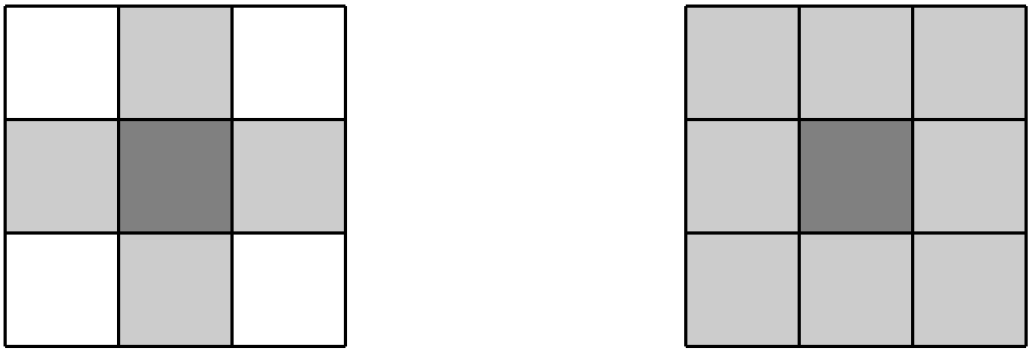

Figure 1.1: von Neumann neighbourhood (left) and Moore neighbourhood (right).

usually[1] characterized by an infinite two-dimensional lattice of cells, which can be in an *alive* or in a *dead* state. The neighbourhood scheme can be the Moore neighbourhood or the von Neumann neighbourhood (usually the former). The update rule is the following [Gam70]:

- Every *alive* cell with two or three neighbours stays in *alive* state
- Every *alive* cell with four or more neighbours *dies* from overpopulation
- Every *alive* cell with one or none neighbours *dies* from isolation
- Every *dead* cell with exactly *three* neighbours changes its state to *alive*

Conway's Game of Life is very fascinating because it is an example of emergent phenomenon from very simple rules. The quest for stationary configurations– namely configurations which do not change over time steps, or pattern behaving in chaotic or, on the other side, strongly predictable ways – is a challenge which continues also at the present days, even if quite exaustive classifications of well known patterns have been published and are available online [GoL].

2. FROM CLASSICAL TO QUANTUM CELLULAR AUTOMATA

Classical CA (or simply CA) have many applications in complex systems physics and also in understanding the physiology of muscular fibers, or in modelling traffic (Wolfram's Rule 184 is the simplest car traffic simulation provided by an automaton). What about the Feynman's desideratum of describing physics through

[1] many versions have been studied, here I will describe the most common configuration

algorithms? Physical phenomena include an extremely wide range of situations and, as stated before, they include quantum physics. So, how quantum physics can be described through such a paradigm? Can we see quantum system and hopefully quantum field theory (QFT) as an epiphenomenon of a sort of *quantum* cellular automaton?
In order to provide a satisfactory answer to these questions the theory of Quantum Cellular Automata (QCA) has been developed.
As one can imagine, QCA are a bit more recent than their classical counterpart. In a sense they were born with Feynman's idea on quantum computing, but the locution *Quantum Cellular Automata* was firstly used by Grössing and Zeilinger [GZ88]. The definition of QCA they provide is the following [Wie08]

Definition 1.2.1. *A Grössing- Zeilinger QCA is a triple (A,$\mathcal{H}$,U), where $A \subseteq \mathbb{Z}$ is an infinite 1-dimensional lattice where each site at each time represents the basis $\{\psi_{t,i}\}$ of an Hilbert space $\mathcal{H}$ and U is an r-diagonal unitary operator.*

Since a QCA is often required to be homogeneous, i.e. each cell is treated the same way by the update rule, in this case U must commute with the translational operator T and in particular this implies it must be invariant under its action:

$$UT - TU = 0 \Longrightarrow U = TUT^{\dagger} \tag{1.1}$$

and T defined as

$$T = \begin{pmatrix} \ddots & & & & & & \\ \dots & 1 & 0 & 0 & \dots & & \\ & \dots & 1 & 0 & 0 & \dots & \\ & & \dots & 1 & 0 & 0 & \dots \\ & & & & & & \ddots \end{pmatrix} \tag{1.2}$$

namely the operator version of the permutation matrix with 1s on the subdiagonal.

In matrix representation this QCA with homogeneity hypotesis can be visualized as

$$\begin{pmatrix} \vdots \\ \psi_{t+1,-1} \\ \psi_{t+1,0} \\ \psi_{t+1,1} \\ \vdots \end{pmatrix} = \begin{pmatrix} \ddots & & & & & & \\ & \delta_{-r} & \dots & \delta_r & & & \\ & & \delta_{-r} & \dots & \delta_r & & \\ & & & \delta_{-r} & \dots & \delta_r & \\ & & & & & & \ddots \end{pmatrix} = \begin{pmatrix} \vdots \\ \psi_{t,-1} \\ \psi_{t,0} \\ \psi_{t,1} \\ \vdots \end{pmatrix} \tag{1.3}$$

Meyer proved [Mey96] that *every band r-diagonal unitary matrix U which commutes with one-step translation matrix T is also a translation matrix T^k for some $k \in \mathbb{Z}$, times a phase*, result also known by the name of *No-go Lemma*. This means that in this picture there is no nontrivial, homogeneous, local[2], scalar QCA– namely we cannot observe nontrivial dynamics or nearest-neighbour interaction.
Another QCA with the unitarity constraint relaxed in order to approximate unitarity was introduced by Grössing- Zeilinger, but turned out to manifest a strong undesired non-local behaviour.

After this first researches on the topic, Watrous [Wat95] introduced another model of one-dimensional QCA, which has the following definition:

Definition 1.2.2. *A one-dimensional QCA A is a quadruple (S_A, f_A, k, S), where S_A is a finite set of states (including a distinguished quiescent state called ε), f_A is a local transition function, k is an integer denoting the acceptance cell, and $S \subseteq S_A$ is a set of accepting states. A is composed by a two-way infinite sequence of cells, indexed by $i \in \mathbb{Z}$ and the neighbourhood of a cell is defined by the cell itself and its nearest neighbours.*

Watrous introduced also the idea of *configuration* for his QCA, namely

Definition 1.2.3. *A configuration of a one-dimensional QCA A is a map*

$$a : \mathbb{Z} \longrightarrow S_A \tag{1.4}$$

where $\forall n \in \mathbb{Z}$ $a(n)$ denotes the state of the cell indexed by n.

Given $\mathcal{C} = \mathcal{C}(A)$ the set of all configurations of A, any $a \in \mathcal{C}$ in which the cell indexed by k contains an element of S is called *accepting configuration*. Furthermore, a definition for the local transition rule is provided:

Definition 1.2.4. *The local transition rule f_A is a map:*

$$f_A : S^4 \longrightarrow \mathbb{C} \tag{1.5}$$

such that in particular

$$f_A(\varepsilon, \varepsilon, \varepsilon, s) = \begin{cases} 1 & \text{if } s = \varepsilon \\ 0 & \text{if } s \neq \varepsilon \end{cases} \tag{1.6}$$

describing the evolution of A

[2]Locality, intuitively the action of U for a single basis element is confined in its neighbourhood, is given by the band structure of U operator

As an example, let us consider that at some given time t A has a cell with a neighbourhood (s_1, s_2, s_3). For every state $s \in S_A$, s_2 will be updated to the state s with *amplitude* $f_A(s_1, s_2, s_3, s)$. With this definition, if A is in configuration $a \in \mathcal{C}$ at time t, the probability (amplitude) that we observe a transition $a \longrightarrow b$ at time $t + 1$ is

$$\prod_{n \in \mathbb{Z}} f_A(a(n-1), a(n), a(n+1), b(n)) \tag{1.7}$$

The revolutionary idea here is the fact that A evolves into many new configurations simultaneously and each new configuration has an associated *transition probability amplitude* and this means that A, if the evolution proceeds as if all of these transitions occur at the same time, after m steps will be in a *superposition configuration*. This idea allows each configuration to be seen as a vector in an $\ell^2(\mathcal{C})$ space, which is an Hilbert space with defined norm and scalar product.
Since however no notion of unitarity of the configuration states evolution is given, this definition also allows non-physical properties.
In the same paper Watrous provided also a definition for a *Partitioned QCA*

Definition 1.2.5. *A one-dimensional Partitioned QCA is a one-dimensional QCA in which each cell is partitioned into three subcells: a left subcell, a middle subcell and a right subcell. In this partitioned scheme also the set of states S_A is partitioned such that*

$$S_A = S_{A,l} \times S_{A,m} \times S_{A,r} \tag{1.8}$$

The updated state of any cell can now depend only upon the states of the left subcell of the right neighbour, the middle subcell of the cell itself and the right subcell of the left neighbour.
The local transition function is defined in a more complicated way. In fact, let us consider a $|S_A| \times |S_A|$ matrix Σ over $\mathbb{C}$, such that

$$\Sigma = \begin{pmatrix} \sigma(s_1, s_1) & \sigma(s_1, s_2) & \dots & \sigma(s_1, s_{|S_A|}) \\ \sigma(s_2, s_1) & \sigma(s_2, s_2) & \dots & \sigma(s_2, s_{|S_A|}) \\ \vdots & \vdots & \ddots & \vdots \\ \sigma(s_{|S_A|}, s_1) & \sigma(s_{|S_A|}, s_2) & \dots & \sigma(s_{|S_A|}, s_{|S_A|}) \end{pmatrix} \tag{1.9}$$

with $\sigma : S_A \times S_A \Longrightarrow \mathbb{C}$ such that

$$\sigma(\varepsilon, s) = \sigma(s, \varepsilon) = \begin{cases} 1 & \text{if } s = \varepsilon \\ 0 & \text{if } s \neq \varepsilon \end{cases} \tag{1.10}$$

and since now a state is tripartite, it can be represented with a triple, $s = (s_l, s_m, s_r)$

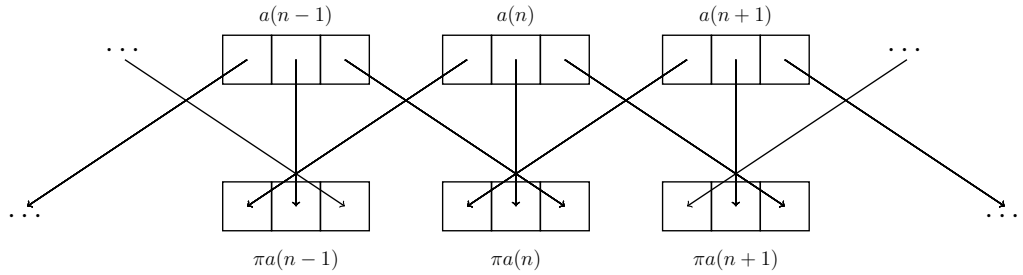

Figure 1.2: Partitioned Watrous scheme with permutation.

$$\begin{aligned} l(s) &= s_l \\ m(s) &= s_m \\ r(s) &= s_r \end{aligned} \tag{1.11}$$

and the transition function is now

$$\begin{aligned} f_A(a(n-1), a(n), a(n+1)) = \sigma((l(a(n+1)), m(a(n)), r(a(n-1))), s) = \\ = \sigma(\pi a(n), s) \end{aligned} \tag{1.12}$$

As we can see, the transition function for the partitioned scheme involves also a permutation π between subcells defined as

$$\pi a(n) := (l(a(n+1)), m(a(n)), r(a(n-1)) \tag{1.13}$$

It is possible to prove that this class of QCA is computationally universal, i.e. any quantum Turing machine can be efficiently simulated by a partitioned QCA. We conclude this paragraph providing the definition of quantum Turing machine for the sake of completeness [Wat95, BV97].

Definition 1.2.6. *A Quantum Turing Machine (QTM) is a quintuple* (K, Σ, μ, k, A)*, where* K *is a finite set of states,* Σ *is a finite tape alphabet including also a* b *(blank) symbol,* μ *is a local transition function – namely a map* $\mu : K \times \Sigma \times \Sigma \times K \times \{L, R\} \longrightarrow \mathbb{C}$ *with* $\{L, R\}$ *instructions for moving left or right the tape –, k is an integer denoting the acceptance tape square (the starting cell of the machine) and* $A \subseteq \Sigma$ *is a set of states for the acceptance tape square. The machine is also assumed to have an head for reading and writing on the tape and an indexing for the cells of the tape (indices* $\in \mathbb{Z}$*)*

3. AN ASIDE: C^* -ALGEBRAS

In the following section and throughout this work we will need to deal with technical tools a little bit different from the ones reviewed so far. In particular, we will work with the algebra of operators on a Hilbert space. In order to make sure that the structure of C^*-algebras is known by the reader, we will spend a few words on the topic.

Definition 1.3.1. *An ring is a set S equipped with two binary operations: addition and multiplication, such that the following axioms are respected:*

- *S is an abelian group under addition*
- *S is a monoid under multiplication (i.e. multiplication is associative and there exists the identity for multiplication in S)*
- *Multiplication is distributive with respect to addition*

If multiplication for S is commutative, S is a *commutative ring*.

Definition 1.3.2. *Let S be a ring with identity and 1 as identity for multiplication. A left $S-module$ M is an abelian group $(M,+)$ and an operation $\cdot : S \times M \longrightarrow M$ such that $\forall r, s$ in S and x, y in M:*

- $r \cdot (x+y) = r \cdot x + r \cdot y$
- $(r+s) \cdot x = r \cdot x + s \cdot x$
- $(rs) \cdot x = r \cdot (s \cdot x)$
- $1 \cdot x = x$

A left $S-module$ has the same properties, but the multiplicative operation is defined as $\cdot : M \times S \longrightarrow M$

Definition 1.3.3. *Let S be a commutative ring. An associative $S-algebra$ A is a ring that is also an $S-module$ such that the ring addition and the module addition coincide and the multiplication has the property, $\forall s \in S$ and $x, y \in A$*

$$s \cdot (xy) = (s \cdot x)y = x(s \cdot y) \tag{1.14}$$

We need some more definitions on Banach space and Banach algebras in order to be ready for the C^*- algebra definition.

Definition 1.3.4. *A normed space V is a vector space over K field (real or complex) on which a norm is defined, i.e. a function $v \mapsto \|v\|$ with the properties:*

- $\|v\| \geq 0 \, \forall v \in V$
- $\|v\| = 0 \iff v = 0$
- $\|kv\| = |k|\|v\| \, \forall k \in K$ *and* $v \in V$
- *The triangle inequality holds:* $\|v + w\| \leq \|v\| + \|w\| \, \forall v, w \in V$

Definition 1.3.5. *A metric induced by a norm is a function* $d : V \times V \longrightarrow \mathbb{R}$ *such that*

$$d(v, w) = \|v - w\| \tag{1.15}$$

Definition 1.3.6. *Given a metric space V (a set equipped with a metric on the set), a sequence of elements of V is a Cauchy sequence if* $\forall \varepsilon > 0$ *there exists a positive integer N such that* $\forall m, n > N$*,*

$$d(v_m, v_n) < \varepsilon.$$

Definition 1.3.7. *A metric space V is complete if every Cauchy sequence of points in V has a limit that is also in V*

Definition 1.3.8. *A Banach space is a normed space that is complete in the metric induced by its norm.*

Definition 1.3.9. *A Banach algebra is an associative algebra* A *over* $\mathbb{R}$ *or* $\mathbb{C}$ *such that it is at the same time also a Banach space. The norm must satisfy*

$$\forall v, w \in A : \|vw\| \leq \|v\|\|w\|. \tag{1.16}$$

We are ready to formalize C^*- algebra:

Definition 1.3.10. *A* C^*- *algebra* $\mathcal{A}$ *is a Banach algebra on* $\mathbb{C}$ *equipped with an adjoint map* $A \mapsto A^*$ *with the properties (in the following* $A, B \in \mathcal{A}$*)*

- $A^{**} = (A^*)^* = A$
- $(A + B)^* = A^* + B^*$
- $(AB)^* = B^* A^*$
- $(kA)^* = \bar{k} A^* \, \forall k \in \mathbb{C}$
- $\|A^* A\| = \|A\|\|A^*\|$

We will usually write also $A^\dagger := A^*$ for the adjoint of an operator on Hilbert spaces.

It can be useful also defining the concept of tensor product of C^*-algebras:

Definition 1.3.11. *Given a finite set J of indexes the tensor product of C^*-algebras $\mathcal{A} = \bigotimes_j \mathcal{A}_j$ $j \in J$ is the usual vector space tensor product of the operators in the algebra with product defined as*

$$\left(\bigotimes_j A_j\right)\left(\bigotimes_j B_j\right) = \bigotimes_j (A_j B_j) \tag{1.17}$$

and the adjoint

$$\left(\bigotimes_j A_j\right)^* = \bigotimes_j A_j^*. \tag{1.18}$$

The tensor product is formed by taking the tensor product of the underlying Hilbert spaces and the algebra generated by all tensor product operators.

The norm for the operators involved is defined in the following way:

Definition 1.3.12. *Given A in $\mathcal{A}$, we define the norm $\|A\|$ as*

$$\|A\| := \inf_\lambda \{\lambda > 0 | \exists B A^* A + B^* B = \lambda^2 I\} \tag{1.19}$$

with I identity operator.

4. REVERSIBLE QCA

The journey taken so far involved a philosophy based on the Schrödinger picture, namely the evolution of states living in an Hilbert space. A different approach comes from Schumacher and Werner [SW04], who proposed a definition of QCA based on evolution of observables, i.e. an approach based on Heisenberg picture. Before describing Schumacher and Werner's point of view we need to define the concept of *Reversible QCA*, since their study (and ours) is directed towards this class of QCA

The scenario in which this class of QCA live is the same intuitive scenario presented before: we have a lattice or array of cells labelled by an index $i \in \mathbb{Z}$ in the monodimensional case or by an integer vector $\vec{i} \in \mathbb{Z}^d$, with $d > 1$ dimension of the lattice. In each cell we consider an n-level quantum system with $n \geq 2$. A quantum system in Schumacher and Werner model is an observable algebra $\mathcal{A}_i$ isomorphic to the algebra of complex $n \times n$ matrices. They consider the *local algebra* given by the observable algebras over a finite subset of cells and call *Quasi-local algebra* their algebraic closure under the norm of the tensor product of their operators. They thus define an automation as an homomorfism of quasi-local algebras on a defined neighbourhood scheme.

Definition 1.4.1 (Reversible QCA)**.** *A reversible QCA with neighbourhood scheme $\mathcal{N} \subset \mathbb{Z}^d$ is an homomorfism $T : \mathcal{A}(\mathbb{Z}^d) \longrightarrow \mathcal{A}(\mathbb{Z}^d)$ of the quasi-local algebra, which commutes with the translation operator on the lattice and satisfies the locality condition $T(\mathcal{A}(\Lambda)) \subset \mathcal{A}(\Lambda + \mathcal{N})$ for every finite set $\Lambda \subset \mathbb{Z}^d$. The local transition rule of the reversible QCA is the homomorfism $T_0 : \mathcal{A}_0 \longrightarrow \mathcal{A}(\mathcal{N})$.*

The time evolution in this scenario follows the Heisenberg picture, intended as measuring an observable $A \in \mathcal{A}(\Lambda)$ at time $t + 1$ is equivalent to measuring $T(A)$ at time t.

It can be useful decomposing reversible QCAs into local unitary operators. To this purpose, some partitioning schemes were proposed, such as the Margolus generalized partition scheme [SW04], whose main problem is the impossibility to implement the shift operator through local unitaries in dimensions higher than one [Wie08, Far20, ANW07].
However, it has been proposed a general recipe which allows to obtain the desidered partition despite introducing an additional QCA [ANW09, Far20]. It is valid both for qudit and Fermionic and Bosonic systems [FS14].
Given an automaton A with dynamics U_A, the main idea is considering its identical copy with inverse dynamics U_B^{-1} and taking the QCA with dynamics $U_A \otimes U_B^{-1}$. It is then defined the *global swap operator*, which swaps the system at each site n of the automaton A with the one at the same site of the automaton B. We can thus write

$$\begin{aligned} U_A U_B^{-1} &= S_{AB} U_B S_{AB} U_B^{-1} = \\ &= \left(\prod_m S_m\right) U_B \left(\prod_n S_n\right) U_B^{-1} \\ &= \left(\prod_m S_m\right) \left(\prod_n U_B S_n U_B^\dagger\right) \end{aligned} \tag{1.20}$$

where S_n is a local unitary for each site n and in particular this is true also for $U_B S_n U_B^\dagger$ [ANW09]. Thus we can implement in parallel both the S_m and the $U_B S_n U_B^\dagger$ and write the QCA composed by A and B using only local unitaries.

5. FERMIONIC QCA

The motivation behind defining Fermionic QCA is bounded to what we have presented so far: we are looking for an *algorithm* capable of describing quantum phenomena and in particular quantum field theory.

The objective of re-derive QFT from informational principle and in particular exploiting QCA is surely challenging. There are many problems related, starting from the fact that any QCA discretization breaks Lorentz covariance, i.e. the laws of physics remain the same in all inertial frames. Some clever proposal on how to solve this problem have been the object of recent papers [BDP16b, AFF14]. Furthermore, such a reductionistic descrete approach requires a lot of work (also in term of calculations) to be done before showing, as emergent phenomena, results comparable to the ones already known. We also need to formulate models that hopefully can *predict* and not only *emulate* results and even if many results have been reached, the theory is still at its beginnings and many verifications must be done. Moreover, on the epistemological side, we must consider that our yardstick is QFT, an effective theory which has its own restricted field of validity. In other words, we are far from having *the big picture* clear even when we talk about QFT. Anyway is worth exploring this path and, as we will see in more details, some promising results are already on the table.
Now that we have introduced the topic, we need to present Fermions and in particular, since we are talking about QCA in Heisenberg picture, we need to describe in depth the Fermionic algebra.

6. Fermionic Algebra and CAR

Let us consider a set of operators $\{a_i\}$ acting on a finite-dimensional Hilbert space $\mathcal{H}$. Defining the anticommutator as

$$\{A, B\} := AB + BA \tag{1.21}$$

if the relation

$$\{a_i, a_j^\dagger\} = \delta_{ij} I;\ \{a_i, a_j\} = 0 \tag{1.22}$$

holds, then the set of operators satisfies the Canonical Anticommutation Relations (CAR).

Given this definition, we can ask ourselves what properties these operators have. The first one is thee following

Property 1.6.1. *The operators $a_i^\dagger a_i$ are positive Hermitian with eigenvalues 0 and 1*

Proof. Let us evaluate

$$\begin{aligned}(a_j^\dagger a_j)^2 &= a_j^\dagger a_j a_j^\dagger a_j = \\ &= (\{a_j^\dagger, a_j\} - a_j a_j^\dagger) a_j^\dagger a_j = \\ &= a_j^\dagger a_j - (a_j^\dagger)^2 a_j^2\end{aligned} \tag{1.23}$$

but from the second of (1.22) we have $a_j^2 = 0$. Thus $(a_j^\dagger a_j)^2 = a_j^\dagger a_j$, which means that its eigenvalues are 0 or 1. Furthermore we notice that it is trivial to verify that it is Hermitian, instead for the positivity we notice that $\langle v|a_j^\dagger a_j v\rangle = \langle v a_j|a_j v\rangle \geq 0$ for all $v \in \mathcal{H}$ □

Property 1.6.2. *a_j are lowering operators*

Proof. Let $|\psi\rangle$ a normalized eigenstate of $a_j^\dagger a_j$ with eigenvalue 1. We want to show that $a_j|\psi\rangle$ is a normalized eigenstate of $a_j^\dagger a_j$ with eigenvalue 0.
But this is straightforward, in fact

$$a_j^\dagger a_j a_j|\psi\rangle = a_j^\dagger (a_j)^2|\psi\rangle = 0 \tag{1.24}$$

and for the normalization, $\langle\psi|a_j^\dagger a_j|\psi\rangle$

If $|\psi\rangle$ is a normalized eigenstate of $a_j^\dagger a_j$ with eigenvalue 0, then (1.24) holds again.

□

The fact that property 1.6.2 holds and in particular $(a_j)^2 = 0$ tell us that the operators we are working with respect the *Pauli's exclusion principle*, which characterizes Fermions.

Property 1.6.3. *$a_j^\dagger$ are raising operators*

Proof. Let $|\psi\rangle$ a normalized eigenstate of $a_j^\dagger a_j$ with eigenvalue 0. We want to show that $a_j^\dagger|\psi\rangle$ is a normalized eigenstate of $a_j^\dagger a_j$ with eigenvalue 1.
We observe that

$$\langle\psi|a_j a_j^\dagger|\psi\rangle = -\langle\psi|a_j^\dagger a_j|\psi\rangle + \langle\psi|\psi\rangle \tag{1.25}$$

but $a_j^\dagger a_j|\psi\rangle = 0$, thus we have proved normalization. We also have to show that $a_j^\dagger|\psi\rangle$ is eigenvector of $a_j^\dagger a_j$ with eigenvalue 1.

$$\begin{aligned}a_j^\dagger a_j a_j^\dagger|\psi\rangle &= a_j^\dagger (I - a_j^\dagger a_j)|\psi\rangle = \\ &= a_j^\dagger|\psi\rangle\end{aligned} \tag{1.26}$$

If $|\psi\rangle$ is a normalized eigenstate of $a_j^\dagger a_j$ with eigenvalue 1, since $(a_j^\dagger)^2 = (a_j^2)^\dagger$, we have instead

$$a_j^\dagger|\psi\rangle = a_j^\dagger a_j^\dagger a_j|\psi\rangle = (a_j^\dagger)^2 a_j|\psi\rangle = 0 \tag{1.27}$$

□

Property 1.6.4. *$\{a_j^\dagger a_j\}_j$ forms a set of mutually commuting observables*

Proof It can be proven applying iteratively the CAR. □

Property 1.6.5. *There exists a common eigenbasis of the $\{a_j^\dagger a_j\}_j$ operators*

proof. Since the $\{a_j^\dagger a_j\}_j$ are a set of mutually commuting observables the property holds. □

The common eigenspace of operators $a_j^\dagger a_j$ with eigenvalue 0 needs not to be one-dimensional.
Given a state $|\mathbf{0}\rangle$ in this eigenspace, it is straightforward defining an orthonormal basis:

$$|\mathbf{b}\rangle = (a_1^\dagger)^{b_1} \dots (a_n^\dagger)^{b_n}|\mathbf{0}\rangle \tag{1.28}$$

for any tuple of the form $\mathbf{b} := (b_1, ..., b_n)$.
We also observe that what we have seen so far reflects the behaviour of the CAR, in fact if $b_j = 0$, then $b_j|\mathbf{b}\rangle = 0$ and if we have $b_j = 1$ and we define $\mathbf{b}'$ as the vector equal to $\mathbf{b}$ except for the jth entry changed to 0, we have

$$a_j|\mathbf{b}\rangle = -(-1)^{s_\mathbf{b}^j}|\mathbf{b}'\rangle \tag{1.29}$$

where $s_\mathbf{b}^j := \sum_{k=1}^{j-1} b_k$.
For $a_j^\dagger$ instead we have $a_j^\dagger|\mathbf{b}\rangle = 0$ if $b_j = 0$, while $a_j^\dagger|\mathbf{b}\rangle = -(-1)^{s_\mathbf{b}^j}|\mathbf{b}'\rangle$ when $b_j = 0$ and $\mathbf{b}'$ is the vector where the jth entry is changed to 1.
So far we have seen the action of the raising and lowering operators for the subspace spanned by the states of the form $|\mathbf{b}\rangle$. What about the action on the orthogonal complement? Let us call B the space spanned by $\{|\mathbf{b}\rangle\}_{\mathbf{b}\in\{0,1\}^n}$ and $B^\perp$ its orthogonal complement.
Since B is closed under the action of a_j and $a_j^\dagger$, then also $B^\perp$ is closed under the action of the same operators. Thus $a_j|\mathbf{b}^\perp\rangle$ and $a_j^\dagger|\mathbf{b}^\perp\rangle$ with $|\mathbf{b}^\perp\rangle$ in $B^\perp$ are also in $B^\perp$.
We shall now consider the operators $\tilde{a}_j$, restriction of a_j to $B^\perp$. If $B^\perp$ is not the trivial space, the $\tilde{a}_j$s respect the CAR and identify a 2^n-dimensional subspace of

$B^{\perp 3}$. Since by our initial hypotesis $\mathcal{H}$ is finite dimensional, by iterating this procedure we obtain a finite number of 2^n-dimensional subspaces, which at the end of the procedure identify an orthonormal basis $|\mathbf{b}, k\rangle$, where the index k identifies the subspace of $\mathcal{H}$ invariant under the action of raising and lowering operators.
In particular the action of a_j and $a_j^\dagger$ in this representation, which involves a total space $\mathbb{C}^{2^n} \otimes \mathbb{C}^d$, is trivial on the $\mathbb{C}^d$ subspace, while acts as described before on the other subspace. This representation is also called *occupation number representation* for the Fermi algebra a_j [Nie05].

7. TECHNICAL BACKGROUND FOR FERMIONIC QCAS

In the previous section, we have presented the main properties of the Fermionic algebra and the CARs, now we need to describe the general background, i.e. the hypothesis we need for providing a complete explanation of the class of Fermionic QCA we will work with. By making these hypothesis we are imposing precise constraints to our algorithm.

1.7.1 Homogeneity

The first constraint we are imposing is, unsurprisingly, homogeneity, which has been required also for other examples of QCA we have studied so far. The principle of homogeneity is, roughly speaking, a principle of undistinguishability of the cells of the QCA's lattice. We have no reason to consider privileged cells with respect to others. Following [Per20b], we define an *Homogeneous update rule*:

Definition 1.7.1 (Homogeneous update rule)**.** *Every two memory cells cannot be distinguished by the way in which the rule updates their state, unless one establishes a reference cell, which can be any.*

The update rule is thus unaware of cell address in the lattice. So far it seems that we have formulated only a *spatial* homogeneity principle, but with definition 1.7.1 we actually mean also a *time* homogeneity principle, i.e. the update rule is also independent of the time step of the evolution of the QCA.

1.7.2 Reversibility

We will now specify what we intend as reversibility.
First of all, we have an *operational invertibility*,

[3] Analogous for $a_j^\dagger$

Definition 1.7.2 (Operational invertibility)**.** *A transformation is operationally invertible if there exists another one that inverts its effects.*

We remark that this principle works theoretically and mathematically, but a physical law cannot be *in practice* inverted [Per20b]. However, we have also a notion of *invertibility*

Definition 1.7.3. *We call invertibility the possibility of using the knowledge of the state of a cell or a group of cells to mathematically reconstruct the state of another group of cells at an earlier evolution step.*

Since in physics the *state* of a system is often determinable, this definition of invertibility may be useful. Unfortunately, this is not our case [Per20b, DY96]. Nevertheless, we can provide a notion of *reversibility*

Definition 1.7.4. *An evolution is reversible if it is equivalent to its inverse except for operationally reversible local transformations.*

In order to show the importance of this definition, let us suppose that we have an invertible evolution rule, $\mathcal{A}$, with mathematical inverse $\mathcal{A}^{-1}$ such that they are not reversible in the sense of the definition 1.7.4. How can we build a reversible rule starting from $\mathcal{A}$ and $\mathcal{A}^{-1}$? One can consider a two layers memory array, such that each cell can be identified by a couple (a, i), with $a \in \mathbb{N}$ address of the cell in its layer and $i \in \{0, 1\}$ address of the layer. On this geometry we build the rule $\mathcal{A} \otimes \mathcal{A}^{-1}$. But now this rule is in accordance with definition 1.7.4, since it is equivalent to its inverse, namely $\mathcal{A}^{-1} \otimes \mathcal{A}$ modulo a local swap between $(a, 0)$ and $(a, 1)$, $\forall a \in \mathbb{N}$.
We can thus add reversibility to the requirements for our automata.

1.7.3 Locality

Locality is a property that has been subliminally considered also in the previous section, but has to be detailed a little more. The notion of locality is bound to the geometry of the systems we are considering, in particular to the notion of *close system*, where defining the *closeness* needs to have an underlying geometry. Since so far we have talked about lattices and cells containing *information* at a very fundamental level, we need to explicit at least a metric or a notion of distance on the lattice.

Definition 1.7.5 (Neighbours)**.** *Two cells a and b are neighbours if the update rule that changes a at step t affects b at step $t + 1$.*

The definition above can be generalized to a notion of distance defining the distance d between two cells as the number of steps required by the update rule to affect one of them after the other has been changed.
This is undoubtedly a useful operative way to define a distance, but we can provide a better definition through the identification of a structure of group on the lattice, which brings us to the identification of the lattice with a *Cayley graph*, i.e. the graphical representation of a group.

Definition 1.7.6. *A group is a set G equipped with a binary operation (let us call it $\cdot$) such that for all a, b, c in G*

- $(a \cdot b) \cdot c = a \cdot (b \cdot c)$. *This property is called associativity*
- *There exists e in G such that $e \cdot a = a \cdot e = a$, called identity*
- *Given $a \in G$ there exists $a' \in G$ such that $a' \cdot a = a \cdot a' = e$. a' is called inverse*

Definition 1.7.7. *A graph is a pair (V, E), where V is a set of vertices (nodes or points) and E is a set of edges (lines or arcs), pairing vertices. A directed graph is a graph in which edges have orientation. Orientation is defined through an incidence function $\phi : E \longrightarrow V^2$ which maps every edge to an ordered pair of vertices. With little abuse of notation we will often refer to E as the set $\phi(E)$, identifying edges with ordered pairs of vertices $\in V^2$. Furthermore, a graph is edge-colored if a label (color) is assigned to the edges of the graph such that no vertex is incident to two edges of the same color.*

Definition 1.7.8. *Let G be a group and S the set of generators of G, namely a subset of G such that each element of G can be expressed as a combination under the group operation of elements of S, the Cayley Graph of G, (V, E) with respect to the set S is an edge-colored directed graph with the following properties:*

- *A vertex is assigned to each element of G*
- *A color c_s is assigned to each element of S*
- *$\forall g \in G$, $\forall s \in S$ there is a directed edge of color c_s from the vertex assigned to g to the one assigned to $g \cdot s$. If $s = s^{-1}$ then the edges are left undirected. This happens also when the set of generators is symmetric, namely $S \equiv S^{-1}$ and S does not contain the identity.*

Connecting these definitions with our preliminary notion of distance, in our case the vertices set V is identified with the group G and the edge set E contains

all pairs (a, b) such that if a is changed at step t, then b can be affected by a change at step $t + 1$.
We have also to take into account homogeneity of the update rule: all vertices are treated the same by the rule. Thus one can choose a reference cell e and identify the set of generators as the set of its neighbour cells, $S := \{h_i\}_i$. We can also use this procedure to identify the neighbour for each $g \in G$ and rewriting the set of edges as

$$E = \{(g, g')|g \in G,\ g' = gh_i, i \in S\} \subseteq G^2. \tag{1.30}$$

We will also use the notion of relators R, namely a set of group elements of the form $h_{i_1}^{s_1} h_{i_2}^{s_2} ... h_{i_k}^{s_k}$ with $s_k \in \{+1, -1\}$ which are set equal to the identity of the group e.
With this construction we are now ready to define a notion of locality. Let $p := (g_1, g_2, ..., g_n)$ be a path in G, i.e. a collection of vertices connected with edges $(g_i, g_{i'})$ that connects g_1 to g_n. Calling $g_1 = a$ and $g_n = b$ and considering the set $\pi(a, b)$ of all the possible paths from a to b, the distance on the graph is defined as

$$d(a, b) := \min_{\pi(a,b)} \sum_{i=1}^{n-1} d(g_i, g_{i+1}) \tag{1.31}$$

with $d(g_i, g_{i+1})$ distance between neighbours in the sense of the definition 1.7.5.
We also require that a must have a neighbourhood of bounded size. That is because otherwise we would have arbitrarily large groups of connected cells, a condition not compatible with a reasonable notion of locality.
Furthermore, we need something more than homogeneity and locality in the sense that a property holds pointwise and only local experiments are sufficient to give enough information about that property. We are not just verifying a property, we are actually specifying an update rule which makes evolve a theoretically infinite graph. This means that we also require that every closed paths can be decomposed into elementary closed paths with an uniformly bounded lenght, i.e. there exists an $M \in \mathbb{R}$ such that given l_{ii} the set of lengths of the closed paths in which the larger one is decomposed, $l_i \leq M\ \forall i$. Thus the important thing is that we have uniform boundness of the elementary paths. All these observations are condensed in the following definition [Per20b, Per20a]:

Definition 1.7.9 (Local Update Rule)**.** *The size of the neighbourhood of every cell is uniformly bounded, and closed paths on the graph of the update rule are decomposable into elementary closed paths of uniformly bounded length.*

The concepts presented here can be used to provide the definition of Cellular Automaton intended in the next sections [Per20a]:

Definition 1.7.10 (Cellular Automaton)**.** *A memory array with homogeneous, reversible and local update rule is a Cellular Automaton (CA).*

and in particular we can define a Fermionic QCA as

Definition 1.7.11. *A Fermionic QCA is a CA in the sense of definition 1.7.10, such that the memory array is made of local Fermionic modes (LFMs).*

8. QCA AND QUANTUM WALKS

Defining Fermionic QCA, namely QCA with a memory array made of LFMs, means working with Fermionic operators (presented in Sec. 1.6) in Heisenberg picture. From the perspective of QFT, this also means that we are working in *second quantization*, privileging fields over states and in fact working with an arbitrary number of Fermionic particles.
The QCA formalism developed in the previous section however, with some slight modifications, can be applied also to states of single particles, in a *first quantization* framework. In this case we speak about *Quantum Walks* (QW).
In order to be a bit more formal, we go back to Fermionic QCA and define the reversible evolution for the QCA as a reversible map $\mathcal{A}$, automorphism of the Fermionic algebra. The most general $\mathcal{A}$, is a polynomial in the Fermionic field operators a_j. A common constraint on this map, is the fact that it is *number preserving*, namely it contains the same number of operators a_j and $a_j^\dagger$ in order to preserve the number of particles in action.
Now we introduce a further crucial constraint: $\mathcal{A}$ must be linear, i.e. its action must be representable through a linear combination of matrices associated to each generator $h_i \in S$,

$$\mathcal{A}[a_j(g)] = \sum_{h_i \in S, j'} W_{jj'}(h_i) a_j(g h_i^{-1}) \tag{1.32}$$

Where $W(h_i)$ is called *transition matrix* with elements $W_{jj'}(h_i)$ corresponding to the generator $h_i \in S$, and the notation $a_j(g)$ indicates that the field operator belongs to the site labeled as g.
At this point we notice that, since $\mathcal{A}$ is a linear map and the matrices are representation of linear applications, the transition matrices contain all the information about the dynamics of the system. We can state that, if we exploit the framework of first quantization, the transition matrices realize the evolution of states of a single excitation. In formulas, if at step t we have a single excitation in the state

$$|a(t)\rangle = \sum_{g \in G,\, j} \phi_j(g,t) |g\rangle |j\rangle, \tag{1.33}$$

where j indicates the index associated to a Fermionic mode, it takes into account the internal structure of the cell, at time step $t+1$ the state becomes

$$|a(t+1)\rangle = \sum_{g\in G, j, j', h_i \in S} W^*_{jj'}(h_i)\phi_j(g,t)|gh_i^{-1}\rangle|j'\rangle \tag{1.34}$$

where we used $W^*_{j,j'}(h_i)$ instead of $W_{j,j'}(h_i)$ because we are interested in the evolution (1.32) for $a_j^\dagger$, since Fermionic states are defined as in (1.28).
Looking at the evolved coefficients, we obtain

$$\phi_s(g,t+1) = \sum_{j', h_i \in S} W^*_{jj'}(h_i)\phi_j(gh_i^{-1},t) \tag{1.35}$$

in particular multiple excitations evolve independently and $\phi_j(g,t)$ can be interpreted as a "single particle" wavefunction in the Hilbert space $\ell^2(G)\otimes\mathcal{C}^n$, with n number of Fermionic modes. The evolution rule in first quantization can be thus defined as

$$W = \sum_{h_i \in S} T_{h_i} \otimes W(h_i) \tag{1.36}$$

with T_{h_i} translation operator in direction h_i, also known as *right-regular representation* of the group G, it acts on the $\ell^2(G)$ part of the system with the rule

$$T_{h_i}|g\rangle = |gh_i^{-1}\rangle \tag{1.37}$$

and $W(h_i)$ transition matrix with elements $W_{jj'}(h_i)$. The evolution rule (1.36) is the *Quantum Walk* we anticipated at the beginning of the section. Its name is reminiscent of the classical *Random Walk*, with the main difference that this acts on quantum systems. We can recognize, as in the classical case, the operator acting on the *walker*, represented by T_{h_i}, and the operator acting on the *coin*, i.e. the transition matrix.

9. ISOTROPY

The introduction of the transition matrices in the previous section, allows us to introduce another technical principle we will exploit in the next Chapters, the notion of *isotropy*.
In Physics the word *isotropy* is associated to the equivalence of every direction in space. Since we are setting our framework in a Cayley graph as topological background, we need to translate this principle in precise terms to our context.
The isotropy requirement in our case means that every generator S must be equivalent for our graph. In other words, if we permute the labels for elements in S, we

obtain another generator set S for which the physical laws are not changed. It can be interpreted as a sort of *rotational invariance* for the Cayley graph. In formal terms

Definition 1.9.1 (L-isotropic QW)**.** *Let L be a group of automorphism of the Cayley graph (G, S), with $l \in L$ such that $l : G \longrightarrow G$ and l acts as permutations λ of edges of the graph, namely for $g \in G$ with $g = h_{i_1}^{s_1} h_{i_2}^{s_2} ... h_{i_k}^{s_k}$, $l(g) = \lambda(h_{i_1}^{s_1})\lambda(h_{i_2}^{s_2})...\lambda(h_{i_k}^{s_k})$.*
We define the QW on graph (G, E) L-isotropic if there exists a unitary injective operator $U : L \longrightarrow \mathcal{U}(\mathbb{C}^d)$ ($\mathcal{U}(\mathbb{C}^d)$ is the set of unitary operators over $\mathbb{C}^d$) such that

$$W_{l(h_i)} = U_l W_{h_i} U_l^{-1} \tag{1.38}$$

for $l \in L$, $W_{l(h_i)} \neq W_{h_i}$. The group L acts transitively on S, i.e. S is non-empty and $\forall h_{i_1}, h_{i_2} \in S \, \exists \, l \in L$ such that $l(h_{i_1}) = h_{i_2}$.

We can now complete our setting defining

Definition 1.9.2 (Isotropic Update Rule)**.** *A QW is isotropic if it is L-isotropic in the sense of the definition 1.9.1 for some group L of automorphisms of the graph (G, S).*

Having presented all the properties of our scenario, we are ready to provide the description of the QCA and QW object of our study.

CHAPTER 2

WEYL AND DIRAC QCA: FREE EVOLUTION

In this chapter we will present the two Fermionic QCA of our interest: Weyl and Dirac Cellular Automaton. Their names are justified by the fact that, as we will see, their relativistic limit brings to the dynamics described by Weyl and Dirac equations.
As stated in the previous chapter, these QCA involve identical Fermionic quantum systems. We will start from the description of the quantum systems in each cell, which can be seen as finite-dimensional vectors of Fermionic modes:

$$a(g) = \begin{pmatrix} a_1(x) \\ a_2(x) \\ \vdots \\ a_n(x) \end{pmatrix} \tag{2.1}$$

where their dimension is denoted by n and they live on a d-dimensional lattice. The hypotesis we will consider for our automaton are the ones discussed before: unitarity, homogeneity, locality, linearity and discrete isotropy.

Reversibility actually is replaced with a constraint which is necessary for reversibility, but not sufficient, that is the unitarity of the evolution rule. Defining as $W(h_i)$ the transition matrices in direction $h_i \in S$, this means

$$\sum_{h_i \in S} W_{h_i}^\dagger W_{h_i} = \sum_{h_i \in S} W_{h_i} W_{h_i}^\dagger = I \tag{2.2}$$

and

$$\sum_{h_{i_1} h_{i_2}^{-1} = h_{i_3}} W_{h_{i_2}}^\dagger W_{h_{i_1}} = \sum_{h_{i_1} h_{i_2}^{-1} = h_{i_3}} W_{h_{i_1}} W_{h_{i_2}}^\dagger = 0. \tag{2.3}$$

Furthermore, a little clarification on the group G (and the generators set S): it has to be intended as an abelian group under the sum as the group composition. Thus the second of the previous equations can be rewritten as

$$\sum_{\mathbf{h}_{i_1}-\mathbf{h}_{i_2}=\mathbf{h}_{i_3}} W^{\dagger}_{\mathbf{h}_{i_2}} W_{\mathbf{h}_{i_1}} = \sum_{\mathbf{h}_{i_1}-\mathbf{h}_{i_2}=\mathbf{h}_{i_3}} W_{\mathbf{h}_{i_1}} W^{\dagger}_{\mathbf{h}_{i_2}} = 0. \tag{2.4}$$

and, in general, $\mathbf{h}_i^{-1} = -\mathbf{h}_i$, where we used the boldfaced vector notation $\mathbf{h}_i$ for elements of S, since they are intended as d-dimensional vectors on the lattice (a similar notation is extended also to elements of G).
Lastly, a remark on the set S: we exclude the identity e from S, since it is physically related to the possibility of self interaction for each system, which is an assumption we do not intend to make at this level. Moreover, it can be useful to split S into two subsets, S_+ and S_-, where S_- is the set of inverses of the elements in S_+.

1. AN ASIDE: ELEMENTS OF GROUP THEORY

Before proceeding further it is important to give some basic definitions of group theory. In the previous chapter we have used them intuitively, but in this chapter we will use them more consistently. We start introducing the concept of *Group action*:

Definition 2.1.1 (Left group action)**.** *Given a group L with identity denoted with e and a set G (it can be another group), the (left) group action λ of L on G, is a function*

$$\begin{aligned} &\lambda : L \times G \longrightarrow G \\ &\lambda(l, g) \mapsto l \cdot g (= lg = l(g)) \end{aligned} \tag{2.5}$$

that satisfies the axioms, for $l, l' \in L$ and $g \in G$

- $e \cdot g = g$ *(Identity)*
- $l'(l \cdot g) = (l'l) \cdot g$ *(Compatibility)*

There is also a *Right action*, which has identical definition except for the order in which the product ll' acts on g in the *compatibility axiom*.

Since for a fixed $l \in L$ the function $\tilde{\lambda} : G \longrightarrow G$ such that $\tilde{\lambda}(g) = l \cdot g$ is a bijection, an equivalent definition is

Definition 2.1.2 (Group Action)**.** *The action of a group L on a set (or another group) G is a group of homomorphisms from L into the group of all bijections from G to itself.*

We now need two more definitions which will be taken from granted

Definition 2.1.3 (Transitive action)**.** *The action of L on G is transitive if G is non empty and $\forall g, g' \in G\, \exists\, l \in L |\, l \cdot g = g'$.*

Definition 2.1.4 (Faithful action)**.** *The action of L on G is faithful if $\forall l, l' \in L\, \exists\, g \in G | l \cdot g \neq l' \cdot g$.*

It is also important the concept of *orbit* and *stabilizer*.

Definition 2.1.5 (Orbit)**.** *Let L be a group acting on a set G. The orbit of an element $g \in G$ is the set:*

$$L \cdot g := \{l \cdot g | g \in G\} \tag{2.6}$$

that is the set of elements in G that are images through the action of L on the element $g \in G$.

thus the action of a group is transitive if and only if it has a unique orbit.

Definition 2.1.6 (Stabilizer)**.** *Given L, G and $g \in G$ as in the previous definitions, the stabilizer or isotropy group is the set*

$$L_g := \{l \in L | l \cdot g = g\}. \tag{2.7}$$

The action of L on G is said to be free if and only if all the stabilizers are the singleton $\{e\}$.

2. WEYL QW AND QCA

Starting from the hypothesis discussed in Sec. 1.7, we define our automaton. Unitarity and homogeneity bring us to the following unitary operator over the Hilbert space $\ell^2(G) \otimes \mathbb{C}^d$:

$$W = \sum_{\mathbf{h}_i \in S} T_{\mathbf{h}_i} \otimes W_{\mathbf{h}_i}. \tag{2.8}$$

[DEP19] which is clearly of the form (1.36), with $T_{\mathbf{h}_i}$ translation operator over the lattice considered. The unitarity is granted if and only if equations (2.2) and (2.4) hold. We notice that we have not imposed any constraint on the geometry of the lattice. This problem will be faced further on.
For now let us put our magnifying glass on the translation operator. In Dirac *ket* notation, it can be considered as

$$T_{\mathbf{h}_i} := \sum_{g \in G} |\mathbf{g} + \mathbf{h}_i\rangle\langle \mathbf{g}|. \tag{2.9}$$

We now consider the set S and its elements. They are generally linearly dependent, thus it can be useful taking all the subsets D_k of linearly independent elements of S:

$$D_k := \{\mathbf{h}_{i_1}, \mathbf{h}_{i_2}, ..., \mathbf{h}_{i_d}\} \tag{2.10}$$

where d is the dimension of the lattice. We can also define the duals subsets $\tilde{D}_k$

$$\tilde{D}_k := \{\tilde{\mathbf{h}}_1^{(\mathbf{k})}, \tilde{\mathbf{h}}_2^{(\mathbf{k})}, ..., \tilde{\mathbf{h}}_d^{(\mathbf{k})}\} \tag{2.11}$$

such that

$$\tilde{\mathbf{h}}_j^{(\mathbf{k})} \cdot \mathbf{h}_{i_s} = \delta_{j,s} \tag{2.12}$$

and the set

$$\tilde{D} := \bigcup_k \tilde{D}_k. \tag{2.13}$$

This allows us to define the *Brillouin zone*:

Definition 2.2.1 (Brillouin Zone)**.** *We call Brillouin zone the polytope $B \subseteq \mathbb{R}^d$ of the form*

$$B = \bigcap_{\tilde{\boldsymbol{h}} \in \tilde{D}} \{\boldsymbol{k} \in \mathbb{R}^d | -\pi|\tilde{\boldsymbol{h}}|^2 \leq \boldsymbol{k} \cdot \tilde{\boldsymbol{h}} \leq \pi|\tilde{\boldsymbol{h}}|^2\}. \tag{2.14}$$

We notice that (2.9) is unitary[1] and is the representation of an abelian group since G is abelian and

$$T_{\mathbf{h}_i} T_{\mathbf{h}_j} = \left(\sum_{\mathbf{g} \in G} |\mathbf{g} + \mathbf{h}_i\rangle\langle \mathbf{g}|\right) \left(\sum_{\mathbf{g}' \in G} |\mathbf{g}' + \mathbf{h}_j\rangle\langle \mathbf{g}'|\right) = \sum_{\mathbf{g}' \in G} |\mathbf{g}' + \mathbf{h}_i + \mathbf{h}_j\rangle\langle \mathbf{g}'| = T_{\mathbf{h}_i + \mathbf{h}_j} \tag{2.15}$$

and

$$T_{\mathbf{h}_i} T_{-\mathbf{h}_i} = T_{\mathbf{0}} = I_G \tag{2.16}$$

which respects the definition of representation of a group on an Hilbert space $\mathcal{H}$. We have also $[W, T_{\mathbf{h}_i} \otimes I_d] = 0$. We observe that $T_{\mathbf{h}_i}$ is also irreducible, thus is an irreps of an abelian group and thus is monodimensional. This implies

[1] It is straightforward that $T_{\mathbf{h}_i}^\dagger T_{\mathbf{h}_i} = T_{\mathbf{h}_i} T_{\mathbf{h}_i}^\dagger = I_G$

$$T_{\mathbf{h}_i}|\mathbf{k}\rangle := e^{-i\mathbf{k}\cdot\mathbf{h}_i}|\mathbf{k}\rangle \tag{2.17}$$

with $\{|\mathbf{k}\rangle\}$ eigenvectors. A simple check tells us that

$$|\mathbf{k}\rangle := \frac{1}{\sqrt{|B|}}\sum_{\mathbf{g}\in G} e^{i\mathbf{k}\cdot\mathbf{g}}|\mathbf{g}\rangle \tag{2.18}$$

which is the discrete Fourier transform for the basis $\{|\mathbf{g}\rangle\}$, while the antitransform is defined as

$$|\mathbf{g}\rangle = \frac{1}{\sqrt{|B|}}\int_B d\mathbf{k}\, e^{-i\mathbf{k}\cdot\mathbf{g}}|\mathbf{k}\rangle \tag{2.19}$$

with the normalization condition

$$\langle\mathbf{k}|\mathbf{k}'\rangle = \frac{1}{|B|}\sum_{\mathbf{g}\in G} e^{(\mathbf{k}-\mathbf{k}')\cdot g} = \delta_{2\pi}(\mathbf{k}-\mathbf{k}'). \tag{2.20}$$

These observations allow us to block- diagonalize W:

$$W = \int_B d\mathbf{k}\,|\mathbf{k}\rangle\langle\mathbf{k}|\otimes W(\mathbf{k}) \tag{2.21}$$

with $W(\mathbf{k})$ Fourier transform of $W(\mathbf{h}_i)$

$$W(\mathbf{k}) = \sum_{\mathbf{h}_i} e^{ik\cdot\mathbf{h}_i} W(\mathbf{h}_i). \tag{2.22}$$

We can now investigate which lattices are ammitted by our assumption and their dimensionality. We will sum up the arguments contained in [DEP17]. A crucial assumption for the geometry of the lattice is the isotropy assumption (cfr. sect. 1.9), which involves the action of a group L of automorphisms on the Cayley graph. We remark that this action is transitive on S, in particular on S_+, and it is extended by linearity on all $\mathbb{Z}^d$. In [DEP17] it is proved that L *is isomorphic to a finite permutation group acting transitively on* S_+ *when all generators have the same order*[2], thus L can be treated as a group of permutations.
Let us consider M as a representation on integers of L, $M_l M_f = M_{lf}$, for $l, f \in L$. if a matrix P is defined as

$$P := \sum_{l\in L} M_l^\top M_l \tag{2.23}$$

[2]The *order* of a generator is an integer ω such that, given the generator $h \in S$, $h^\omega = e$. In our case is straightforward that $\omega = +\infty$.

then we have

$$PM_f = \sum_{l\in L} M_l^\top M_{lf} = \sum_{l'\in L} M_{l'f^{-1}}^\top M_{l'} = \sum_{l'\in L} (M_{f^{-1}} M_{l'})^\top M_{l'} = M_{f^{-1}}^\top P. \quad (2.24)$$

We observe that both $M_l^\top M_l$ and P are positive operators and M_l are invertible. Thus P has a trivial kernel, because the only possibile $|m\rangle$ solving $\langle m|P|m\rangle = 0$ is $|m\rangle = 0$. This allows us to define the invertible operator

$$\tilde{M}_l := P^{\frac{1}{2}} M_l P^{-\frac{1}{2}} \quad (2.25)$$

which acts as a change of representation and brings to the relation

$$\tilde{M}_l^\top \tilde{M}_l = I \quad (2.26)$$

this means that $\tilde{M}_l$ is an orthogonal matrix and thus L can be represented orthogonally, when the underlying Cayley graph is embedded in $\mathbb{R}^d$.
Thus the finite subgroups of $\mathbb{GL}(d,\mathbb{Z})$ which are also subgroups of $\mathbb{O}(d)$ are isomorphic, varying the value of d, to [DEP17, Mac96, Tah71]:

- If $d = 3$, $\mathbb{Z}_n$, D_n with $n \in \{1, 2, 3, 4, 6\}$, A_4 (group of *even* permutations on a set of 4 elements), S_4 (group of the permutations over a set of 4 elements) and the direct product of these groups with $\mathbb{Z}_2$
- If $d = 2$, $\mathbb{Z}_n$ and D_n with $n \in \{1, 2, 3, 4, 6\}$
- If $d = 1$, $\{e\}$ and $\mathbb{Z}_2$.

We can now show how to derive the Weyl QW from the scenario presented, for d=1,2 and 3.
We start from considering the polar decomposition of the transition matrix $W(\mathbf{h})$[3], namely

$$W(\mathbf{h}) = V_{\mathbf{h}} |W(\mathbf{h})| \quad (2.27)$$

for $|W(\mathbf{h})| := \sqrt{W(\mathbf{h})^\dagger W(\mathbf{h})}$ and $V_{\mathbf{h}}$ unitary. If we take $\mathbf{h}_{i_1} = \mathbf{h}_{i_2} = h$ and $\mathbf{h}_{i_3} = 2h$ in (2.4), we get $W(\mathbf{h})W(-\mathbf{h})^\dagger = 0$ and thus $V_{\mathbf{h}}|W(\mathbf{h})||W(-\mathbf{h})|V_{-\mathbf{h}}^\dagger = 0 \implies |W(\mathbf{h})||W(-\mathbf{h})| = 0$, since the transition matrices are non null.
We conclude that $|W(\mathbf{h})|$ and $|W(-\mathbf{h})|$ must have orthogonal supports.
Now we have to make an assumption on the dimension of the Fermionic system, $n = 2$, since $n = 1$ would just give a trivial QCA and $n = 2$ is the smallest non-trivial case, and thus the transition matrices will be considered as 2×2 matrices. In this case in order to have orthogonal supports, the transition matrices must

[3]When there is no confusion we omit the index i and denote with h the elements of S

have rank $Rnk(W(\pm h)) = 1$. Therefore, there must exist an orthonormal basis $|w_{\mathbf{h}}\rangle, |w_{-\mathbf{h}}\rangle$ and $\omega_{\pm\mathbf{h}} > 0$ such that

$$\begin{aligned} W(\mathbf{h}) &=: \omega_{\mathbf{h}} V_{\mathbf{h}} |w_{\mathbf{h}}\rangle\langle w_{\mathbf{h}}| \\ W(-\mathbf{h}) &=: \omega_{-\mathbf{h}} V_{-\mathbf{h}} |w_{-\mathbf{h}}\rangle\langle w_{-\mathbf{h}}|. \end{aligned} \tag{2.28}$$

Now, $W(\mathbf{h})^\dagger W(-\mathbf{h}) = 0 \implies |W(\mathbf{h})| V_{\mathbf{h}}^\dagger V_{-\mathbf{h}} |W(-\mathbf{h})| = 0$, but $|W(\pm h)| = \omega_{\pm\mathbf{h}} |w_{\pm\mathbf{h}}\rangle\langle w_{\pm\mathbf{h}}|$ and $V_{\mathbf{h}}^\dagger V_{-\mathbf{h}}$ unitary, thus $V_{\mathbf{h}}^\dagger V_{-\mathbf{h}}$ must be diagonal in the basis $\{|w_{\pm\mathbf{h}}\rangle\}$. We then notice that $|W(\pm h)|$ are not full rank, thus the polar decomposition is not unique and in particular $V(\mathbf{h})(|w_{\mathbf{h}}\rangle\langle w_{\mathbf{h}}| + e^{i\phi_{\mathbf{h}}} |w_{-\mathbf{h}}\rangle\langle w_{-\mathbf{h}}|)$ gives the same decomposition of $V_{\mathbf{h}}$ for all $h \in S$. $\phi_{\mathbf{h}}$ can thus be chosen such that $V_{\mathbf{h}}^\dagger V_{-\mathbf{h}} = I$ which implies $V_{\mathbf{h}} = V_{-\mathbf{h}}$ for every h. Furthermore, we have the isotropy condition which brings to $\omega_{\pm\mathbf{h}} = \omega_{\pm\mathbf{h}'}$ for all $h, h' \in S$ and thus $\omega_{\pm\mathbf{h}}$ can be considered as $\omega_\pm$ independent of $\mathbf{h}$ [DEPT15].
Let us now consider L, group of automorphisms of the Cayley graph for which the isotropy requirement is fullfilled. We suppose that exists a subgroup $K \subseteq L$ such that, fixing $\mathbf{h}_1 \in S_+$ and considered its orbit under the action of K, $\mathcal{O}_K(\mathbf{h}_1)$, $\forall \mathbf{h}_i, \mathbf{h}_j \in \mathcal{O}_K(\mathbf{h}_1)$ with $\mathbf{h}_i \neq \mathbf{h}_j$ and for elements in the orbit of L (or null vectors) $\mathbf{h}_l, \mathbf{h}_m \in \{\mathbf{0}\} \cup \mathcal{O}_L(\mathbf{h}_1)$, we have

$$\mathbf{h}_i - \mathbf{h}_j = \mathbf{h}_l - \mathbf{h}_m \iff (\mathbf{h}_i = \mathbf{h}_l) \vee (\mathbf{h}_i = -\mathbf{h}_m). \tag{2.29}$$

This allows us to write two new relations of the kind (2.4):

$$\begin{aligned} W(\mathbf{h}_1) W^\dagger(\mathbf{h}_j) + W(-\mathbf{h}_j) W^\dagger(-\mathbf{h}_1) &= 0 \\ W^\dagger(\mathbf{h}_1) W(\mathbf{h}_j) + W^\dagger(-\mathbf{h}_j) W(-\mathbf{h}_1) &= 0. \end{aligned} \tag{2.30}$$

Multiplying the first equation by $W(\mathbf{h}_1)$ on the right or by $W^\dagger(\mathbf{h}_j)$ on the left and exploiting (2.2)

$$W^\dagger(\mathbf{h}_j) W(\mathbf{h}_1) W^\dagger(\mathbf{h}_j) = W(\mathbf{h}_1) W^\dagger(\mathbf{h}_j) W(\mathbf{h}_1) = 0. \tag{2.31}$$

and by the isotropy requirement, imposing $W(\mathbf{h}_j) = U_k W(\mathbf{h}_1) U_k^\dagger$ for some suitable representation U_k of the isotropy group

$$U_k W^\dagger(\mathbf{h}_1) U_k^\dagger W(\mathbf{h}_1) U_k W^\dagger(\mathbf{h}_1) U_k^\dagger = W(\mathbf{h}_1) U_k W(\mathbf{h}_1) U_k^\dagger W(\mathbf{h}_1) = 0. \tag{2.32}$$

but we know that $W(\mathbf{h}) = \omega_\pm V_{\mathbf{h}} |w_{\mathbf{h}}\rangle\langle w_{\mathbf{h}}|$ and (2.32) becomes

$$\langle w_{\mathbf{h}_1} | V_{\mathbf{h}_1}^\dagger U_k^\dagger V_{\mathbf{h}_1} | w_{\mathbf{h}_1}\rangle \langle w_{\mathbf{h}_1} | U_k | w_{\mathbf{h}_1}\rangle = 0. \tag{2.33}$$

Therefore either $\langle w_{\mathbf{h}_1}|V_{\mathbf{h}_1}^\dagger U_k^\dagger V_{\mathbf{h}_1}|w_{\mathbf{h}_1}\rangle$ or $\langle w_{\mathbf{h}_1}|U_k|w_{\mathbf{h}_1}\rangle$ must be equal to zero. The generic form for the unitary representation U_k is $U_k = \cos\theta I + i\sin\theta \mathbf{n}_k \cdot \boldsymbol{\sigma}$, where $\mathbf{n}_k$ is a generic versor and $\boldsymbol{\sigma}$ is a vector of Pauli sigma matrices. From (2.33) we conclude that θ must be equal to $m\frac{\pi}{2}$, $m \in \mathbb{Z}$

$$U_k = i\mathbf{n}_k \cdot \boldsymbol{\sigma} \tag{2.34}$$

and exploiting the identity

$$U_k U_{k'} = -\mathbf{n}_k \cdot \mathbf{n}_{k'} I - i(\mathbf{n}_k \times \mathbf{n}_{k'}) \cdot \sigma \tag{2.35}$$

we conclude that, in order to mantain the form (2.34) (U_k are representations of an isotropy group), the $\mathbf{n}_k$ have to be mutually orthogonal, then the cardinality of the subgroup K must be ≤ 4.
Therefore, the subgroups of L satisfying the condition presented in this section are:

- $\{I, \sigma_x, \sigma_y, \sigma_z\}$, with σ_i Pauli sigma matrix
- one of the following groups: $\{I, i\sigma_x\}$, $\{I, -V_{\mathbf{h}_1}(i\sigma_x)V_{\mathbf{h}_1}^\dagger\}$, $\{I, i\sigma_x, -I, -i\sigma_x\}$ and $\{I, -V_{\mathbf{h}_1}(i\sigma_x)V_{\mathbf{h}_1}^\dagger, -I, V_{\mathbf{h}_1}(i\sigma_x)V_{\mathbf{h}_1}^\dagger\}$
- The singleton $\{I\}$

In [DEP17] a complete derivation of these results is provided, as well as a complete proof of the following fact on the structure of the admittable Cayley graphs:

Theorem 2.2.1. *The primitive cells associated to the unique graphs admitting isotropic QWs in dimensions $d = 1, 2, 3$ are the following:*

- *Integer lattice with generators $S_+ = \{\boldsymbol{h}_1\}$ and $S_+ \equiv S_- = \{\boldsymbol{h}_1, -\boldsymbol{h}_1\}$ corrisponding to the isotropy groups $U_L = \{I\}$ and $U_L = \{I, i\sigma_x\}$*
- *Simple square lattice with generators $S_+ = \{\boldsymbol{h}_1, \boldsymbol{h}_2\}$ and $S_+ \equiv S_- = \{\boldsymbol{h}_1, \boldsymbol{h}_2, -\boldsymbol{h}_1, -\boldsymbol{h}_2\}$ corrisponding to the isotropy groups $U_L = \{I, i\sigma_x\}, \{I, i\sigma_z\}$ and $U_L = \{I, i\sigma_x, i\sigma_y, i\sigma_z\}$*
- *Body centered lattice (BCC) with generator $S_+ = \{\boldsymbol{h}_1, \boldsymbol{h}_2, \boldsymbol{h}_3, \boldsymbol{h}_4\}$, relator $\boldsymbol{h}_1 + \boldsymbol{h}_2 + \boldsymbol{h}_3 + \boldsymbol{h}_4 = 0$ and isotropy group $U_L = \{I, i\sigma_x, i\sigma_y, i\sigma_z\}$*

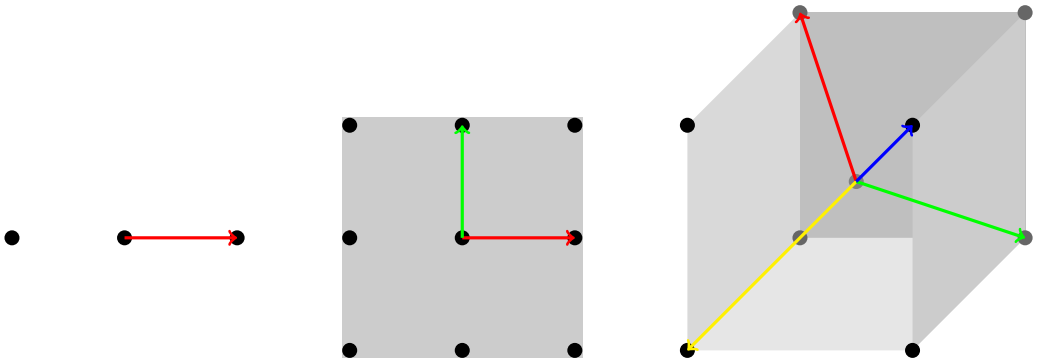

Figure 2.1: Lattices for Weyl's automaton for $d = 1$, $d = 2$ and $d = 3$ with generators.

2.2.1 d=1

We can now consider the automaton on a $1d$ lattice. The generators set is composed by $\{\mathbf{h}_1, -\mathbf{h}_1\}$, thanks to (2.28) we can write

$$\begin{aligned} W(\mathbf{h}_1) &= \omega_+ V |w_{\mathbf{h}_1}\rangle\langle w_{\mathbf{h}_1}| \\ W(\mathbf{h}_1) &= \omega_- V |w_{-\mathbf{h}_1}\rangle\langle w_{-\mathbf{h}_1}| \end{aligned} \tag{2.36}$$

for the discussion made, $V_{\mathbf{h}_1} = V_{-\mathbf{h}_1} = V$. Exploiting the unitarity conditions multiplied on the right for $W(\mathbf{h}_1)$ and $W(-\mathbf{h}_1)^\dagger$ we get

$$\begin{aligned} W(\mathbf{h}_1)W(\mathbf{0})^\dagger + W(\mathbf{0})W(-\mathbf{h}_1)^\dagger &= 0 \\ W(\mathbf{0})^\dagger W(\mathbf{h}_1) + W(-\mathbf{h}_1)^\dagger W(\mathbf{0}) &= 0 \end{aligned} \tag{2.37}$$

and since $W(\mathbf{h}_i)W^\dagger(-\mathbf{h}_i) = W^\dagger(-\mathbf{h}_i)W(\mathbf{h}_i) = 0$ for unitarity conditions, multiplying on left and right for the matrices realizing the condition, we obtain

$$W(\pm\mathbf{h}_1)W^\dagger(\mathbf{0})W(\pm\mathbf{h}_1) = 0 \tag{2.38}$$

this means

$$\langle w_{\pm\mathbf{h}_1}|W^\dagger(\mathbf{0})V|w_{\pm\mathbf{h}_1}\rangle = 0 \tag{2.39}$$

which implies that $W^\dagger(\mathbf{0})$ must have form VW_e, with W_e with off-diagonal elements in the basis $\{|w_{\pm\mathbf{h}_1}\rangle\}$ (V is a unitary responsible for the change of basis from $|w_{\pm\mathbf{h}_1}\rangle$ to $V|w_{\pm\mathbf{h}_1}\rangle$).
Making the substitutions:

- $W(\mathbf{0}) = V(\alpha|w_{-\mathbf{h}_1}\rangle\langle w_{\mathbf{h}_1}| + \beta|w_{\mathbf{h}_1}\rangle\langle w_{-\mathbf{h}_1}|)$
- $W(\mathbf{h}_1) = \omega_+ V|w_{\mathbf{h}_1}\rangle\langle w_{\mathbf{h}_1}|$
- $W(-\mathbf{h}_1) = \omega_- V|w_{-\mathbf{h}_1}\rangle\langle w_{-\mathbf{h}_1}|$

into Eqs. (2.37), and remebering that $\omega_\pm$ are real numbers, we obtain that the relations are satisfied for $\omega_+ = \omega_- =: n$ and for $\alpha = \beta =: im$, and $m \geq 0$. The condition

$$\sum_{h\in S} W(\mathbf{h})^\dagger W(\mathbf{h}) = I_{2\times 2} \tag{2.40}$$

brings us to conclude that $n^2 + m^2 = 1$. Then we must consider the isotropy groups admitted, i.e. $\{I\}$ and $\{I, i\sigma_x\}$. If we consider the first one, the matrices of the automation assume the form

$$\begin{aligned} W(\mathbf{h}_1) &= V \begin{pmatrix} n & 0 \\ 0 & 0 \end{pmatrix}, \\ W(-\mathbf{h}_1) &= V \begin{pmatrix} 0 & 0 \\ 0 & n \end{pmatrix}, \\ W(\mathbf{0}) &= V \begin{pmatrix} 0 & im \\ im & 0 \end{pmatrix} \end{aligned} \tag{2.41}$$

with V arbitrary unitary matrix, while for $\{I, i\sigma_x\}$, if we take V unitary commuting with σ_x we fullfill the completeness relation $\sum_{h\in S} W(\mathbf{h}) = I_{2\times 2}$.
We remark that we are not interested in the case of self interaction, thus we will consider as our automaton the one with $n = 1, m = 0$ and V will be taken as the identity matrix for simplicity:

$$\begin{aligned} W(\mathbf{h}_1) &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \\ W(-\mathbf{h}_1) &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \end{aligned} \quad . \tag{2.42}$$

2.2.2 d=2

In this case we have $S_+ = \{\mathbf{h}_1, \mathbf{h}_2\}$ or $S_+ \equiv S_- = \{\mathbf{h}_1, \mathbf{h}_2, -\mathbf{h}_1, -\mathbf{h}_2\}$ and the transition matrices become

$$W(\pm\mathbf{h}_1) = \omega_\pm V_{\mathbf{h}_1}|w_{\pm\mathbf{h}_1}\rangle\langle w_{\pm\mathbf{h}_1}|, W(\pm\mathbf{h}_2) = \omega_\pm V_{\mathbf{h}_2}|w_{\pm\mathbf{h}_2}\rangle\langle w_{\pm\mathbf{h}_2}|, \tag{2.43}$$

while the unitarity conditions we consider are

$$W(\mathbf{h}_1)W^\dagger(\pm\mathbf{h}_2) + W(\mp\mathbf{h}_2)W^\dagger(-\mathbf{h}_1) = 0, \tag{2.44}$$

thus multiplying (2.44) on the right by $W(\mathbf{h}_1)$,

$$W(\mathbf{h}_1)W^\dagger(\pm\mathbf{h}_2)W(\mathbf{h}_1) = 0. \tag{2.45}$$

By similar arguments as in the 1-d case, we can conclude that

- we have either $|w_{\pm\mathbf{h}_1}\rangle = |w_{\pm\mathbf{h}_2}\rangle$ or $|w_{\pm\mathbf{h}_1}\rangle = |w_{\mp\mathbf{h}_2}\rangle$
- $V_{\mathbf{h}_1} = V_{\mathbf{h}_2}(i\sigma_y)$ can be chosen up to a change of basis
- $\omega_+ = \omega_- =: \omega$ and in particular $\omega = \frac{1}{\sqrt{2}}$

if $V := V_{\mathbf{h}_2}$, we obtain

$$W(\pm\mathbf{h}_1) = \pm\omega V|w_{\pm\mathbf{h}_1}\rangle\langle w_{\pm\mathbf{h}_1}|, W(\pm\mathbf{h}_2) = \omega V|w_{\pm\mathbf{h}_1}\rangle\langle w_{\pm\mathbf{h}_1}|, \tag{2.46}$$

for the first choice of base vectors, while

$$W(\pm\mathbf{h}_1) = \pm\omega V|w_{\pm\mathbf{h}_1}\rangle\langle w_{\pm\mathbf{h}_1}|, W(\pm\mathbf{h}_2) = \omega V|w_{\mp\mathbf{h}_1}\rangle\langle w_{\mp\mathbf{h}_1}|, \tag{2.47}$$

for the second one.
Regarding the self-interaction $W(\mathbf{0})$, we observe that

$$W(\mathbf{h})W^\dagger(\mathbf{0}) + W(\mathbf{0})W^\dagger(-\mathbf{h}) = W^\dagger(\mathbf{h})W(\mathbf{0}) + W(\mathbf{0})^\dagger W(-\mathbf{h}) = 0, \qquad \forall h \in S \tag{2.48}$$

is satisfied only if $W(\mathbf{0}) = 0$.
As we have seen, we have multiple choices for the isotropy group: $\{I, i\sigma_z\}$ or $\{I, i\sigma_x, i\sigma_y, i\sigma_z\}$ for the case $|w_{\pm\mathbf{h}_1}\rangle = |w_{\pm\mathbf{h}_2}\rangle$ and $\{I, i\sigma_x\}$ or $\{I, i\sigma_x, i\sigma_y, i\sigma_z\}$ for the case $|w_{\pm\mathbf{h}_1}\rangle = |w_{\mp\mathbf{h}_2}\rangle$.
The transition matrices in the first case are:

$$\begin{aligned} W(\mathbf{h}_1) &= \frac{1}{2}V\begin{pmatrix}1 & 0\\ 1 & 0\end{pmatrix} \\ W(\mathbf{h}_2) &= \frac{1}{2}V\begin{pmatrix}0 & -1\\ 0 & 1\end{pmatrix} \\ W(-\mathbf{h}_1) &= \frac{1}{2}V\begin{pmatrix}1 & 0\\ -1 & 0\end{pmatrix} \\ W(-\mathbf{h}_2) &= \frac{1}{2}V\begin{pmatrix}0 & 1\\ 0 & 1\end{pmatrix} \end{aligned} \tag{2.49}$$

where V is a unitary matrix commuting with σ_z. For the second case it is sufficient to exchange $\mathbf{h}_2$ with $-\mathbf{h}_2$ and taking V as a unitary matrix commuting with σ_x. In both cases it is convenient to take $V = I$.

2.2.3 d=3

We start from the derivation of $V_{\mathbf{h}_1}$. From (2.33) and the fact that the isotropy group is $\{I, i\sigma_x, i\sigma_y, i\sigma_z\}$ we conclude that the condition $\langle w_{\mathbf{h}_1}|i\sigma_z|w_{\mathbf{h}_1}\rangle$ cannot be satisfied, thus must be satisfied

$$\langle w_{\mathbf{h}_1}|V_{\mathbf{h}_1}^\dagger i\sigma_z V_{\mathbf{h}_1}|w_{\mathbf{h}_1}\rangle = 0 \tag{2.50}$$

but this brings to

$$Tr\left[V_{\mathbf{h}_1}^\dagger \sigma_z V_{\mathbf{h}_1}\sigma_z\right] = 0 \tag{2.51}$$

and since $V_{\mathbf{h}_1}$ is unitary, its general form is

$$V_{\mathbf{h}_1} = \kappa \begin{pmatrix} \zeta & -\nu^* \\ \nu & \zeta^* \end{pmatrix} \tag{2.52}$$

with $|\kappa|^2 = |\zeta|^2 + |\nu|^2 = 1$ and the condition on the trace implies that $|\zeta| = |\nu| = \frac{1}{\sqrt{2}}$ which brings to

$$W(\mathbf{h}_1) = \frac{\omega_+}{\sqrt{2}} \begin{pmatrix} \xi & 0 \\ \upsilon & 0 \end{pmatrix}, \qquad W(-\mathbf{h}_1) = \frac{\omega_-}{\sqrt{2}} \begin{pmatrix} 0 & -\upsilon^* \\ 0 & \xi^* \end{pmatrix} \tag{2.53}$$

The orbit of these matrices under the isotropy group $\{I, i\sigma_x, i\sigma_y, i\sigma_z\}$ completes the set of transition matrices:

$$\begin{aligned} W(\mathbf{h}_2) &= \frac{\omega_+}{\sqrt{2}} \begin{pmatrix} 0 & \upsilon \\ 0 & \xi \end{pmatrix}, & W(-\mathbf{h}_2) &= \frac{\omega_-}{\sqrt{2}} \begin{pmatrix} \xi^* & 0 \\ -\upsilon^* & 0 \end{pmatrix} \\ W(\mathbf{h}_3) &= \frac{\omega_+}{\sqrt{2}} \begin{pmatrix} 0 & -\upsilon \\ 0 & \xi \end{pmatrix}, & W(-\mathbf{h}_3) &= \frac{\omega_-}{\sqrt{2}} \begin{pmatrix} \xi^* & 0 \\ \upsilon^* & 0 \end{pmatrix} \\ W(\mathbf{h}_4) &= \frac{\omega_+}{\sqrt{2}} \begin{pmatrix} \xi & 0 \\ -\upsilon & 0 \end{pmatrix}, & W(-\mathbf{h}_4) &= \frac{\omega_-}{\sqrt{2}} \begin{pmatrix} 0 & \upsilon^* \\ 0 & \xi^* \end{pmatrix} \end{aligned} \tag{2.54}$$

It can be useful writing the Fourier transform of the transition matrices

$$W(\mathbf{k}) = \sum_{i=1}^{4} \left(W(\mathbf{h}_i) e^{i\mathbf{h}_i \cdot k} + W(-\mathbf{h}_i) e^{-i\mathbf{h}_i \cdot k} \right) \tag{2.55}$$

which must be unitary, and thus we obtain

$$\begin{aligned} \omega_+^2 = \omega_-^2 = \frac{1}{4}, \\ \xi^{*2} + \xi^2 = \upsilon^{*2} + \upsilon^2 = 0 \end{aligned} \tag{2.56}$$

and the possible solutions are

$$\begin{aligned} \pm\,\alpha^+ := \pm\frac{1+i}{\sqrt{2}} \\ \pm\,\alpha^- := \pm\frac{1-i}{\sqrt{2}} \end{aligned} \tag{2.57}$$

There are many equivalent choices for υ and ξ. In particular they are connected each other by a phase factor and conjugation by $e^{\pm i\frac{\pi}{4}\sigma_z}$. In particular we can choose $\xi = \upsilon = \alpha^{\pm}$. This concludes our derivation. Since the evolution is linear, the map associated to the corresponding QCA will be in corrispondence with the transition matrices according to the discussion in Sec. 1.8.

2.2.4 From the Automaton to Weyl Equation

In the previous section we have derived the automaton imposing only the principles discussed at the beginning and provided a classification of the QW and the correspondig QCA obtained according to the dimensionality of the lattice. We now want to study the solutions of the walk dynamics in the *small wave-vector regime* approximation.
We can effectively talk about waves because the overall eigenstate of the automaton is

$$|\psi\rangle = \int_B d^3k \, \left(\psi_+(\mathbf{k})|\mathbf{k}\rangle|w_k^+\rangle + \psi_-(\mathbf{k})|\mathbf{k}\rangle|w_k^-\rangle\right), \tag{2.58}$$

with $|w_k^{\pm}\rangle$ such that $W(\mathbf{k})|w_k^{\pm}\rangle = e^{i\pm\omega_k^{\pm}}|w_k^{\pm}\rangle$,
which is a superposition of plane waves $|\mathbf{k}\rangle$ around a value $\mathbf{k}_0$ such that

$$|\psi_{\pm}(\mathbf{k})| < \varepsilon \qquad \forall k : |\mathbf{k} - \mathbf{k}_0| \geq \delta. \tag{2.59}$$

we restrict the domain of our wave to the *first Brillouin zone*, thus $k, \mathbf{k}_0 \in B$ and in particular $|\mathbf{k}_0| << \pi$.

The dynamics is studied defining the *interpolating Hamiltonian*, $H_I(\mathbf{k})$:

$$W(\mathbf{k}) =: e^{-iH_I(\mathbf{k})}. \tag{2.60}$$

We also take into account the following definitions:

Definition 2.2.2 (Quasi-isometry)**.** *A quasi-isometry is a function f between two metric spaces (S_1, d_1), $(S_2, d2)$ such that, there exist three constants $A \geq 1$, $B \geq 0$ and $C \geq 0$ with the properties:*

- $\forall s, t \in S_1 \ \frac{1}{A} d_1(s,t) - B \leq d_2(f(s), f(t)) \leq A d_1(s,t) + B$,
- $\forall r \in S_2 \ \exists s \in S_1 | d_2(r, f(s)) \leq C$

Definition 2.2.3 (Quasi-isometric embedding)**.** *A function f is a quasi isometric embedding if it satisfies the first property of definition 2.2.2, but not necessarily the second.*

The discrete lattice $(\mathbf{g}, t)$, with $\mathbf{g}$ three-dimensional can be embedded quasi-isometrically in $\mathbb{R}^4$, i.e. there exists an f with the properties of definition 2.2.3. Exploiting the existence of f and extending the domain of k from the first Brillouin zone to all $\mathbb{R}^3$, the interpolating Hamiltonian is well defined on $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ and we can define the unitary evolution:

$$U(t) := \int_{\mathbb{R}^3} d^3k \, |\mathbf{k}\rangle\langle\mathbf{k}| \otimes e^{-i\mathbf{h}_I(\mathbf{k})t}. \tag{2.61}$$

and we observe that given the spinor $\psi(\mathbf{k}) = (\psi_+(\mathbf{k}), \psi_-(\mathbf{k}))$ and applying (2.61) to it, the solution $\psi(\mathbf{k}, t) = (\psi_+(\mathbf{k}, t), \psi_-(\mathbf{k}, t))$ gives rise to

$$i\partial_t \psi(\mathbf{k}, t) = \mathbf{h}_I(\mathbf{k}) \psi(\mathbf{k}, t) \tag{2.62}$$

which is the *Scrödinger's equation*.
Now, (2.55) can be written in the following form [DP14, Per20b]:

$$W(\mathbf{k}) = d_k^{\pm} I - i\mathbf{n}_k^{\pm} \cdot \boldsymbol{\sigma}^{\pm} \tag{2.63}$$

where the $\pm$ signs take into account different choices for the solutions (2.57), while $\boldsymbol{\sigma}^+ = (\sigma_x, \sigma_y, \sigma_z)$ and $\boldsymbol{\sigma}^- = (\sigma_x, -\sigma_y, \sigma_z)$. Furthermore:

- $s_i := \sin k_i$, $c_i := \cos k_i$, $i = x, y, z$
- $\mathbf{n}_k^{\pm} := \begin{pmatrix} s_x c_y c_z \pm c_x s_y s_z \\ s_y c_x c_z \pm c_y s_x s_z \\ s_z c_x c_y \mp c_z s_x s_y \end{pmatrix}$
- $d_k^{\pm} := c_x c_y c_z \pm s_x s_y s_z$.

Applying the *small-wave vector regime* means that $\mathbf{k}$ must be taken small enough so that non-linear terms in $\mathbf{k}$ can be ignored, i.e. we have to expand at the first order (2.63). Since $s_i = k_i$, $c_i = 1 \, \forall i$ and products of s_i vanish because are at superior orders, we obtain

$$W(\mathbf{k})_{\text{ f.o.}} = I \pm i\mathbf{k}\cdot\boldsymbol{\sigma}. \tag{2.64}$$

Remembering (2.60), at first order:

$$\mathbf{h}_I(\mathbf{k})_{\text{ f.o.}} = \pm\mathbf{k}\cdot\boldsymbol{\sigma} \tag{2.65}$$

and thus for (2.62)

$$i\partial_t\psi(\mathbf{k},t) = \pm\mathbf{k}\cdot\boldsymbol{\sigma}\psi(\mathbf{k},t) \tag{2.66}$$

which are exactly Weyl's equations in the **k** domain.

3. DIRAC QW AND QCA

In this section we will focus on the reversibility constraint, which we have replaced with unitarity (necessary, but not sufficient for reversibility) and we will build a reversibile automaton coupling two Weyl automata. We will call this automaton *Dirac QCA* because its dynamics under certain condition brings to the *Dirac equation*.
We observe that in the case of the Weyl QWs, unitarity alone does not guarantee the reversibility because every local transformation acting independently and identically on every cell is not sufficient to reverse the sign of $\mathbf{n}_k^{\pm}$.
However, as stated in Sec. 1.7.2, taking

$$D^{\pm} = W^{\pm}\otimes W^{\pm\dagger} \tag{2.67}$$

allows to build a reversible automaton. The general form of the coupling in Fourier's basis is the following:

$$D'(\mathbf{k}) := \begin{pmatrix} xF_k & yB \\ zC & tG_k \end{pmatrix} \tag{2.68}$$

Since we required locality, the blocks B and C have to be independent of k, while the blocks on diagonal are the direct sum of the Weyl's automata in Fourier's basis. First of all, we require unitarity. It can be proved [DP14] that this corresponds to the requirements:

$$\begin{aligned} B^\dagger B = C^\dagger C = BB^\dagger = CC^\dagger = I \\ y^2 = z^2 \\ xF_k = -t^* BG_k^\dagger C|x|^2 + y^2 = z^2 + |t|^2 = 1 \end{aligned} \tag{2.69}$$

imposing $k = 0$, $F_0 = D_0 = I$ and $C = e^{i\theta}B^\dagger$ with $e^{i\theta} := -e^{i\arg[xt]}$. Identifying $F_k = W(\mathbf{k})$, we get

$$D'(\mathbf{k}) = \begin{pmatrix} xW(\mathbf{k}) & yB \\ ye^{i\theta}B^\dagger & -x^*e^{i\theta}B^\dagger W^\dagger(\mathbf{k})B \end{pmatrix} = UD(\mathbf{k})U^\dagger \tag{2.70}$$

with

$$\begin{aligned} U &:= \begin{pmatrix} I & 0 \\ 0 & iB \end{pmatrix} \\ D(\mathbf{k}) &= \begin{pmatrix} xW(\mathbf{k}) & iyI \\ -iye^{i\theta}I & -x^*e^{i\theta}W^\dagger(\mathbf{k}) \end{pmatrix} \end{aligned} \tag{2.71}$$

and we can choose as a valid automaton the one with $y = n \in \mathbb{R}$, $x = m \in \mathbb{R}$ and $e^{i\theta} = \pm 1$:

$$D(\mathbf{k}) = \begin{pmatrix} nW(\mathbf{k}) & imI \\ imI & nW^\dagger(\mathbf{k}) \end{pmatrix} \tag{2.72}$$

with $n^2 + m^2 = 1$. We notice that this expression is independent of the dimensionality of the lattice
The Dirac automaton can be rewritten in a form corresponding to (2.63) for the Weyl automaton:

$$D(\mathbf{k}) = Id_k^{D\pm} - i\gamma_0\boldsymbol{\gamma}^\pm \cdot \mathbf{n}_k^{D\pm} + im\gamma_0 \tag{2.73}$$

with

- $d_k^{D\pm} = nd_k^\pm$
- $\mathbf{n}_k^{D\pm} = n\mathbf{n}_k^\pm$
- $$\gamma_0 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \qquad \gamma_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$
$$\gamma_2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}, \qquad \gamma_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{2.74}$$
- $\boldsymbol{\gamma}^\pm = (\gamma_1, \pm\gamma_2, \gamma_3)$

The γ_i matrices are called *Dirac gamma matrices*. We will see their properties in major detail in the next chapter.
In the small-wave limit the Fourier transform of (2.73) becomes

$$i\partial_t\psi(\mathbf{g},t) = (\pm in\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} - m\beta)\,\psi(\mathbf{g},t) \tag{2.75}$$

with $\psi(\mathbf{g},t)$ four-components spinor or *bispinor*, $\boldsymbol{\alpha} = \gamma_0\boldsymbol{\gamma}$ and $b = \gamma_0$. m here assumes the role of mass parameter, which can be taken such that $m << n$ in the relativistic limit and this brings to, in Einstein's notation,

$$(i\gamma_\mu\partial_\mu - mI)\psi(\mathbf{g},t) = 0. \tag{2.76}$$

i.e. the Dirac equation.

CHAPTER 3

INTERACTIONS IN QUANTUM CELLULAR AUTOMATA: OVERVIEW AND CLASSIFICATION

So far we have reviewed some remarkable results on the theory of QCA and introduced Weyl and Dirac QW and QCA having as objective a re-derivation of the most important dynamical equation in QFT. These results are known as *free* evolution, namely we consider the Fermionic modes in each system as non interacting and studying their standalone evolution. The desideratum is now studying local interactions between modes at each site. Some steps in this direction have been made, but this is mostly an unexplored path. We indicate [CKSS10, CSB07] as examples of systems in which interactions are mediated by decoherence, [BDT13, AAM$^+$11] for interactions with external fields, [NBPR07, LKanN15] for non-linear interactions, which are also the object of our study and [BDPT18, BDM$^+$18] for the Thirring model for Fermionic QWs, which has particularly inspired this work.
In this chapter, we will provide a complete classification of the local isotropic number preserving interactions for Weyl and Dirac QCA and in particular we will focus on interactions between two particles located in the same site.
In the next chapter we will recover the correspondence between QW and QCA and we will study in detail a non trivial interaction.

3.0.1 Overview on Interactions in QCA

In the previous chapter we have treated Fermionic QCAs as arrays of memory cells evolved *linearly*, namely the evolution of the modes in a cell was ruled by

transition matrices applied on a vector of Fermionic modes, acting as internal degrees of freedom for the quantum system and a translation operator, namely the left-right regular representation for the group of sites on the lattice, acting on the position degree of freedom.
Describing an interaction, instead, involves unitary operators, which are *non-linear* in the fields. We must also consider the fact that the interactions considered shall not change the total number of the modes involved, a property that is realized through the number preservation, i.e. we will consider the same number of $a_i^\dagger$ and a_i operators. We are interested in particular on operators of the form

$$J = \prod_g e^{iH_g} \tag{3.1}$$

where H_g is an "Hamiltonian" intended as an Hermitian operator acting as an Hamiltonian in describing the interaction even potentially in a non-perturbative approach, while the *capital pi* notation indicates that the operator acts on all the points of the lattice and the ordering in the product is immaterial since, being the unitary operators U_g number preserving and localized on site g, they commute.
Until now, we have not considered the geometry of the lattice yet. This aspect affects the number of interactions we should take into account. That is because we need that the most general interaction admissible respects the invariance under the action of the isotropy group for the lattice chosen.
Remembering Sec. 2.2, for the 1D lattice we have $U_L = \{I\}$ and $U_L = \{I, i\sigma_x\}$, for the 2D case $U_L = \{I, i\sigma_x\}, \{I, i\sigma_z\}$ and $U_L = \{I, i\sigma_x, i\sigma_y, i\sigma_z\}$, while for the 3D case $U_L = \{I, i\sigma_x, i\sigma_y, i\sigma_z\}$. We will provide a complete classification for the 3D case, namely the interaction operator must be invariant under $U_L = \{I, i\sigma_x, i\sigma_y, i\sigma_z\}$.
Before proceeding with the classification, we highlight that it is possible to write out the automaton resulting from a free evolution step and a local interaction step. Taking J in the form (3.1) for the Weyl or the Dirac and F in the form (2.8) or (2.67), we have

$$A := JF. \tag{3.2}$$

1. INTERACTIONS FOR THE WEYL QCA

The Weyl QCA involves spinors of the form

$$\psi = \begin{pmatrix} a_u \\ a_d \end{pmatrix} \tag{3.3}$$

The most general interaction will be in the form (3.1) and in particular H_g will be a polynomial in the fields operator with the number preserving constraint:

$$H_{g,\text{Weyl}} = \lambda_1 a_u^\dagger a_u + \lambda_2 a_u^\dagger a_d + \lambda_3 a_d^\dagger a_u + \lambda_4 a_d^\dagger a_d + \lambda_5 a_u^\dagger a_u a_d^\dagger a_d. \tag{3.4}$$

where for lightier notation we omitted the spatial degree of freedom, namely $a_i := a_i(g)$, $i \in \{u, d\}$. Now we consider invariance under the group $U_L = \{I, i\sigma_x, i\sigma_y, i\sigma_z\}$. A representation useful for our purposes is

$$\begin{aligned} I &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \tag{3.5}$$

acting on spinors (3.3). This means that the mixed terms in (3.4), $a_d^\dagger a_u$ and $a_u^\dagger a_d$ do not satisfy the isotropy requirements, and thus $\lambda_2 = \lambda_3 = 0$. We then observe that λ_4 must be equal to λ_1, since σ_x exchanges u and d internal degrees of freedom, but we need invariance of the operator under its action. At the end, we find that

$$J_{\text{Weyl}} = \prod_g e^{iH_{g,\text{Weyl}}} \tag{3.6}$$

is the interaction operator with Hamiltonian

$$H_{g,\text{Weyl}} = \lambda_1 \left(a_d^\dagger a_d + a_u^\dagger a_u \right) + \lambda_5 a_u^\dagger a_u a_d^\dagger a_d \tag{3.7}$$

is the most general interaction operator for the Weyl automaton.

2. INTERACTIONS FOR THE DIRAC QCA

In the Dirac QCA, the free evolution acts linearly on *bispinors* of the form

$$\psi_D = \begin{pmatrix} a_{u1} \\ a_{d1} \\ a_{u2} \\ a_{d2} \end{pmatrix}. \tag{3.8}$$

In fact, the Dirac QCA is a reversible QCA built from the Weyl automaton in the form $D = W \otimes W^\dagger$. This means that the isotropy group in this case will be $U_L = \{I, i\sigma_x, i\sigma_y, i\sigma_z\}$ for each of the spinors in the bispinor separately.

The most general polynomial describing the Hamiltonian of the interaction operator is far more complex than in the Weyl case. To study its invariance under the action of the isotropy group calculations "by hand" may bring easily to mistakes. Therefore, we decided to write a code in *sympy*, a Python module for symbolic mathematics, in order to handle matrices and the properties of the Fermions' algebra, which have to be heavily used. The details of the algorithms and the full code of the library written can be found in Appendix A.
We start noticing that the Hamiltonian of the local interaction, denoted $H_{g,\text{Dirac}}$, will have at most 8-linear number preserving terms. Overall, it is composed by 69 terms:

- 16 2-linear terms:

$$\begin{array}{llll} a^\dagger_{u_1}a_{u_1}, & a^\dagger_{d_1}a_{d_1}, & a^\dagger_{u_1}a_{d_1}, & a_{u_1}a^\dagger_{d_1}, \\ a^\dagger_{u_2}a_{u_2}, & a^\dagger_{d_2}a_{d_2}, & a^\dagger_{u_2}a_{d_2}, & a_{u_2}a^\dagger_{d_2}, \\ a^\dagger_{u_1}a_{d_2}, & a_{d_1}a^\dagger_{u_2}, & a^\dagger_{d_1}a_{u_2}, & a_{u_1}a^\dagger_{d_2}, \\ a^\dagger_{u_1}a_{u_2}, & a_{u_1}a^\dagger_{u_2}, & a^\dagger_{d_1}a_{d_2}, & a_{d_1}a^\dagger_{d_2} \end{array}$$

- 36 4-linear terms:

$$\begin{array}{ll} a_{d_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2}, & a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}, \\ a^\dagger_{d_1}a_{d_1}a^\dagger_{d_2}a_{d_2}, & a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{d_2}, \\ a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}, & a^\dagger_{d_1}a_{d_1}a_{u_2}a^\dagger_{d_2}, \\ a^\dagger_{d_1}a^\dagger_{u_2}a_{u_2}a_{d_2}, & a^\dagger_{d_1}a_{u_2}a^\dagger_{d_2}a_{d_2}, \\ a^\dagger_{u_1}a_{d_1}a^\dagger_{d_2}a_{d_2}, & a^\dagger_{u_1}a_{d_1}a^\dagger_{u_2}a_{d_2}, \\ a^\dagger_{u_1}a_{d_1}a^\dagger_{u_2}a_{u_2}, & a^\dagger_{u_1}a_{d_1}a_{u_2}a^\dagger_{d_2}, \\ a^\dagger_{u_1}a^\dagger_{d_1}a_{d_1}a_{d_2}, & a^\dagger_{u_1}a^\dagger_{d_1}a_{d_1}a_{u_2}, \\ a^\dagger_{u_1}a^\dagger_{d_1}a_{u_2}a_{d_2}, & a^\dagger_{u_1}a^\dagger_{u_2}a_{u_2}a_{d_2}, \\ a^\dagger_{u_1}a_{u_1}a_{d_1}a^\dagger_{d_2}, & a^\dagger_{u_1}a_{u_1}a_{d_1}a^\dagger_{u_2}, \\ a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}, & a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_2}, \\ a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{u_2}, & a^\dagger_{u_1}a_{u_1}a^\dagger_{d_2}a_{d_2}, \\ a^\dagger_{u_1}a_{u_1}a^\dagger_{u_2}a_{d_2}, & a^\dagger_{u_1}a_{u_1}a^\dagger_{u_2}a_{u_2}, \\ a^\dagger_{u_1}a_{u_1}a_{u_2}a^\dagger_{d_2}, & a^\dagger_{u_1}a_{u_2}a^\dagger_{d_2}a_{d_2}, \\ a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2}, & a_{u_1}a_{d_1}a^\dagger_{u_2}a^\dagger_{d_2}, \\ a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{d_2}, & a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}, \end{array}$$

$$a_{u_1}a^\dagger_{d_1}a^\dagger_{d_2}a_{d_2}, \qquad a_{u_1}a^\dagger_{d_1}a^\dagger_{u_2}a_{d_2},$$
$$a_{u_1}a^\dagger_{d_1}a^\dagger_{u_2}a_{u_2}, \qquad a_{u_1}a^\dagger_{d_1}a_{u_2}a^\dagger_{d_2},$$
$$a_{u_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2}, \qquad a_{u_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}$$

- 16 6-linear terms:

$$a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2}, \qquad a_{u_1}a^\dagger_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2},$$
$$a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2}, \qquad a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2},$$
$$a^\dagger_{u_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2}, \qquad a^\dagger_{u_1}a_{u_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2},$$
$$a^\dagger_{u_1}a_{u_1}a_{d_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2}, \qquad a^\dagger_{u_1}a_{u_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2},$$
$$a^\dagger_{u_1}a^\dagger_{d_1}a_{d_1}a_{u_2}a^\dagger_{d_2}a_{d_2}, \qquad a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{u_2}a^\dagger_{d_2}a_{d_2},$$
$$a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{d_2}a_{d_2}, \qquad a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}a_{u_2}a^\dagger_{d_2},$$
$$a^\dagger_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a_{d_2}, \qquad a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a^\dagger_{u_2}a_{u_2}a_{d_2},$$
$$a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{d_2}, \qquad a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}$$

- 1 8-linear term: $a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2}$

each one multiplied for a λ_i, coupling constant $\in \mathbb{C}$.
The resulting polynomial invariant under the action of the isotropy group is

$$\begin{aligned}
H_{g,\text{Dirac}} =&\lambda_1 a^\dagger_{d_1}a_{d_1}+\\
&\lambda_1 a^\dagger_{u_1}a_{u_1}+\\
&\lambda_5 a^\dagger_{d_2}a_{d_2}+\\
&\lambda_5 a^\dagger_{u_2}a_{u_2}+\\
&\lambda_{13} a^\dagger_{d_1}a_{d_2}+\\
&\lambda_{13} a^\dagger_{u_1}a_{u_2}+\\
&\lambda_{14} a_{d_1}a^\dagger_{d_2}+\\
&\lambda_{14} a_{u_1}a^\dagger_{u_2}+\\
&\lambda_{18} a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}+\\
&\lambda_{18} a_{u_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2}+\\
&\lambda_{19} a^\dagger_{d_1}a_{d_1}a^\dagger_{d_2}a_{d_2}+\\
&\lambda_{19} a^\dagger_{u_1}a_{u_1}a^\dagger_{u_2}a_{u_2}+\\
&\lambda_{21} a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}+
\end{aligned}$$

$$
\begin{aligned}
&\lambda_{21} a^\dagger_{u_1} a_{u_1} a^\dagger_{d_2} a_{d_2} + \\
&\lambda_{23} a^\dagger_{d_1} a^\dagger_{u_2} a_{u_2} a_{d_2} + \\
&\lambda_{23} a^\dagger_{u_1} a_{u_2} a^\dagger_{d_2} a_{d_2} + \\
&\lambda_{26} a_{u_1} a^\dagger_{d_1} a_{u_2} a^\dagger_{d_2} + \\
&\lambda_{26} a^\dagger_{u_1} a_{d_1} a^\dagger_{u_2} a_{d_2} + \\
&\lambda_{28} a_{u_1} a^\dagger_{d_1} a^\dagger_{u_2} a_{d_2} + \\
&\lambda_{28} a^\dagger_{u_1} a_{d_1} a_{u_2} a^\dagger_{d_2} + \\
&\lambda_{30} a^\dagger_{u_1} a_{u_1} a^\dagger_{d_1} a_{d_2} + \\
&\lambda_{30} a^\dagger_{u_1} a^\dagger_{d_1} a_{d_1} a_{u_2} + \\
&\lambda_{31} a^\dagger_{u_1} a^\dagger_{d_1} a_{u_2} a_{d_2} + \\
&\lambda_{33} a_{u_1} a^\dagger_{d_1} a_{d_1} a^\dagger_{u_2} + \\
&\lambda_{33} a^\dagger_{u_1} a_{u_1} a_{d_1} a^\dagger_{d_2} + \\
&\lambda_{35} a^\dagger_{u_1} a_{u_1} a^\dagger_{d_1} a_{d_1} + \\
&\lambda_{43} a^\dagger_{u_2} a_{u_2} a^\dagger_{d_2} a_{d_2} + \\
&\lambda_{44} a_{u_1} a_{d_1} a^\dagger_{u_2} a^\dagger_{d_2} + \\
&\lambda_{53} a^\dagger_{d_1} a_{d_1} a^\dagger_{u_2} a_{u_2} a^\dagger_{d_2} a_{d_2} + \\
&\lambda_{53} a^\dagger_{u_1} a_{u_1} a^\dagger_{u_2} a_{u_2} a^\dagger_{d_2} a_{d_2} + \\
&\lambda_{55} a_{u_1} a^\dagger_{d_1} a_{d_1} a^\dagger_{u_2} a^\dagger_{d_2} a_{d_2} + \\
&\lambda_{55} a^\dagger_{u_1} a_{u_1} a_{d_1} a^\dagger_{u_2} a_{u_2} a^\dagger_{d_2} + \\
&\lambda_{61} a^\dagger_{u_1} a_{u_1} a^\dagger_{d_1} a^\dagger_{u_2} a_{u_2} a_{d_2} + \\
&\lambda_{61} a^\dagger_{u_1} a^\dagger_{d_1} a_{d_1} a_{u_2} a^\dagger_{d_2} a_{d_2} + \\
&\lambda_{63} a^\dagger_{u_1} a_{u_1} a^\dagger_{d_1} a_{d_1} a^\dagger_{d_2} a_{d_2} + \\
&\lambda_{63} a^\dagger_{u_1} a_{u_1} a^\dagger_{d_1} a_{d_1} a^\dagger_{u_2} a_{u_2} + \\
&\lambda_{69} a^\dagger_{u_1} a_{u_1} a^\dagger_{d_1} a_{d_1} a^\dagger_{u_2} a_{u_2} a^\dagger_{d_2} a_{d_2}
\end{aligned}
\tag{3.9}
$$

but we have not finished yet, since the Hermiticity of $H_{g,\text{Dirac}}$ is yet to impose. With this further constraint we obtain

$$
\begin{aligned}
H_{x,\text{Dirac}} =& \lambda_1 (a^\dagger_{d_1} a_{d_1} + a^\dagger_{u_1} a_{u_1}) + \\
& \lambda_5 (a^\dagger_{d_2} a_{d_2} + a^\dagger_{u_2} a_{u_2}) + \\
& \lambda_{13} (a^\dagger_{d_1} a_{d_2} + a^\dagger_{u_1} a_{u_2}) + \overline{\lambda_{13}} (a_{d_1} a^\dagger_{d_2} + a_{u_1} a^\dagger_{u_2}) +
\end{aligned}
$$

$$\lambda_{18}(a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2} + a_{u_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2}) + \overline{\lambda_{18}}(a^\dagger_{d_1}a^\dagger_{u_2}a_{u_2}a_{d_2} + a^\dagger_{u_1}a_{u_2}a^\dagger_{d_2}a_{d_2})+$$
$$\lambda_{19}(a^\dagger_{d_1}a_{d_1}a^\dagger_{d_2}a_{d_2} + a^\dagger_{u_1}a_{u_1}a^\dagger_{u_2}a_{u_2})+$$
$$\lambda_{21}(a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2} + a^\dagger_{u_1}a_{u_1}a^\dagger_{d_2}a_{d_2})+$$
$$\lambda_{26}(a_{u_1}a^\dagger_{d_1}a_{u_2}a^\dagger_{d_2} + a^\dagger_{u_1}a_{d_1}a^\dagger_{u_2}a_{d_2})+$$
$$\lambda_{28}(a_{u_1}a^\dagger_{d_1}a^\dagger_{u_2}a_{d_2} + a^\dagger_{u_1}a_{d_1}a_{u_2}a^\dagger_{d_2})+$$
$$\lambda_{30}(a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_2} + a^\dagger_{u_1}a^\dagger_{d_1}a_{d_1}a_{u_2}) + \overline{\lambda_{30}}(a^\dagger_{u_1}a_{u_1}a_{d_1}a^\dagger_{d_2} + a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2})+$$
$$\lambda_{31}a^\dagger_{u_1}a^\dagger_{d_1}a_{u_2}a_{d_2} + \overline{\lambda_{31}}a_{u_1}a_{d_1}a^\dagger_{u_2}a^\dagger_{d_2}+$$
$$\lambda_{35}a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}+$$
$$\lambda_{43}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2}+$$
$$\lambda_{53}(a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2} + a^\dagger_{u_1}a_{u_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2})+$$
$$\lambda_{55}(a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2} + a^\dagger_{u_1}a_{u_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2})+$$
$$\overline{\lambda_{55}}(a^\dagger_{u_1}a^\dagger_{d_1}a_{d_1}a_{u_2}a^\dagger_{d_2}a_{d_2} + a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a^\dagger_{u_2}a_{u_2}a_{d_2})+$$
$$\lambda_{63}(a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{d_2}a_{d_2} + a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2})+$$
$$\lambda_{69}a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2} \tag{3.10}$$

3. CLASSIFICATION OF THE 4-LINEAR TERMS

We want to put our magnifying glass on the 4-linear terms of $H_{g,\text{Dirac}}$.
These terms are important because they are involved in the most general interaction in the two particle sector, which we will consider later in this work. In fact, the 8-linear and the 6-linear terms applied on a two-Fermions state, return zero as a result. As an example, taking the 8-linear term:

$$\lambda_{69}a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2}|f_1\rangle|f_2\rangle|0\rangle|0\rangle = 0 \tag{3.11}$$

where f_1 and f_2 indicate the occupation number for the state of the two Fermions. The problem now is finding a suitable way of classifying these terms. Since the objective is working in the direction of providing a re-derivation of the results known in QFT (and possibly using this approach to discover new phenomenology), it can be particularly useful investigating the relationship between these interactions and the Dirac γ matrices, which we will now review briefly.

3.3.1 Dirac γ Matrices

The Dirac γ matrices are important because they can be defined as the set of 4×4 matrices fulfilling the anticommutation relation for the *Clifford Algebra*:

$$\{\gamma^\mu, \gamma^\nu\} := \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu} I. \tag{3.12}$$

with $\eta^{\mu\nu}$ metric tensor, such that

$$\eta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{3.13}$$

They can have different representations. The one we will use is

$$\gamma_0 = \sigma_x \otimes I == \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \qquad \gamma_1 = i\sigma_y \otimes \sigma_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$
$$\gamma_2 = i\sigma_y \otimes \sigma_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}, \qquad \gamma_3 = i\sigma_y \otimes \sigma_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{3.14}$$

It is useful to define also a γ_5 matrix as

$$\gamma_5 = \sigma_z \otimes I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{3.15}$$

Another widely used representation is

$$\begin{aligned} \gamma_0 &= \sigma_z \otimes I, \\ \gamma_1 &= i\sigma_y \otimes \sigma_x, \\ \gamma_2 &= i\sigma_y \otimes \sigma_y, \\ \gamma_3 &= i\sigma_y \otimes \sigma_z, \\ \gamma_5 &= \sigma_x \otimes I. \end{aligned}$$

The Clifford algebra is related to the Lorentz group thanks to the property of its commutator:

$$S^{\rho\sigma} = \frac{1}{4}\left[\gamma^\rho, \gamma^\sigma\right] = \frac{1}{2}\gamma^\rho\gamma^\sigma - \frac{1}{2}\eta^{\rho\sigma} = \begin{cases} 0, & \rho = \sigma \\ \frac{1}{2}\gamma^\rho\gamma^\sigma, & \rho \neq \sigma \end{cases} \tag{3.16}$$

This definition leads to two properties.

Property 3.3.1. $[S^{\mu\nu}, \gamma^\rho] = \gamma^\mu\eta^{\nu\rho} - \gamma^\nu\eta^{\rho\mu}$

Proof. If $\mu \neq \nu$, the property is proved by the following calculation:

$$\begin{aligned}
&[S^{\mu\nu}, \gamma^\rho] = \frac{1}{2}\left[\gamma^\mu\gamma^\nu, \gamma^\rho\right] \\
&= \frac{1}{2}\gamma^\mu\gamma^\nu\gamma^\rho - \frac{1}{2}\gamma^\rho\gamma^\mu\gamma^\nu \\
&= \frac{1}{2}\gamma^\mu\left\{\gamma^\nu, \gamma^\rho\right\} - \frac{1}{2}\gamma^\mu\gamma^\rho\gamma^\nu - \frac{1}{2}\left\{\gamma^\rho, \gamma^\mu\right\}\gamma^\nu + \frac{1}{2}\gamma^\mu\gamma^\rho\gamma^\nu \\
&= \gamma^\mu\eta^{\nu\rho} - \gamma^\nu\eta^{\rho\mu}
\end{aligned}$$

□

Before stating the other property, we recall briefly the definition of Lorentz algebra. Given a matrix in the Lorentz group, namely the group of the matrices $\Lambda^{\mu\nu}$ such that $\Lambda^\mu_\sigma\Lambda^\nu_\rho\eta^{\sigma\rho} = \eta^{\mu\nu}$ describing all the transformations of Minkowski spacetime, we can take $\Lambda^{\mu\nu}$ as an infinitesimal transformation

$$\Lambda^\mu_\nu = \delta^\mu_\nu + \omega^\mu_\nu \tag{3.17}$$

and study the algebraic structure of $\omega^{\mu\nu}$, which must be antisymmetric in order to fullfill $\Lambda^\mu_\sigma\Lambda^\nu_\rho\eta^{\sigma\rho} = \eta^{\mu\nu}$. In particular it fulfills the structure of *Lorentz Lie Algebra*:

Definition 3.3.1 (Lorentz Lie Algebra)**.** *A Lorentz Lie Algebra is a vector space M of complex 4×4 matrices over $\mathbb{C}$ equipped with a commutator $[\cdot,\cdot] : M \times M \longrightarrow M$ such that*

$$[\mathcal{M}^{\rho\sigma}, \mathcal{M}^{\tau\nu}] = \eta^{\sigma\tau}\mathcal{M}^{\rho\nu} - \eta^{\rho\tau}\mathcal{M}^{\sigma\nu} + \eta^{\rho\nu}\mathcal{M}^{\sigma\tau} - \eta^{\sigma\nu}\mathcal{M}^{\rho\tau} \tag{3.18}$$

Back to our properties, we discover that $S^{\mu\nu}$ forms a representation of the Lorentz Lie Algebra:

Property 3.3.2. $[S^{\mu\nu}, S^{\rho\sigma}] = \eta^{\nu\rho}S^{\mu\sigma} - \eta^{\mu\rho}S^{\nu\sigma} + \eta^{\mu\sigma}S^{\nu\rho} - \eta^{\nu\sigma}S^{\mu\rho}$.

Proof. Considering $\rho \neq \sigma$ and exploiting Property 3.3.1,

$$\begin{aligned}
&[S^{\mu\nu}, S^{\rho\sigma}] \\
&= \frac{1}{2}\left[S^{\mu\nu}, \gamma^{\rho}\gamma^{\sigma}\right] \\
&= \frac{1}{2}\left[S^{\mu\nu}, \gamma^{\rho}\right]\gamma^{\sigma} + \frac{1}{2}\gamma^{\rho}\left[S^{\mu\nu}, \gamma^{\sigma}\right] \\
&= \frac{1}{2}\gamma^{\mu}\gamma^{\sigma}\eta^{\nu\rho} - \frac{1}{2}\gamma^{\nu}\gamma^{\sigma}\eta^{\rho\mu} + \frac{1}{2}\gamma^{\rho}\gamma^{\mu}\eta^{\nu\sigma} - \frac{1}{2}\gamma^{\rho}\gamma^{\nu}\eta^{\sigma\mu}
\end{aligned}$$

but $\gamma^{\mu}\gamma^{\sigma} = 2S^{\mu\sigma} + \eta^{\mu\sigma}$ and thus we obtain the statement. □

It is clear that having a classification of the interactions derived from our hypothesis which exploits the Dirac γ matrices can be helpful in order to build interactions with properties particularly interesting in a relativistic setting, as in the case of Lorentz invariant interactions.

3.3.2 Classification

Given a set of 4×4 complex matrices $\{M_i\}_i$ and $\psi := \left(a_{u_1}, a_{d_1}, a_{u_2}, a_{d_2}\right)^{\top}$ bispinor, we can write a 4-linear polynomial in the fields in the following way:

$$\left(\psi^{\dagger} \otimes \psi^{\dagger}\right)^{\top} \left(M_i \otimes M_j\right) \left(\psi \otimes \psi\right) \tag{3.19}$$

where $\otimes$ is the usual tensor or *Krönecker product*, and $\psi^{\dagger} = \left(a^{\dagger}_{u_1}, a^{\dagger}_{d_1}, a^{\dagger}_{u_2}, a^{\dagger}_{d_2}\right)$

If we replace M_i and M_j with γ_i, $\gamma_i\gamma_j$ or $\gamma_i\gamma_j\gamma_k$ $i, j, k \in \{0, 1, 2, 3, 5\}$, we can recover polynomials contained in the 4-linear part of (3.10). This allows us to obtain a classification based on Dirac γ matrices or products of γs. We sum up our results in a table:

Interaction	λ_{35}	λ_{43}	λ_{19}	λ_{21}	λ_{18+}	λ_{18-}	λ_{30+}	λ_{30-}	λ_{26}	λ_{28}	λ_{31+}	λ_{31-}
$\gamma_0 \otimes \gamma_0$	-2	-2	2	2	0	0	0	0	0	0	0	0
$\gamma_1 \otimes \gamma_1$	0	0	0	-2	0	0	0	0	-2	0	-4	0
$\gamma_2 \otimes \gamma_2$	0	0	0	-2	0	0	0	0	2	0	-4	0
$\gamma_3 \otimes \gamma_3$	0	0	-2	0	0	0	0	0	0	-2	-4	0
$\gamma_5 \otimes \gamma_5$	0	0	2	0	0	0	0	0	0	-2	4	0
$\gamma_0 \otimes \gamma_0\gamma_0$	-2	2	0	0	0	0	0	0	0	0	0	0
$\gamma_1 \otimes \gamma_0\gamma_1$	0	0	0	0	0	0	0	0	0	0	0	-4
$\gamma_2 \otimes \gamma_0\gamma_2$	0	0	0	0	0	0	0	0	0	0	0	-4
$\gamma_3 \otimes \gamma_0\gamma_3$	0	0	0	0	0	0	0	0	0	0	0	-4
$\gamma_5 \otimes \gamma_0\gamma_5$	0	0	0	0	0	0	0	0	0	0	0	4
$\gamma_0 \otimes \gamma_5\gamma_0$	0	0	0	0	-2	0	2	0	0	0	0	0
$\gamma_1 \otimes \gamma_5\gamma_1$	0	0	0	0	2	0	-2	0	0	0	0	0
$\gamma_2 \otimes \gamma_5\gamma_2$	0	0	0	0	2	0	-2	0	0	0	0	0
$\gamma_3 \otimes \gamma_5\gamma_3$	0	0	0	0	2	0	-2	0	0	0	0	0
$\gamma_5 \otimes \gamma_5\gamma_5$	0	0	0	0	0	2	0	-2	0	0	0	0
$\gamma_0\gamma_0 \otimes \gamma_0\gamma_0$	-2	-2	-2	-2	0	0	0	0	0	0	0	0
$\gamma_0\gamma_1 \otimes \gamma_0\gamma_1$	0	0	0	2	0	0	0	0	2	0	-4	0
$\gamma_0\gamma_2 \otimes \gamma_0\gamma_2$	0	0	0	2	0	0	0	0	-2	0	-4	0
$\gamma_0\gamma_3 \otimes \gamma_0\gamma_3$	0	0	2	0	0	0	0	0	0	2	-4	0
$\gamma_0\gamma_5 \otimes \gamma_0\gamma_5$	0	0	-2	0	0	0	0	0	0	2	4	0
$\gamma_5\gamma_0 \otimes \gamma_5\gamma_0$	0	0	-2	0	0	0	0	0	0	2	4	0
$\gamma_5\gamma_1 \otimes \gamma_5\gamma_1$	2	2	0	0	0	0	0	0	2	-2	0	0
$\gamma_5\gamma_2 \otimes \gamma_5\gamma_2$	2	2	0	0	0	0	0	0	-2	-2	0	0
$\gamma_5\gamma_3 \otimes \gamma_5\gamma_3$	2	2	2	-2	0	0	0	0	0	0	0	0
$\gamma_5\gamma_5 \otimes \gamma_5\gamma_5$	-2	-2	-2	-2	0	0	0	0	0	0	0	0
$\gamma_0 \otimes \gamma_5\gamma_0\gamma_0$	0	0	0	0	0	-2	0	-2	0	0	0	0
$\gamma_1 \otimes \gamma_5\gamma_0\gamma_1$	0	0	0	0	2	0	2	0	0	0	0	0
$\gamma_2 \otimes \gamma_5\gamma_0\gamma_2$	0	0	0	0	2	0	2	0	0	0	0	0
$\gamma_3 \otimes \gamma_5\gamma_0\gamma_3$	0	0	0	0	2	0	2	0	0	0	0	0
$\gamma_5 \otimes \gamma_5\gamma_0\gamma_5$	0	0	0	0	0	2	0	2	0	0	0	0
$\gamma_0\gamma_0 \otimes \gamma_5\gamma_0\gamma_0$	0	0	0	0	0	2	0	-2	0	0	0	0
$\gamma_0\gamma_1 \otimes \gamma_5\gamma_0\gamma_1$	0	0	0	0	0	-2	0	2	0	0	0	0
$\gamma_0\gamma_2 \otimes \gamma_5\gamma_0\gamma_2$	0	0	0	0	0	-2	0	2	0	0	0	0
$\gamma_0\gamma_3 \otimes \gamma_5\gamma_0\gamma_3$	0	0	0	0	0	-2	0	2	0	0	0	0
$\gamma_0\gamma_5 \otimes \gamma_5\gamma_0\gamma_5$	0	0	0	0	-2	0	2	0	0	0	0	0
$\gamma_5\gamma_0 \otimes \gamma_5\gamma_0\gamma_0$	0	0	0	0	0	0	0	0	0	0	0	-4
$\gamma_5\gamma_1 \otimes \gamma_5\gamma_0\gamma_1$	-2	2	0	0	0	0	0	0	0	0	0	0
$\gamma_5\gamma_2 \otimes \gamma_5\gamma_0\gamma_2$	-2	2	0	0	0	0	0	0	0	0	0	0
$\gamma_5\gamma_3 \otimes \gamma_5\gamma_0\gamma_3$	-2	2	0	0	0	0	0	0	0	0	0	0
$\gamma_5\gamma_5 \otimes \gamma_5\gamma_0\gamma_5$	2	-2	0	0	0	0	0	0	0	0	0	0

Where $\lambda_{i\pm} = \lambda_i \pm \bar{\lambda}_i$. As an example on how to read the table, let us consider the case $\gamma_5\gamma_5 \otimes \gamma_5\gamma_0\gamma_5$:

$$\left(\psi^\dagger \otimes \psi^\dagger\right)^\top (\gamma_5\gamma_5 \otimes \gamma_5\gamma_0\gamma_5)\,(\psi \otimes \psi) = 2a^\dagger_{u_1} a_{u_1} a^\dagger_{d_1} a_{d_1} - 2\lambda_{43} a^\dagger_{u_2} a_{u_2} a^\dagger_{d_2} a_{d_2}. \tag{3.20}$$

Comparing with (3.10), this means that $\lambda_{35} = 2$, $\lambda_{43} = -2$, while $\lambda_i = 0$, $i \neq \{35, 43\}$.

We can also group in *families* the tensor products giving rise to the same tuple of coefficients (here called *representative*) modulo a constant. We obtain:

Representative	Family
[-2, -2, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0]	$\gamma_0 \otimes \gamma_0$
[0, 0, 0, -2, 0, 0, 0, 0, -2, 0, -4, 0]	$\gamma_1 \otimes \gamma_1$
[0, 0, 0, -2, 0, 0, 0, 0, 2, 0, -4, 0]	$\gamma_2 \otimes \gamma_2$
[0, 0, -2, 0, 0, 0, 0, 0, 0, -2, -4, 0]	$\gamma_3 \otimes \gamma_3$
[0, 0, 2, 0, 0, 0, 0, 0, 0, -2, 4, 0]	$\gamma_5 \otimes \gamma_5$
[-2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]	$\gamma_0 \otimes \gamma_0\gamma_0$ $\gamma_5\gamma_1 \otimes \gamma_5\gamma_0\gamma_1$ $\gamma_5\gamma_2 \otimes \gamma_5\gamma_0\gamma_2$ $\gamma_5\gamma_3 \otimes \gamma_5\gamma_0\gamma_3$ $\gamma_5\gamma_5 \otimes \gamma_5\gamma_0\gamma_5$
[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -4]	$\gamma_1 \otimes \gamma_0\gamma_1$ $\gamma_2 \otimes \gamma_0\gamma_2$ $\gamma_3 \otimes \gamma_0\gamma_3$ $\gamma_5 \otimes \gamma_0\gamma_5$ $\gamma_5\gamma_0 \otimes \gamma_5\gamma_0\gamma_0$
[0, 0, 0, 0, -2, 0, 2, 0, 0, 0, 0, 0]	$\gamma_0 \otimes \gamma_5\gamma_0$ $\gamma_1 \otimes \gamma_5\gamma_1$ $\gamma_2 \otimes \gamma_5\gamma_2$ $\gamma_3 \otimes \gamma_5\gamma_3$ $\gamma_0\gamma_5 \otimes \gamma_5\gamma_0\gamma_5$
[0, 0, 0, 0, 0, 2, 0, -2, 0, 0, 0, 0]	$\gamma_5 \otimes \gamma_5\gamma_5$ $\gamma_0\gamma_0 \otimes \gamma_5\gamma_0\gamma_0$ $\gamma_0\gamma_1 \otimes \gamma_5\gamma_0\gamma_1$ $\gamma_0\gamma_2 \otimes \gamma_5\gamma_0\gamma_2$ $\gamma_0\gamma_3 \otimes \gamma_5\gamma_0\gamma_3$
[-2, -2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0]	$\gamma_0\gamma_0 \otimes \gamma_0\gamma_0$ $\gamma_5\gamma_5 \otimes \gamma_5\gamma_5$
[0, 0, 0, 2, 0, 0, 0, 0, 2, 0, -4, 0]	$\gamma_0\gamma_1 \otimes \gamma_0\gamma_1$
[0, 0, 0, 2, 0, 0, 0, 0, -2, 0, -4, 0]	$\gamma_0\gamma_2 \otimes \gamma_0\gamma_2$
[0, 0, 2, 0, 0, 0, 0, 0, 0, 2, -4, 0]	$\gamma_0\gamma_3 \otimes \gamma_0\gamma_3$
[0, 0, -2, 0, 0, 0, 0, 0, 0, 2, 4, 0]	$\gamma_0\gamma_5 \otimes \gamma_0\gamma_5$ $\gamma_5\gamma_0 \otimes \gamma_5\gamma_0$
[2, 2, 0, 0, 0, 0, 0, 0, 2, -2, 0, 0]	$\gamma_5\gamma_1 \otimes \gamma_5\gamma_1$
[2, 2, 0, 0, 0, 0, 0, 0, -2, -2, 0, 0]	$\gamma_5\gamma_2 \otimes \gamma_5\gamma_2$
[2, 2, 2, -2, 0, 0, 0, 0, 0, 0, 0, 0]	$\gamma_5\gamma_3 \otimes \gamma_5\gamma_3$
[0, 0, 0, 0, 0, -2, 0, -2, 0, 0, 0, 0]	$\gamma_0 \otimes \gamma_5\gamma_0\gamma_0$ $\gamma_5 \otimes \gamma_5\gamma_0\gamma_5$
[0, 0, 0, 0, 2, 0, 2, 0, 0, 0, 0, 0]	$\gamma_1 \otimes \gamma_5\gamma_0\gamma_1$ $\gamma_2 \otimes \gamma_5\gamma_0\gamma_2$ $\gamma_3 \otimes \gamma_5\gamma_0\gamma_3$

For our purposes, it is sufficient taking 12 of them, since the vectors obtained in this way span a 12- dimensional space. In particular we can ignore families from line 11 to line 17, which are redundant. Remembering that $\gamma_0\gamma_0 = I$, $\gamma_5\gamma_5 = I$ and $\gamma_5\gamma_0\gamma_5 = -\gamma_0$, we get:

Representative	Family
[-2, -2, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0]	$\gamma_0 \otimes \gamma_0$
[0, 0, 0, -2, 0, 0, 0, 0, -2, 0, -4, 0]	$\gamma_1 \otimes \gamma_1$
[0, 0, 0, -2, 0, 0, 0, 0, 2, 0, -4, 0]	$\gamma_2 \otimes \gamma_2$
[0, 0, -2, 0, 0, 0, 0, 0, 0, -2, -4, 0]	$\gamma_3 \otimes \gamma_3$
[0, 0, 2, 0, 0, 0, 0, 0, 0, -2, 4, 0]	$\gamma_5 \otimes \gamma_5$
[-2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]	$\gamma_0 \otimes I$ $\gamma_5\gamma_1 \otimes \gamma_5\gamma_0\gamma_1$ $\gamma_5\gamma_2 \otimes \gamma_5\gamma_0\gamma_2$ $\gamma_5\gamma_3 \otimes \gamma_5\gamma_0\gamma_3$ $-I \otimes \gamma_0$
[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -4]	$\gamma_1 \otimes \gamma_0\gamma_1$ $\gamma_2 \otimes \gamma_0\gamma_2$ $\gamma_3 \otimes \gamma_0\gamma_3$ $\gamma_5 \otimes \gamma_0\gamma_5$ $\gamma_5\gamma_0 \otimes \gamma_5$
[0, 0, 0, 0, -2, 0, 2, 0, 0, 0, 0, 0]	$\gamma_0 \otimes \gamma_5\gamma_0$ $\gamma_1 \otimes \gamma_5\gamma_1$ $\gamma_2 \otimes \gamma_5\gamma_2$ $\gamma_3 \otimes \gamma_5\gamma_3$ $-\gamma_0\gamma_5 \otimes \gamma_0$
[0, 0, 0, 0, 0, 2, 0, -2, 0, 0, 0, 0]	$\gamma_5 \otimes I$ $I \otimes \gamma_5$ $\gamma_0\gamma_1 \otimes \gamma_5\gamma_0\gamma_1$ $\gamma_0\gamma_2 \otimes \gamma_5\gamma_0\gamma_2$ $\gamma_0\gamma_3 \otimes \gamma_5\gamma_0\gamma_3$
[-2, -2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0]	$I \otimes I$
[0, 0, 0, 0, 0, -2, 0, -2, 0, 0, 0, 0]	$\gamma_0 \otimes \gamma_5$ $-\gamma_5 \otimes \gamma_0$
[0, 0, 0, 0, 2, 0, 2, 0, 0, 0, 0, 0]	$\gamma_1 \otimes \gamma_5\gamma_0\gamma_1$ $\gamma_2 \otimes \gamma_5\gamma_0\gamma_2$ $\gamma_3 \otimes \gamma_5\gamma_0\gamma_3$

As an example, we show that this procedure allows to obtain 12 independent λ_is with the following (clearly not unique) linear combination of the vectors:

$$
\begin{aligned}
\lambda_{35} =&(-\frac{1}{8},0,0,0,0,-\frac{1}{4},0,0,0,-\frac{1}{8},0,0)\\
\lambda_{43} =&(-\frac{1}{8},0,0,0,0,\frac{1}{4},0,0,0,-\frac{1}{8},0,0)\\
\lambda_{19} =&(\frac{1}{8},\frac{1}{8},\frac{1}{8},-\frac{1}{8},\frac{1}{8},0,0,0,0,-\frac{1}{8},0,0)\\
\lambda_{21} =&(\frac{1}{8},-\frac{1}{8},-\frac{1}{8},\frac{1}{8},-\frac{1}{8},0,0,0,0,-\frac{1}{8},0,0)\\
\lambda_{18+} =&(0,0,0,0,0,0,0,-\frac{1}{4},0,0,0,\frac{1}{4})\\
\lambda_{18-} =&(0,0,0,0,0,0,0,0,\frac{1}{4},0,-\frac{1}{4},0)\\
\lambda_{30+} =&(0,0,0,0,0,0,0,\frac{1}{4},0,0,0,\frac{1}{4})\\
\lambda_{30-} =&(0,0,0,0,0,0,0,0,-\frac{1}{4},0,-\frac{1}{4},0)\\
\lambda_{26} =&(0,-\frac{1}{4},\frac{1}{4},0,0,0,0,0,0,0,0,0)\\
\lambda_{28} =&(0,0,0,-\frac{1}{4},-\frac{1}{4},0,0,0,0,0,0,0)\\
\lambda_{31+} =&(-\frac{1}{16},-\frac{1}{16},-\frac{1}{16},-\frac{1}{16},\frac{1}{16},0,0,0,0,\frac{1}{16},0,0)\\
\lambda_{31-} =&(0,0,0,0,0,0,-\frac{1}{4},0,0,0,0,0)
\end{aligned}
\tag{3.21}
$$

where each entry acts as coefficient for each representative found in the previous table (the ordering of the entries is arbitrary and in this case given by the representative ordering in the table).

These 4-linear terms can be used to study interactions in the *two particle sector*. In the next chapter we will study the Dirac QW for two particles and we concentrate on one non-trivial special interaction.

CHAPTER 4

A SPECIAL INTERACTION IN THE TWO PARTICLE SECTOR

Given the quadrilinear polynomial describing the most general isotropic number preserving interaction for the Dirac automata, namely

$$\begin{aligned}
H_{x,\text{Dirac},4} =& \lambda_{18}(a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2} + a_{u_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2}) + \overline{\lambda_{18}}(a^\dagger_{d_1}a^\dagger_{u_2}a_{u_2}a_{d_2} + a^\dagger_{u_1}a_{u_2}a^\dagger_{d_2}a_{d_2}) + \\
& \lambda_{19}(a^\dagger_{d_1}a_{d_1}a^\dagger_{d_2}a_{d_2} + a^\dagger_{u_1}a_{u_1}a^\dagger_{u_2}a_{u_2}) + \\
& \lambda_{21}(a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}a_{u_2} + a^\dagger_{u_1}a_{u_1}a^\dagger_{d_2}a_{d_2}) + \\
& \lambda_{26}(a_{u_1}a^\dagger_{d_1}a_{u_2}a^\dagger_{d_2} + a^\dagger_{u_1}a_{d_1}a^\dagger_{u_2}a_{d_2}) + \\
& \lambda_{28}(a_{u_1}a^\dagger_{d_1}a^\dagger_{u_2}a_{d_2} + a^\dagger_{u_1}a_{d_1}a_{u_2}a^\dagger_{d_2}) + \\
& \lambda_{30}(a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_2} + a^\dagger_{u_1}a^\dagger_{d_1}a_{d_1}a_{u_2}) + \overline{\lambda_{30}}(a^\dagger_{u_1}a_{u_1}a_{d_1}a^\dagger_{d_2} + a_{u_1}a^\dagger_{d_1}a_{d_1}a^\dagger_{u_2}) + \\
& \lambda_{31}a^\dagger_{u_1}a^\dagger_{d_1}a_{u_2}a_{d_2} + \overline{\lambda_{31}}a_{u_1}a_{d_1}a^\dagger_{u_2}a^\dagger_{d_2} + \\
& \lambda_{35}a^\dagger_{u_1}a_{u_1}a^\dagger_{d_1}a_{d_1} + \\
& \lambda_{43}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2}a_{d_2},
\end{aligned} \tag{4.1}$$

we intend to identify a class of non trivial interactions for systems of two particles evolved through the Dirac automaton. We will restrict the geometry of the lattice to the monodimensional case, even if we will consider the interaction Hamiltonian for the 3D case described in the prevoius chapter. This hypothesis is meant for allowing us to treat more easily the problem of finding analytical solutions. This is possible since the isotropy group for our interaction Hamiltonian, $U_L = \{I, i\sigma_x, i\sigma_y, i\sigma_z\}$ is more restrictive than $U_L = \{I\}$ and $\{I, i\sigma_x\}$, isotropy groups for the 1D lattice.

1. FREE EVOLUTION IN THE TWO-PARTICLE SECTOR

Before approaching the study of interactions, we need to explain how the free evolution for the Dirac QW works provided a state of two particles. In particular we need to explicit (2.67) for our case.
A single particle with two internal degrees of freedom is evolved linearly through the Weyl QW, namely

$$W = \sum_{\mathbf{h}_i \in S} T_{\mathbf{h}_i} \otimes W(\mathbf{h}_i). \tag{4.2}$$

For the 1D lattice, ignoring self interactions (i.e. $W(\mathbf{0})$) we have

$$W(\mathbf{h}_1) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad W(\mathbf{h}_1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{4.3}$$

Since we are evolving a spinor $(a_u, a_d)^\top$, we can rewrite the Weyl QW as a matrix acting on the space of the internal degrees of freedom:

$$W = \begin{pmatrix} T_{\mathbf{h}_1} & 0 \\ 0 & T_{-\mathbf{h}_1} \end{pmatrix} = \begin{pmatrix} T_{\mathbf{h}_1} & 0 \\ 0 & T^\dagger_{\mathbf{h}_1} \end{pmatrix} \tag{4.4}$$

with $T_{\mathbf{h}_1} = T^\dagger_{\mathbf{h}_1}$ since its action on the lattice reverses the action of $T_{\mathbf{h}_1}$.

The Dirac QW describes the evolution of a single particle with four internal degrees of freedom, in particular the evolution is obtained through the coupling of two Weyl QW. Rewriting (2.67) with $m = 0$ in (4.4) form:

$$D = \begin{pmatrix} T_{\mathbf{h}_1} & 0 & 0 & 0 \\ 0 & T^\dagger_{\mathbf{h}_1} & 0 & 0 \\ 0 & 0 & T^\dagger_{\mathbf{h}_1} & 0 \\ 0 & 0 & 0 & T_{\mathbf{h}_1} \end{pmatrix}. \tag{4.5}$$

A remark on the algebra: $\otimes$ is usually intended as Kronecker product, but in (2.67) case it has to be interpreted as Fermionic tensor product for the internal DoF, where we couple two spinors obtaining a bispinor $|\psi\rangle = (a_{u_1}, a_{u_1}, a_{d_2}, a_{d_2})^\top \in \mathcal{H}$. This means that, algebraically, in the massless case we have a direct sum of the two Weyl QW involved in the coupling.

If we consider two particles states, each one with 4 Fermionic internal DoF evolved through a Dirac automaton, we have to take the (Kronecker) tensor product of (4.5), $D \otimes D$, acting on the anti-symmetric subspace of $\ell^2(G) \otimes \ell^2(G) \otimes$

$\mathcal{H} \otimes \mathcal{H}$. This is called the *Two- particle sector* of the evolution.

Explicitly, defining $T_{++} := T_h \otimes T_h$,$T_{+-} := T_h \otimes T_h^\dagger$,$T_{-+} := T_h^\dagger \otimes T_h$,$T_{--} := T_h^\dagger \otimes T_h^\dagger$, we have (the order of the rows is $|u_1\rangle|u_1\rangle$, $|u_1\rangle|d_1\rangle$, $|u_1\rangle|u_2\rangle$, $|u_1\rangle|d_2\rangle$, $|d_1\rangle|u_1\rangle$, $|d_1\rangle|d_1\rangle$, $|d_1\rangle|u_2\rangle$, $|d_1\rangle|d_2\rangle$, $|u_2\rangle|u_1\rangle$, $|u_2\rangle|d_1\rangle$, $|u_2\rangle|u_2\rangle$, $|u_2\rangle|d_2\rangle$, $|d_2\rangle|u_1\rangle$, $|d_2\rangle|d_1\rangle$, $|d_2\rangle|u_2\rangle$, $|d_2\rangle|d_2\rangle$):

$$D = D \otimes D =$$
$$\begin{pmatrix}
T_{++} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & T_{+-} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & T_{+-} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & T_{++} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & T_{-+} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & T_{--} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & T_{--} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{-+} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{-+} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{--} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{--} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{-+} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{++} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{+-} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{+-} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{++}
\end{pmatrix}$$

Another useful basis for the spatial degrees of freedom is the $|y\rangle|w\rangle$ basis, with $y := x_1 - x_2$ and $w := x_1 + x_2$. In this case we have to map the action of T_h in the new basis and then rewrite the two particles sector matrix:

$$\begin{aligned}
T_h \otimes T_h |i\rangle|j\rangle|x_1\rangle|x_2\rangle &= |i\rangle|j\rangle|x_1 + h\rangle|x_2 + h\rangle \mapsto |i\rangle|j\rangle|y\rangle|w + 2h\rangle = I_y \otimes T_h^2 |i\rangle|j\rangle|y\rangle|w\rangle \\
T_h \otimes T_h^\dagger |i\rangle|j\rangle|x_1\rangle|x_2\rangle &= |i\rangle|j\rangle|x_1 + h\rangle|x_2 - h\rangle \mapsto |i\rangle|j\rangle|y + 2h\rangle|w\rangle = T_h^2 \otimes I_w |i\rangle|j\rangle|y\rangle|w\rangle \\
T_h^\dagger \otimes T_h |i\rangle|j\rangle|x_1\rangle|x_2\rangle &= |i\rangle|j\rangle|x_1 - h\rangle|x_2 + h\rangle \mapsto |i\rangle|j\rangle|y - 2h\rangle|w\rangle = T_h^{\dagger 2} \otimes I_w |i\rangle|j\rangle|y\rangle|w\rangle \\
T_h^\dagger \otimes T_h^\dagger |i\rangle|j\rangle|x_1\rangle|x_2\rangle &= |i\rangle|j\rangle|x_1 - h\rangle|x_2 - h\rangle \mapsto |i\rangle|j\rangle|y\rangle|w - 2h\rangle = I_y \otimes T_h^{\dagger 2} |i\rangle|j\rangle|y\rangle|w\rangle
\end{aligned} \tag{4.6}$$

And the matrix becomes, defining $T_w^2 := I_y \otimes T_h^2$, $T_y^2 := T_h^2 \otimes I_w$, $T_w^{\dagger 2} := I_y \otimes T_h^{\dagger 2}$, $T_y^{\dagger 2} := T_h^{\dagger 2} \otimes I_w$

$$D = D \otimes D =$$

$$\begin{pmatrix}
T_w^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & T_y^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & T_y^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & T_w^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & T_y^{\dagger 2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & T_w^{\dagger 2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & T_w^{\dagger 2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & T_y^{\dagger 2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_y^{\dagger 2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_w^{\dagger 2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_w^{\dagger 2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_y^{\dagger 2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_w^2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_y^2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_y^2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & T_w^2
\end{pmatrix}$$

As we will see, we can even consider only smaller sectors of the matrices presented in this section depending on the subspace of $\mathcal{H} \otimes \mathcal{H}$ on which the interactions considered acts and the order of the rows is not restrictive.

2. CASE OF STUDY

Observing (4.5), we understand that each internal DoF is associated to a translation on the lattice ruling its propagation. In particular, if we conventionally consider $T_{\mathbf{h}_1}$ as a translation to the right on the lattice, the internal DoF- propagation mapping is the following:

$$\begin{aligned}
u_1 &\longrightarrow \\
d_1 &\longleftarrow \\
u_2 &\longleftarrow \\
d_2 &\longrightarrow
\end{aligned} \tag{4.7}$$

We will now see how this fact is related to the interactions classified and how this allows us to identify the most interesting ones.
As an example let us consider

$$H := a_{u_1}(x)a_{d_1}^\dagger(x)a_{u_2}^\dagger(x)a_{d_2}(x) + a_{u_1}^\dagger(x)a_{d_1}(x)a_{u_2}(x)a_{d_2}^\dagger(x) \tag{4.8}$$

If we consider its action on the basis $\{|i\rangle|j\rangle\}$, with $i, j \in \{u_1, d_1, u_2, d_2\}$, (4.8) gives non-null vectors only on the subspace $\{|u_1\rangle|d_2\rangle, |d_1\rangle|u_2\rangle, |u_2\rangle|d_1\rangle, |d_2\rangle|u_1\rangle, \}$. Taking the free evolution on this subspace, we obtain:

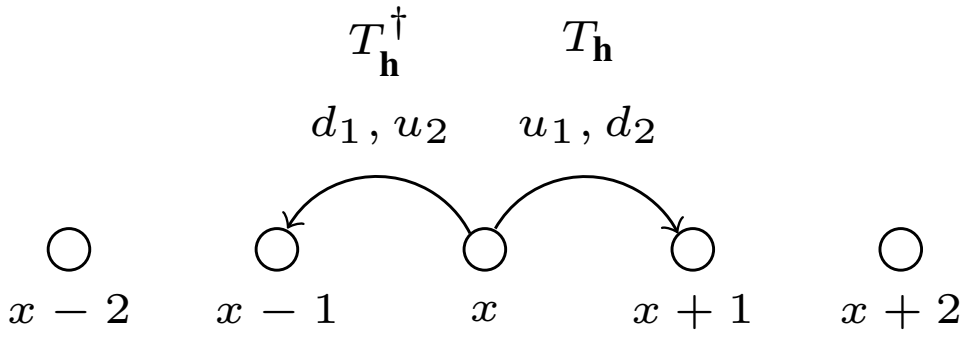

Figure 4.1: Free evolution rule on the 1D lattice for different internal degrees of freedom.

$$\begin{pmatrix} T_{\mathbf{h}_1}\otimes T_{\mathbf{h}_1} & 0 & 0 & 0 \\ 0 & T^{\dagger}_{\mathbf{h}_1}\otimes T^{\dagger}_{\mathbf{h}_1} & 0 & 0 \\ 0 & 0 & T^{\dagger}_{\mathbf{h}_1}\otimes T^{\dagger}_{\mathbf{h}_1} & 0 \\ 0 & 0 & 0 & T_{\mathbf{h}_1}\otimes T_{\mathbf{h}_1} \end{pmatrix}. \tag{4.9}$$

Remembering the action of the operators $T_{\mathbf{h}_1}$ and $T^{\dagger}_{\mathbf{h}_1}$ on $\ell^2(G)$,

$$\begin{aligned} T_{\mathbf{h}_1}|x\rangle &= |x+1\rangle \\ T^{\dagger}_{\mathbf{h}_1}|x\rangle &= |x-1\rangle, \qquad \forall x \in G, \end{aligned}$$

and considering that $T_{\mathbf{h}_1}\otimes T_{\mathbf{h}_1}$ and $T^{\dagger}_{\mathbf{h}_1}\otimes T^{\dagger}_{\mathbf{h}_1}$ act on vectors $|x_1\rangle|x_2\rangle \in \ell^2(G)\otimes \ell^2(G)$, but (4.8) is non trivial only if $x_1 = x_2$, it is convenient performing the following change of basis:

$$|x_1\rangle|x_2\rangle \mapsto |y\rangle|w\rangle := |x_1 - x_2\rangle|x_1 + x_2\rangle. \tag{4.10}$$

The interaction will act non trivially only on vectors with $|y\rangle = |0\rangle$.

On this basis the free evolution becomes, in our subspace of interest,

$$\begin{pmatrix} I\otimes T^2_{\mathbf{h}_1} & 0 & 0 & 0 \\ 0 & I\otimes T^{\dagger 2}_{\mathbf{h}_1} & 0 & 0 \\ 0 & 0 & I^{\dagger}\otimes T^{\dagger 2}_{\mathbf{h}_1} & 0 \\ 0 & 0 & 0 & I\otimes T^2_{\mathbf{h}_1} \end{pmatrix}. \tag{4.11}$$

but this means that in the subspace interested by the interaction it acts always as the identity on the Hilbert space of vectors $|y\rangle$. This means that during the

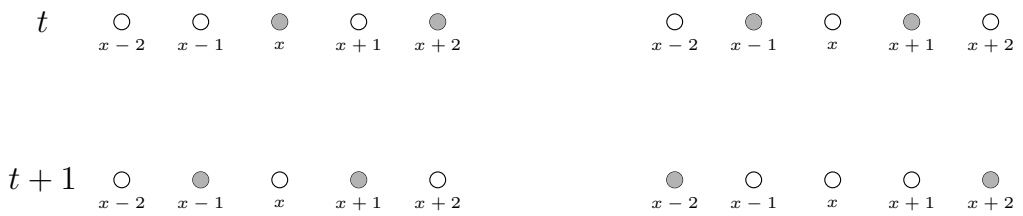

Figure 4.2: Translation of degrees of freedom with the same relative distance (left) and translation of degrees of freedom with different relative distance (right). We are interested in studying non trivial interactions acting on subspaces of the internal DoF Hilbert space translating in different directions.

free evolution step the relative position of the particles does not change and, in particular, that solving the eigenvalue problem $e^{iH}(D \otimes D)|\psi\rangle = e^{-i\omega}|\psi\rangle$ is not of particular interest and it can be proved, with the same techniques we will show later in this chapter, that its solutions are plane waves. This argument could also be inferred observing (4.8): we have the creation of modes d_1 and u_2 and the destruction of the remaining ones (and viceversa for the second term). Remembering (4.7), the interaction acts on modes leaving unaltered their recioprocal direction of propagation. We thus decided to investigate the other class of interactions, namely the ones transforming couples of modes into others with a different reciprocal direction of propagation.

3. A SPECIAL INTERACTION

We are therefore interested in describing the interaction marked with λ_{18} and with λ_{30}. Modulo permutations of the indices, we observe that they are the same interaction, thus we will concentrate on λ_{18}.
Let us consider the interaction Hamiltonian:

$$H_{\text{int}} = \lambda_{18}(a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2} + a_{u_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2}) + \overline{\lambda_{18}}(a^\dagger_{d_1}a^\dagger_{u_2}a_{u_2}a_{d_2} + a^\dagger_{u_1}a_{u_2}a^\dagger_{d_2}a_{d_2}) \tag{4.12}$$

The choice we make for the coupling parameter in order to have an Hermitian operator is $\lambda_{18} = \lambda$ and $\overline{\lambda_{18}} = -\overline{\lambda}$. Thus H_{int} becomes

$$H_{\text{int}} = \lambda(a_{d_1}a^\dagger_{u_2}a_{u_2}a^\dagger_{d_2} + a_{u_1}a^\dagger_{u_2}a^\dagger_{d_2}a_{d_2}) - \overline{\lambda}(a^\dagger_{d_1}a^\dagger_{u_2}a_{u_2}a_{d_2} + a^\dagger_{u_1}a_{u_2}a^\dagger_{d_2}a_{d_2}) \tag{4.13}$$

We can easily see that our subspace of interest is, in the two particles sector, $span\{|u_1\rangle|d_2\rangle,\ |d_1\rangle|u_2\rangle, |u_2\rangle|d_2\rangle,\ |d_2\rangle|u_1\rangle, |u_2\rangle|d_1\rangle, |d_2\rangle|u_2\rangle\}$. The Hamiltonian H_{int} acts in this way:

$$
\begin{aligned}
H_{\text{int}}|u_1\rangle|d_2\rangle &= -\lambda|u_2\rangle|d_2\rangle \\
H_{\text{int}}|d_1\rangle|u_2\rangle &= -\lambda|d_2\rangle|u_2\rangle \\
H_{\text{int}}|u_2\rangle|d_1\rangle &= -\lambda|u_2\rangle|d_2\rangle \\
H_{\text{int}}|u_2\rangle|d_2\rangle &= -\bar{\lambda}|u_2\rangle|d_1\rangle - \bar{\lambda}|u_1\rangle|d_2\rangle \\
H_{\text{int}}|d_2\rangle|u_1\rangle &= -\lambda|d_2\rangle|u_2\rangle \\
H_{\text{int}}|d_2\rangle|u_2\rangle &= -\bar{\lambda}|d_1\rangle|u_2\rangle - \bar{\lambda}|d_2\rangle|u_1\rangle
\end{aligned}
\tag{4.14}
$$

A possible matrix representation is (the order of the rows is $|u_1\rangle|d_2\rangle$, $|u_2\rangle|d_1\rangle$, $|u_2\rangle|d_2\rangle$, $|d_2\rangle|u_1\rangle$, $|d_1\rangle|u_2\rangle$, $|d_2\rangle|u_2\rangle$):

$$
\begin{pmatrix}
0 & 0 & -\bar{\lambda} & 0 & 0 & 0 \\
0 & 0 & -\bar{\lambda} & 0 & 0 & 0 \\
-\lambda & -\lambda & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\bar{\lambda} \\
0 & 0 & 0 & 0 & 0 & -\bar{\lambda} \\
0 & 0 & 0 & -\lambda & -\lambda & 0
\end{pmatrix}
\tag{4.15}
$$

We exponentiate it in order to get $e^{iH_{\text{int}}}$ matrix representation

$$
\begin{pmatrix}
c+\frac{1}{2} & c-\frac{1}{2} & s & 0 & 0 & 0 \\
c-\frac{1}{2} & c+\frac{1}{2} & s & 0 & 0 & 0 \\
\tilde{s} & \tilde{s} & 2c & 0 & 0 & 0 \\
0 & 0 & 0 & c+\frac{1}{2} & c-\frac{1}{2} & s \\
0 & 0 & 0 & c-\frac{1}{2} & c+\frac{1}{2} & s \\
0 & 0 & 0 & \tilde{s} & \tilde{s} & 2c
\end{pmatrix}
\tag{4.16}
$$

with

$$
\begin{aligned}
c &:= \frac{\cos\left(\sqrt{2}|\lambda|\right)}{2} \\
s &:= -\frac{1}{\sqrt{2}}\frac{|\lambda|}{\overline{\lambda}} i \sin\left(\sqrt{2}|\lambda|\right) \\
\tilde{s} &:= -\frac{1}{\sqrt{2}}\frac{\overline{\lambda}}{|\lambda|} i \sin\left(\sqrt{2}|\lambda|\right)
\end{aligned}
\tag{4.17}
$$

We can map the entries of the matrix in the following way:

$$\begin{aligned} A &:= c + \frac{1}{2} \\ B &:= \tilde{s} \\ C &:= c - \frac{1}{2} \\ D &:= 2c \\ E &:= s \end{aligned} \tag{4.18}$$

Obtaining thus

$$\begin{pmatrix} A & C & E & 0 & 0 & 0 \\ C & A & E & 0 & 0 & 0 \\ B & B & D & 0 & 0 & 0 \\ 0 & 0 & 0 & A & C & E \\ 0 & 0 & 0 & C & A & E \\ 0 & 0 & 0 & B & B & D \end{pmatrix} \tag{4.19}$$

It is easy to verify that the determinant of each 3×3 minor is $4c^2 - 2s\tilde{s} = 1$ and thus that the matrix is unitary as we expected, since it is obtained by exponentiating a skew-Hermitian matrix.

In the subspace of our interest we have the following free-evolution:

$$\begin{pmatrix} T_h \otimes T_h & 0 & 0 & 0 & 0 & 0 \\ 0 & T_h^\dagger \otimes T_h^\dagger & 0 & 0 & 0 & 0 \\ 0 & 0 & T_h^\dagger \otimes T_h & 0 & 0 & 0 \\ 0 & 0 & 0 & T_h \otimes T_h & 0 & 0 \\ 0 & 0 & 0 & 0 & T_h^\dagger \otimes T_h^\dagger & 0 \\ 0 & 0 & 0 & 0 & 0 & T_h \otimes T_h^\dagger \end{pmatrix} \tag{4.20}$$

In the $|y\rangle|w\rangle$, $y := x_1 - x_2$ and $w := x_1 + x_2$ basis the free evolution matrix becomes

$$\begin{pmatrix} I_y \otimes T_h^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & I_y \otimes T_h^{\dagger 2} & 0 & 0 & 0 & 0 \\ 0 & 0 & T_h^{\dagger 2} \otimes I_w & 0 & 0 & 0 \\ 0 & 0 & 0 & I_y \otimes T_h^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & I_y \otimes T_h^{\dagger 2} & 0 \\ 0 & 0 & 0 & 0 & 0 & T_h^2 \otimes I_w \end{pmatrix} \tag{4.21}$$

and (4.19) will act only on the subspace with $|y\rangle = |0\rangle$.

Defining $|p\rangle := \frac{1}{2\pi}\sum_w e^{-ipw}|w\rangle$, $p \in (-\pi, \pi]$ we easily see that the free evolution becomes

$$D \otimes D = \begin{pmatrix} e^{2ip} & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{-2ip} & 0 & 0 & 0 & 0 \\ 0 & 0 & T_h^{\dagger 2} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{2ip} & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-2ip} & 0 \\ 0 & 0 & 0 & 0 & 0 & T_h^2 \end{pmatrix} \tag{4.22}$$

Our goal is solving the following equation

$$J(D \otimes D)|\psi\rangle = e^{-i\omega}|\psi\rangle \tag{4.23}$$

Let us write explicitly $|\psi\rangle$:

$$|\psi\rangle = \sum_{i,y} c_{i,y}|i\rangle|y\rangle \tag{4.24}$$

with the new practical mapping for the internal degree of freedom, living in the space of $|i\rangle$ vectors

$$\begin{aligned} |u_1\rangle|d_2\rangle &\mapsto |1\rangle \\ |u_2\rangle|d_1\rangle &\mapsto |\bar{2}\rangle \\ |u_2\rangle|d_2\rangle &\mapsto |3\rangle \\ |d_2\rangle|u_1\rangle &\mapsto |\bar{1}\rangle \\ |d_1\rangle|u_2\rangle &\mapsto |2\rangle \\ |d_2\rangle|u_2\rangle &\mapsto |\bar{3}\rangle \end{aligned} \tag{4.25}$$

Since we are working with Fermions, it can be useful to exploit the antisymmetry of states:

$$|\psi\rangle = \sum_{i,y} c_{i,y}\left(|i\rangle|y\rangle - |\bar{i}\rangle|-y\rangle\right) \tag{4.26}$$

which means $c_{i,y} = -c_{\bar{i},-y}$.

In particular the projection on the antisymmetric space which maps $|i\rangle|y\rangle$ to $|i\rangle|y\rangle - |\bar{i}\rangle|-y\rangle$ commutes with both $D \otimes D$ and J.
We can also observe that, since the interaction acts only on the sector with $y = 0$ and the free evolution shifts $|3\rangle|y\rangle \mapsto |3\rangle|y-2\rangle$ and $|\bar{3}\rangle|y\rangle \mapsto |\bar{3}\rangle|y+2\rangle$, we can

split further $|\psi\rangle$ in an even sector, interested by the interaction, and an odd one, using the following projectors:

$$\begin{aligned} P_{\text{even}} &= \sum_y I \otimes |2y\rangle\langle 2y| \\ P_{\text{odd}} &= \sum_y I \otimes |2y+1\rangle\langle 2y+1| \end{aligned} \tag{4.27}$$

Thus

$$|\psi_e\rangle := P_{\text{even}}|\psi\rangle = \sum_{i,y} c_{i,y} \left(|i\rangle|2y\rangle - |\bar{i}\rangle| - 2y\rangle \right) \tag{4.28}$$

and

$$|\psi_o\rangle := P_{\text{odd}}|\psi\rangle = \sum_{i,y} c_{i,y} \left(|i\rangle|2y+1\rangle - |\bar{i}\rangle| - (2y+1)\rangle \right) \tag{4.29}$$

4.3.1 Applying $J(D \otimes D)$

Acting on $|\psi_o\rangle$ and $|\psi_e\rangle$ with the free evolution:

$$\begin{aligned} (D \otimes D)|\psi_o\rangle = &\sum_y c_{1,2y+1} e^{2ip} (|1\rangle|2y+1\rangle - |\bar{1}\rangle| - (2y+1)\rangle) + \\ &e^{-2ip} c_{2,2y+1} (|2\rangle|2y+1\rangle - |\bar{2}\rangle| - (2y+1)\rangle) + \\ &c_{3,2y+1} (|3\rangle|2(y+1)+1\rangle - |\bar{3}\rangle| - 2(y+1) - 1\rangle) \end{aligned} \tag{4.30}$$

$$\begin{aligned} (D \otimes D)|\psi_e\rangle = &\sum_y e^{2ip} c_{1,2y} (|1\rangle|2y\rangle - |\bar{1}\rangle| - 2y\rangle) + \\ &e^{-2ip} c_{2,2y} (|2\rangle|2y\rangle - |\bar{2}\rangle| - 2y\rangle) + \\ &c_{3,2y} (|3\rangle|2(y+1)\rangle - |\bar{3}\rangle| - 2(y+1)\rangle) \end{aligned} \tag{4.31}$$

Taking P_0, commuting with J, defined as

$$P_0 := \sum_{i \in I} |i\rangle\langle i| \otimes |0\rangle\langle 0| \qquad I := \{1, 2, 3, \bar{1}, \bar{2}, \bar{3}\} \tag{4.32}$$

as projector on the $|i\rangle|0\rangle$ sector, J gives

$$\begin{aligned} P_0 J(D \otimes D)|\psi_e\rangle = &(e^{2ip} c_{1,0} A + c_{3,2} E - e^{-2ip} c_{2,0} C)|1\rangle|0\rangle + \\ &+ (e^{-2ip} c_{2,0} A - e^{2ip} c_{1,0} C - c_{3,2} E)|2\rangle|0\rangle + \\ &+ (e^{2ip} c_{1,0} B + c_{3,2} D - e^{-2ip} c_{2,0} B)|3\rangle|0\rangle - \\ &- (e^{2ip} c_{1,0} A + c_{3,2} E - e^{-2ip} c_{2,0} C)|\bar{1}\rangle|0\rangle - \\ &- (e^{-2ip} c_{2,0} A - e^{2ip} c_{1,0} C - c_{3,2} E)|\bar{2}\rangle|0\rangle - \\ &- (e^{2ip} c_{1,0} B + c_{3,2} D - e^{-2ip} c_{2,0} B)|\bar{3}\rangle|0\rangle \end{aligned} \tag{4.33}$$

While on $(I - P_0)(D \otimes D)|\psi_e\rangle$ and on $|\psi_o\rangle$ J acts trivially as the identity.
Let us now discuss the solutions in the two sectors:

4.3.2 Odd sector

In the following we call $M := J(D \otimes D)$ and we consider the antisymmetry condition, namely $c_{i,y} = c_{\bar{i},-y}$.

$$M|\psi_{1,o}\rangle = e^{2ip}|\psi_{1,o}\rangle \tag{4.34}$$

$$|\psi_{1,o}\rangle = \sum_y c_{1,2y+1}(|1\rangle|2y+1\rangle - |\bar{1}\rangle|-2y-1\rangle) \tag{4.35}$$

$$M|\psi_{2,o}\rangle = e^{-2ip}|\psi_{2,o}\rangle \tag{4.36}$$

$$|\psi_{2,o}\rangle = \sum_y c_{2,2y+1}(|2\rangle|2y+1\rangle - |\bar{2}\rangle|-2y-1\rangle) \tag{4.37}$$

$$M|\psi_{3,o}\rangle = e^{-i\omega}|\psi_{3,o}\rangle \tag{4.38}$$

$$|\psi_{3,o}\rangle = \sum_y c_{3,2y+1}(|3\rangle|2y+1\rangle - |\bar{3}\rangle|-2y-1\rangle) = \sum_y k e^{-i\omega y}(|3\rangle|2y+1\rangle - |\bar{3}\rangle|-2y-1\rangle) \tag{4.39}$$

For k real.

4.3.3 Even sector

For the even sector instead we have:

$$M|\psi_{1,e}\rangle = e^{2ip}|\psi_{1,e}\rangle \tag{4.40}$$

$$|\psi_{1,e}\rangle = \sum_{y\neq 0} c_{1,2y}(|1\rangle|2y\rangle - |\bar{1}\rangle|-2y\rangle) \tag{4.41}$$

$$M|\psi_{2,e}\rangle = e^{-2ip}|\psi_{2,e}\rangle \tag{4.42}$$

$$|\psi_{2,e}\rangle = \sum_{y\neq 0} c_{2,2y}(|2\rangle|2y\rangle - |\bar{2}\rangle|-2y\rangle) \tag{4.43}$$

and the last one, which is involved in the interaction

$$M|\psi_{3,e}\rangle = e^{-i\omega}|\psi_{3,e}\rangle \tag{4.44}$$

$$
\begin{aligned}
|\psi_{3,e}\rangle =& c_{1,0}(c_{3,2},\omega,p)(|1\rangle|0\rangle - |\bar{1}\rangle|0\rangle) \\
&+c_{2,0}(c_{3,2},\omega,p)(|2\rangle|0\rangle - |\bar{2}\rangle|0\rangle) \\
&+c_{3,0}(c_{3,2},\omega,p)(|3\rangle|0\rangle - |\bar{3}\rangle|0\rangle) \\
&+c_{3,2}(|3\rangle|2\rangle - |\bar{3}\rangle|-2\rangle) \\
&+\sum_{y>1} c_{3,2}e^{-i\omega(y-1)}(|3\rangle|2y\rangle - |\bar{3}\rangle|-2y\rangle) \\
&+\sum_{y<0} c_{3,0}(c_{3,2},\omega,p)e^{-i\omega y}(|3\rangle|2y\rangle - |\bar{3}\rangle|-2y\rangle)
\end{aligned}
\tag{4.45}
$$

with $\omega \in (-\pi, \pi]$.

The coefficients yet to determine, namely $c_{1,0}$,$c_{2,0}$,$c_{3,0}$ and $c_{3,2}$, are derived from (4.33) as solution of the following equation

$$
\begin{bmatrix}
Ae^{2ip} & -Ce^{-2ip} & 0 & E \\
-Ce^{2ip} & Ae^{-2ip} & 0 & -E \\
Be^{2ip} & -Be^{-2ip} & 0 & D \\
0 & 0 & 0 & e^{-ik}
\end{bmatrix}
\begin{bmatrix} c_{1,0} \\ c_{2,0} \\ c_{3,0} \\ c_{3,2} \end{bmatrix}
= e^{-i\omega}
\begin{bmatrix} c_{1,0} \\ c_{2,0} \\ c_{3,0} \\ c_{3,2} \end{bmatrix}
\tag{4.46}
$$

The problem is solved for the pair eigenvector- eigenvalue:

$$
e^{-ik}, \quad
\begin{bmatrix}
s(e^{-ik} - e^{-2ip}) \\
s(e^{2ip} - e^{-ik}) \\
(e^{ik} - \cos(2p)) + 2c(e^{-ik} - \cos(2p)) \\
e^{-ik}(e^{-ik} - \cos(2p)) + 2ce^{-ik}(e^{ik} - \cos(2p))
\end{bmatrix}
\tag{4.47}
$$

and k must be equal to ω.
We notice that fourth entry of (4.47) is the complex conjugate of the third entry multiplied by a factor e^{-ik}.

4. COMPLETENESS OF THE SOLUTIONS SET

Let us now redefine the solution set found in the previous section.

$$\begin{aligned}
|\phi_1\rangle :=& \sum_y c_{1,2y+1}(|1\rangle|2y+1\rangle - |\bar{1}\rangle|-2y-1\rangle) \\
|\phi_2\rangle :=& \sum_y c_{2,2y+1}(|2\rangle|2y+1\rangle - |\bar{2}\rangle|-2y-1\rangle) \\
|\phi_3\rangle :=& \sum_y ke^{-i\omega y}(|3\rangle|2y+1\rangle - |\bar{3}\rangle|-2y-1\rangle) \\
|\phi_4\rangle :=& \sum_{y\neq 0} c_{1,2y}(|1\rangle|2y\rangle - |\bar{1}\rangle|-2y\rangle) \\
|\phi_5\rangle :=& \sum_{y\neq 0} c_{2,2y}(|2\rangle|2y\rangle - |\bar{2}\rangle|-2y\rangle) \\
|\phi_6\rangle :=& c_{1,0}(|1\rangle|0\rangle - |\bar{1}\rangle|0\rangle) \\
&+c_{2,0}(|2\rangle|0\rangle - |\bar{2}\rangle|0\rangle) \\
&+c_{3,0}(|3\rangle|0\rangle - |\bar{3}\rangle|0\rangle) \\
&+c_{3,2}(|3\rangle|2\rangle - |\bar{3}\rangle|-2\rangle) \\
&+\sum_{y>1} c_{3,2}e^{-i\omega(y-1)}(|3\rangle|2y\rangle - |\bar{3}\rangle|-2y\rangle) \\
&+\sum_{y<0} c_{3,0}e^{-i\omega y}(|3\rangle|2y\rangle - |\bar{3}\rangle|-2y\rangle)
\end{aligned} \tag{4.48}$$

A set $\{\phi_a\}_{a\in A}$ with A set of indices is complete if, given a vector $|\psi\rangle$, the relationship

$$\langle\phi_a|\psi\rangle = 0 \quad \forall a \in A \tag{4.49}$$

holds only if $|\psi\rangle = 0$. Defining

$$|\psi\rangle = \sum_{i,y} \tilde{c}_{i,y}(|i\rangle|y\rangle - |\bar{i}\rangle|-y\rangle) \tag{4.50}$$

completeness for the set (4.48) becomes:

$$\begin{aligned}
\langle\phi_1|\psi\rangle = 0 \Longrightarrow \quad & \tilde{c}_{1,2y+1} = 0 \quad \forall y \\
\langle\phi_2|\psi\rangle = 0 \Longrightarrow \quad & \tilde{c}_{2,2y+1} = 0 \quad \forall y \\
\langle\phi_3|\psi\rangle = 0 \Longrightarrow \quad & \tilde{c}_{3,2y+1} = 0 \quad \forall y \\
\langle\phi_4|\psi\rangle = 0 \Longrightarrow \quad & \tilde{c}_{1,2y} = 0 \quad \forall y \neq 0 \\
\langle\phi_5|\psi\rangle = 0 \Longrightarrow \quad & \tilde{c}_{2,2y} = 0 \quad \forall y \neq 0 \\
\langle\phi_6|\psi\rangle = 0 \Longrightarrow \quad & \tilde{c}_{3,2y} = 0 \quad \forall y,\ \tilde{c}_{1,0} = 0 \text{ and } \tilde{c}_{2,0} = 0
\end{aligned} \tag{4.51}$$

it thus implies that $|\psi\rangle = 0$.

4.4.1 Case $|\phi_3\rangle$

We focus our attention on the third equation in (4.51). Concluding that $\tilde{c}_{3,2y+1} = 0$ is not straightforward as for other eigenvectors.
A pursuable strategy consists in integrating each term of the sum, multiplied by $e^{i\omega X}$, in ω in the I Brillouin zone:

$$\int_{-\pi}^{\pi} d\omega \, \langle\psi|\phi_3\rangle = \sum_y \int_{-\pi}^{\pi} d\omega \, k\tilde{c}^*_{3,2y+1} e^{-i\omega y} e^{i\omega X} = 0 \tag{4.52}$$

this is the Fourier transform of the scalar product.
We thus obtain

$$k\tilde{c}^*_{3,2y+1}\delta_{y,X} = 0 \tag{4.53}$$

which means, since $k \neq 0$, that $\tilde{c}^*_{3,2y+1} = 0 \; \forall y$.

4.4.2 Case $|\phi_6\rangle$

The last equation in (4.51) must be proved more precisely. The main problem is related to the fact that coefficients in $|\phi_6\rangle$ are functions of ω for each p fixed.
Let us write the scalar product between $|\phi_6\rangle$ and $|\psi\rangle$:

$$\begin{aligned}\langle\psi|\phi_6\rangle =& c_{1,0}(\omega,p)\tilde{c}^*_{1,0} + c_{2,0}(\omega,p)\tilde{c}^*_{2,0} + \\ & \sum_{y\leq 0} c_{3,0}(\omega,p)\tilde{c}^*_{3,2y} e^{-i\omega y} + \sum_{y\geq 1} c_{3,0}(\omega,p)\tilde{c}^*_{3,2y} e^{-i\omega(y-1)}\end{aligned} \tag{4.54}$$

Integrating each term exploiting (4.47) multiplied by $e^{i\omega X}$ in $d\omega$ in the interval $[-\pi, \pi]$ (I Brillouin zone), we get:

$$\int_{-\pi}^{\pi} d\omega \, e^{i\omega X} s(e^{-i\omega} - e^{-2ip})\tilde{c}^*_{1,0} = s\tilde{c}^*_{1,0}\delta_{X,1} - s\tilde{c}^*_{1,0}\delta_{X,0}e^{-2ip} \tag{4.55}$$

$$\int_{-\pi}^{\pi} d\omega \, e^{i\omega X} s(e^{2ip} - e^{-i\omega})\tilde{c}^*_{2,0} = \tilde{c}^*_{2,0} s e^{2ip}\delta_{X,0} - \tilde{c}^*_{2,0} s\delta_{X,1} \tag{4.56}$$

$$\begin{aligned}&\sum_{y\leq 0}\int_{-\pi}^{\pi} d\omega \, e^{i\omega X}\{(e^{i\omega} - \cos(2p)) + 2c(e^{-i\omega} - \cos(2p))\}e^{-i\omega y}\tilde{c}^*_{3,2y} = \\ &\sum_{y\leq 0}\{\delta_{X+1,y} + 2c\delta_{X-1,y} - \cos(2p)(2c+1)\delta_{X,y}\}\tilde{c}^*_{3,2y}\end{aligned} \tag{4.57}$$

$$\begin{aligned}&\sum_{y\geq 1}\int_{-\pi}^{\pi} d\omega \, e^{i\omega X}\{e^{-2i\omega} - e^{-i\omega}\cos(2p) + 2c - 2ce^{-i\omega}\cos(2p)\}e^{-i\omega(y-1)} = \\ &\sum_{y\geq 1}\{\delta_{X-1,y} - \cos(2p)(2c+1)\delta_{X,y} + 2c\delta_{X+1,y}\}\tilde{c}^*_{3,2y}\end{aligned} \tag{4.58}$$

we require that (4.55) + (4.56) + (4.57) + (4.58) = 0 $\forall X$. We thus have the following system:

$$\begin{cases} -s\tilde{c}^*_{1,0}e^{-2ip} + \tilde{c}^*_{2,0}se^{2ip} + 2c\,\tilde{c}^*_{3,-2} - \cos(2p)(2c+1)\tilde{c}^*_{3,0} + 2c\tilde{c}^*_{3,2} = 0 & \text{if } x = 0 \\ s\tilde{c}^*_{1,0} - s\tilde{c}^*_{2,0} + 2c\,\tilde{c}^*_{3,0} + 2c\,\tilde{c}^*_{3,4} - \cos(2p)(2c+1)\tilde{c}^*_{3,2} = 0 & \text{if } x = 1 \\ \tilde{c}^*_{3,2(y+1)} - \cos(2p)(2c+1)\tilde{c}^*_{3,2y} + 2c\,\tilde{c}^*_{3,2(y-1)} = 0 & \text{if } x < 0 \\ \tilde{c}^*_{3,2(y-1)} - \cos(2p)(2c+1)\tilde{c}^*_{3,2y} + 2c\,\tilde{c}^*_{3,2(y+1)} = 0 & \text{if } x > 1 \end{cases} \tag{4.59}$$

We can write the system with the recurring relationships as an operator. Defining $\delta := 2c$ and $\varepsilon := \cos(2p)(2c+1)$,

$$\begin{pmatrix} \ddots & & & & & & \cdots & & & & & \\ & \delta & -\varepsilon & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\ & 0 & \delta & -\varepsilon & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \\ & 0 & 0 & \delta & -\varepsilon & -se^{-2ip} & se^{2ip} & \delta & 0 & 0 & 0 & \\ \vdots & 0 & 0 & 0 & \delta & s & -s & -\varepsilon & \delta & 0 & 0 & \vdots \\ & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\varepsilon & \delta & 0 & \\ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\varepsilon & \delta & \\ & & & & & & \cdots & & & & & \ddots \end{pmatrix} \tag{4.60}$$

We notice that (4.60) is divided into a "tails" part, which is represented by the recurring tridiagonal terms for $X < 0$ and $X > 1$ and a "central" part, which takes into account also coefficients $\tilde{c}^*_{1,0}$ and $\tilde{c}^*_{2,0}$ for $X = 0$ and $X = 1$.
It is easy to verify that the tails verify the difference equation

$$x_{n+1} = \frac{1}{\delta}(\varepsilon x_n - x_{n-1}) \tag{4.61}$$

which can be rewritten in matrix notation

$$\begin{bmatrix} x_{n+1} \\ x_n \end{bmatrix} = \begin{bmatrix} \frac{\varepsilon}{\delta} & -\frac{1}{\delta} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_n \\ x_{n-1} \end{bmatrix} \tag{4.62}$$

or in a more compact form, $v_{n+1,n} = Mv_{n,n-1}$. Exploiting the recurrence we have $v_{n+1,n} = M^n v_{1,0}$, with $v_{1,0}$ initial conditions vector.
We can also diagonalize M and get

$$M^n = (PDP^{-1})^n = PD^nP^{-1} \tag{4.63}$$

with P

$$P = \begin{pmatrix} \frac{\varepsilon - \sqrt{\varepsilon^2 - 4\delta}}{2\delta} & \frac{\varepsilon + \sqrt{\varepsilon^2 - 4\delta}}{2\delta} \\ 1 & 1 \end{pmatrix} \tag{4.64}$$

diagonalizing M and D

$$D = \begin{pmatrix} \frac{\varepsilon}{2\delta} - \frac{\sqrt{\varepsilon^2-4\delta}}{2\delta} & 0 \\ 0 & \frac{\varepsilon}{2\delta} + \frac{\sqrt{\varepsilon^2-4\delta}}{2\delta} \end{pmatrix} \tag{4.65}$$

diagonal matrix.
Studying this matrix is useful because it stores the information on some coefficients of $|\psi\rangle$. If we prove that these coefficients give rise to a vector that is not in $\ell^2(\mathbb{C})$, i.e. $\sum_{i,y} |\tilde{c}_{i,y}|^2$ does not converge, we have to conclude that the only suitable solution for the system (4.59) is zero for all the coefficients of $|\psi\rangle$.
The initial conditions for the problem (4.62) are

$$v_{1,0} = \begin{bmatrix} \tilde{c}^*_{3,4} \\ \tilde{c}^*_{3,2} \end{bmatrix} \text{ for } X > 1 \tag{4.66}$$

and

$$v_{1,0} = \begin{bmatrix} \tilde{c}^*_{3,-2} \\ \tilde{c}^*_{3,0} \end{bmatrix} \text{ for } X < 0 \tag{4.67}$$

these are derived from the kernel of the matrix

$$\begin{bmatrix} \tilde{a} & \tilde{b} & \tilde{c} & \tilde{d} & \tilde{a} & 0 \\ 0 & \tilde{a} & \tilde{e} & \tilde{f} & \tilde{b} & \tilde{a} \end{bmatrix} \tag{4.68}$$

with

$$\begin{aligned} \tilde{a} &= 2c = \delta \\ \tilde{b} &= -\cos(2p)(2c+1) = -\varepsilon \\ \tilde{c} &= -se^{-2ip} \\ \tilde{d} &= se^{2ip} \\ \tilde{e} &= s \\ \tilde{f} &= -s \end{aligned} \tag{4.69}$$

The nullspace has the form:

$$\begin{bmatrix} -\tilde{c} + \frac{\tilde{b}\tilde{e}}{\tilde{a}} \\ -\tilde{e} \\ \tilde{a} \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} -\tilde{d} + \frac{\tilde{b}\tilde{f}}{\tilde{a}} \\ -\tilde{f} \\ 0 \\ \tilde{a} \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} -1 + \frac{\tilde{b}^2}{\tilde{a}^2} \\ -\frac{\tilde{b}}{\tilde{a}} \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} \frac{\tilde{b}}{\tilde{a}} \\ -1 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \tag{4.70}$$

and the initial conditions must be taken from the first two and the last two entries. In particular we observe that

$$\begin{bmatrix} -\tilde{c} + \frac{\tilde{b}\tilde{e}}{\tilde{a}} \\ -\tilde{e} \end{bmatrix}, \begin{bmatrix} -\tilde{d} + \frac{\tilde{b}\tilde{f}}{\tilde{a}} \\ -\tilde{f} \end{bmatrix} \propto \begin{bmatrix} \delta e^{\pm 2ip} + \varepsilon \\ \delta \end{bmatrix}$$

Divergence of the coefficients series

Let us now prove that $\sum_{y \in S} |\tilde{c}^*_{3,y}|^2$ diverges with S set of the coefficients in the "tails".
In particular, defining $|\psi\rangle := (x_0, x_1)^\top$ the divergence is verified if and only if

$$\sum_{n \in S} \langle \psi | M^{n\dagger} M^n | \psi \rangle \text{ diverges.} \tag{4.71}$$

Looking at (4.64) and (4.65), if $\varepsilon^2 - 4\delta > 0$ matrices have real values, while in the other case matrices are complex and in (4.71) we have transpose matrices in place to conjugate transpose.

Real case

Let us start from the real case, i.e. $\varepsilon^2 - 4\delta > 0$. (4.71) becomes

$$\begin{aligned} &\sum_{n \in S} \langle \psi | M^{n\top} M^n | \psi \rangle \\ &= \sum_{n \in S} \langle \psi | (P^\top)^{-1} D^n P^\top P D^n P^{-1} | \psi \rangle \end{aligned} \tag{4.72}$$

we notice that $P^\top P$ is positive definite, thus in particular $P^\top P \geq \min\{\lambda_1, \lambda_2\} I$, with λ_1, λ_2 eigenvalues of $P^\top P$. This allows us to write

$$D^n P^\top P D^n \geq \min\{\lambda_1, \lambda_2\} D^{2n} \tag{4.73}$$

knowing the eigenvalues of M, namely $\frac{\varepsilon}{2\delta} - \frac{\sqrt{\varepsilon^2 - 4\delta}}{2\delta}$ and $\frac{\varepsilon}{2\delta} + \frac{\sqrt{\varepsilon^2 - 4\delta}}{2\delta}$, we have

$$D^{2n} = \begin{pmatrix} \left(\frac{\varepsilon}{2\delta} - \frac{\sqrt{\varepsilon^2 - 4\delta}}{2\delta}\right)^{2n} & 0 \\ 0 & \left(\frac{\varepsilon}{2\delta} + \frac{\sqrt{\varepsilon^2 - 4\delta}}{2\delta}\right)^{2n} \end{pmatrix} = \begin{pmatrix} \mu_1^{2n} & 0 \\ 0 & \mu_2^{2n} \end{pmatrix} \tag{4.74}$$

which in particular is positive definite. Now, defining $|\phi\rangle := P^{-1}|\psi\rangle = (a, b)^\top$ we have to study the divergence of

$$\sum_n \min\{\lambda_1, \lambda_2\} \langle \phi | D^{2n} | \phi \rangle = \sum_n \min\{\lambda_1, \lambda_2\} \left(|a|^2 \mu_1^{2n} + |b|^2 \mu_2^{2n} \right). \tag{4.75}$$

We observe that $det(M) = \frac{1}{\delta} = \mu_1\mu_2$, but its module is always ≥ 1, thus at least one between μ_1 and μ_2 is greater than 1 and (4.75) diverges unless a or b are zero and the non-zero part of the sum does not diverges. These pathological cases will be studied separately.

Complex case

In this case $\varepsilon^2 - 4\delta < 0$. We have

$$D = \begin{pmatrix} \frac{\varepsilon}{2\delta} - i\frac{\sqrt{4\delta-\varepsilon^2}}{2\delta} & 0 \\ 0 & \frac{\varepsilon}{2\delta} + i\frac{\sqrt{4\delta-\varepsilon^2}}{2\delta} \end{pmatrix} := (fI + gZ) \tag{4.76}$$

with $f = \frac{\varepsilon}{2\delta}$ and $g = -i\frac{\sqrt{4\delta-\varepsilon^2}}{2\delta}$.

In the complex case we have to study $D^{n\dagger}P^\dagger PD^n$ in place of $D^nP^\top PD^n$. We observe that $P^\dagger P$ is positive definite with real and positive eigenvalues λ_1 and λ_2. Similarly to the previous case,

$$D^{n\dagger}P^\dagger PD^n \geq \min\{\lambda_1,\lambda_2\}D^{n\dagger}D^n =$$
$$\min\{\lambda_1,\lambda_2\}(fI + g^*Z)^n(fI+gZ)^n = \min\{\lambda_1,\lambda_2\}\left[(f^2+|g|^2)I + f(g+g^*)Z\right]$$

but $g + g^* = 0$, thus

$$(D^\dagger D)^n = (f^2+|g|^2)^n I. \tag{4.77}$$

and the series to study becomes

$$\sum_n (f^2+|g|^2)^n\langle\phi|\phi\rangle. \tag{4.78}$$

We notice that

$$f^2 + |g|^2 = \frac{\varepsilon^2}{4\delta^2} + \frac{4\delta-\varepsilon^2}{4\delta^2} = \frac{1}{\cos(\sqrt{2}|\lambda|)} \tag{4.79}$$

which is always ≥ 1 since we have taken $4\delta > \varepsilon^2$, but δ must necessarily be positive since ε^2 is positive.

This means that (4.78) diverges unless $|\phi\rangle = P^{-1}|\psi\rangle$ is the zero vector, namely $|\psi\rangle$ is in the nullspace of P^{-1}.

4.4.3 Special cases

In the previous section we postponed the analysis of some remarkable cases. Let us describe them in order to understand when we cannot apply the reasoning presented so far.

P is not invertible

If the matrix P is not invertible, then we cannot rely on (4.72). This happens when $\varepsilon^2 = 4\delta$. In this case M becomes

$$M = \begin{bmatrix} \frac{4}{\varepsilon} & -\frac{4}{\varepsilon^2} \\ 1 & 0 \end{bmatrix} \tag{4.80}$$

which is clearly not diagonalizable, since its eigenstates span a space of dimension less than 2.
However, we can always write (4.80) in Jordan form:

$$M = J \begin{pmatrix} \frac{2}{\varepsilon} & 1 \\ 0 & \frac{2}{\varepsilon} \end{pmatrix} J^{-1} \tag{4.81}$$

and in particular, defining $\sigma_+ := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $\sigma_- := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ and $\alpha := \frac{2}{\varepsilon}$

$$\begin{aligned} M^{n\dagger} M^n = \alpha^{2n} J(I + n\alpha^{-1}\sigma_-)(I + n\alpha^{-1}\sigma_+)J^{-1} = \\ \alpha^{2n}\left(I + n\alpha^{-1}X + n^2\alpha^{-2}\frac{I - Z}{2}\right) \end{aligned} \tag{4.82}$$

since $\alpha^2 = \frac{1}{\delta}$ we conclude that the corresponding series diverges unless $|\psi\rangle$ is in the nullspace of $I + n\alpha^{-1}X + n^2\alpha^{-2}\frac{I-Z}{2}$. Since the latter has determinant equal to 1, we conclude that the series diverges unless $|\psi\rangle$ is the zero vector.

Critical cases for $P^{-1}|\psi\rangle$

We study exploiting (4.70) the pathological cases for the divergence of (4.75). Since it is sufficient that one of the "tails" diverges in order to prove completeness, we will study only one tail for each vector in (4.70). Defining $\gamma := \sqrt{\varepsilon^2 - 4\delta}$, we are thus restricted to the following cases:

$$P^{-1}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \propto \begin{pmatrix} -1 \\ 1 \end{pmatrix} \tag{4.83}$$

$$P^{-1}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \propto \begin{pmatrix} \frac{\varepsilon}{2\gamma} + \frac{1}{2} \\ -\frac{\varepsilon}{2\gamma} + \frac{1}{2} \end{pmatrix} \tag{4.84}$$

$$P^{-1}\begin{pmatrix}\delta e^{\pm 2ip}+\varepsilon\\ \delta\end{pmatrix}\propto\begin{pmatrix}-\left(\frac{\delta}{\gamma}e^{\pm 2ip}+\frac{\varepsilon}{2\gamma}\right)+\frac{1}{2}\\ \frac{\delta}{\gamma}e^{\pm 2ip}+\frac{\varepsilon}{2\gamma}+\frac{1}{2}\end{pmatrix}. \tag{4.85}$$

(4.75) always diverges when the initial condition are given by (4.83), since both a and b cannot be zero.
Considering (4.84), If $a=0$, namely $\frac{\varepsilon}{2\gamma}=-\frac{1}{2}$, we conclude that $b=1$ and, from the relation $\gamma^2=\varepsilon^2-4\delta=\gamma^2-4\delta\longrightarrow\delta=0$, μ_2 diverges.
Similarly, if $b=0$, $\frac{\varepsilon}{2\gamma}=-\frac{1}{2}$ and $\delta=0$ thus μ_1 diverges.
If our initial conditions are given by (4.85), we have instead, if $a=0$, namely $\left(\frac{\delta}{\gamma}e^{\pm 2ip}+\frac{\varepsilon}{\gamma}\right)=\frac{1}{2}$, it is then straightforward to verify that $e^{\pm 2ip}=-\mu_1$. Since we are restricted to the real case, this is true only when $e^{\pm 2ip}=\pm 1$. Remembering the relation $\mu_1\mu_2=\frac{1}{\delta}$ we prove the divergence of the series. The case $b=0$ can be proved with the same strategy, exchanging the roles of μ_1 and μ_2.

Critical cases for $|\psi\rangle$

For the complex case, the particular situations to check regard $|\psi\rangle=0$. We observe that this is never the case for the initial conditions for $|\psi\rangle$ enumerated, namely $\begin{pmatrix}1\\0\end{pmatrix}$,$\begin{pmatrix}0\\1\end{pmatrix}$ and $\begin{pmatrix}\delta e^{\pm 2ip}+\varepsilon\\ \delta\end{pmatrix}$.

5. DISCUSSION OF OTHER SOLUTIONS

The matrix on the lhs of (4.46) has other possible eigenvalues and eigenvectors. These are:

$$0,\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$$

$$A\cos(2p)\pm\sqrt{C^2-A^2\sin^2(2p)},$$

$$\begin{pmatrix}-(A+C)e^{-2ip}+A\cos(2p)\pm\sqrt{C^2-A^2\sin^2(2p)}\\ -(A+C)e^{2ip}+A\cos(2p)\pm\sqrt{C^2-A^2\sin^2(2p)}\\ 2i\sin(2p)B\\ 0\end{pmatrix}$$

Since we are looking for eigenvalues in the form $e^{i\omega}$, we need to verify at least that the square modulus of the eigenvalues is 1 in order to declare these further

solutions as admissible. For the first one, it is trivial that it can be thrown away. Let us analyze the other two solutions: the eigenvalues

$$A\cos(2p) \mp \sqrt{C^2 - A^2\sin^2(2p)} \tag{4.86}$$

are real or complex depending on the sign of $C^2 - A^2\sin^2(2p)$, in detail

$$\begin{cases} A\cos(2p) \mp \sqrt{C^2 - A^2\sin^2(2p)} \text{ if } C^2 - A^2\sin^2(2p) \geq 0 \\ A\cos(2p) \mp i\sqrt{A^2\sin^2(2p) - C^2} \text{ if } C^2 - A^2\sin^2(2p) \leq 0 \end{cases} \tag{4.87}$$

We have admissible eigenvalues (i.e. with square modulus equal to 1) in these scenarios:
In the first scenario, we have

$$\begin{aligned} &A\cos(2p) \mp \sqrt{C^2 - A^2\sin^2(2p)} = \pm 1 \\ &A\cos(2p) \mp 1 = \pm\sqrt{C^2 - A^2\sin^2(2p)} \\ &A^2\cos^2(2p) + 1 \mp 2A\cos(2p) = C^2 - A^2\sin^2(2p) \\ &A^2 - C^2 + 1 = \pm 2A\cos(2p) \\ &2c + 1 = \pm(2c+1)\cos(2p) \\ &(2c+1)(1 \mp \cos(2p)) = 0 \end{aligned} \tag{4.88}$$

which holds for $c = -\frac{1}{2}$ and $\cos(2p) = \pm 1$.
In the second case we have instead

$$\begin{aligned} &A^2\cos^2(2p) + A^2\sin^2(2p) - C^2 = 1 \\ &A^2 - C^2 = 0 \\ &c = \frac{1}{2}. \end{aligned} \tag{4.89}$$

We observe that when $C^2 - A^2\sin(2p) < 0$, namely $c = \frac{1}{2}$, $A = 1$, $C, B, E = 0$ while $D = 1$. Remembering (4.19), we conclude that the interaction is the identity, namely only the free evolution acts on the system in this case.
In the case $c = -\frac{1}{2}$ we have instead:

$$\tilde{J} := \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \tag{4.90}$$

In particular we notice that an eigenvector of the problem $\tilde{J}(D \otimes D)|\psi\rangle = e^{-i\omega}|\psi\rangle$ is

$$|\psi\rangle = c_{1,0}(|1\rangle|0\rangle - |\bar{1}\rangle|0\rangle) \pm e^{2ip}c_{1,0}(|2\rangle|0\rangle - |\bar{2}\rangle|0\rangle) \tag{4.91}$$

with $\pm$ sign depending on $e^{i\omega} = \pm 1$. In particular, substituting into the eigenvector at the beginning of the section we have

$$c_{1,0} = \pm e^{-ip}$$
$$c_{2,0} = e^{ip}$$

up to a constant.

CONCLUSIONS

In this work we have widely studied Fermionic QCA with particular regard to interactions for Weyl and Dirac automata.
In Chapter 1 we have reviewed the theory of QCA and we focused on the hypotheses of reversibility, unitarity, linearity, homogeneity and isotropy which are crucial to develop a physical theory of Fermionic QCA.
In Chapter 2 we have described in detail Weyl QCA and QW for 1, 2 and 3 dimensions of the lattices and studied the general form of the Dirac automata, valid for all the dimensions of the lattice.
In Chapter 3 we have approached the topic of interactions, providing a classification of all the possible physical interactions for a 3D lattice, but still valid for lattices of lower dimensions, since they are based on discrete isotropy under the isotropy group $\{I, i\sigma_x, i\sigma_y, i\sigma_z\}$ which is a more restrictive constraint with respect to the isotropy groups for lower dimensionalities.
In particular, we provided a classification based on their representation through Dirac gamma matrices, facilitated by the employement of an algorithm developed specifically for handling polynomials of Fermionic operators, presented in detail in Appendix A.
In Chapter 4 we have restricted the dimensionality of the lattice to the monodimensional case and we have made a distinction between interactions regarding internal DoFs which evolve at constant relative position and interactions regarding DoFs which evolve at variable relative position and we studied an eigenvalue problem for the massless Dirac QW in the two particles sector with an interaction in the latter category.
The solutions we found are proved to be complete and they are in general scattering states or solutions in which the evolution acts trivially, except for a particular case. If $\cos(\sqrt{2}|\lambda|) = -\frac{1}{2}$, we find a bound state as a solution, localized in the subspace spanned by $\{|1\rangle, |2\rangle, |\bar{1}\rangle, |\bar{2}\rangle\}$ and $|y\rangle = |0\rangle$. We have classified the solutions according to the sector of the Hilbert space of relative positions, $\{|y\rangle\}$, in which they live. We highlight in particular the non-trivial solution including states with $|y\rangle = |0\rangle$, which is effectively interested by the interaction. In the subspace

of the internal DoF spanned by $\{|3\rangle, |\bar{3}\rangle\}$ we have also found a solution with a plane-wave structure.
This work is intended as a starting point in the developement of a more general theory of interactions for this class of QCAs aimed at recovering known interactions in QFT by means of an information processing theory, even if we remark that pioneering works on the topic have been performed yet [BDPT18, BDM$^+$18, CKSS10, BDT13, AAM$^+$11, LKanN15]. We have in particular proved the feasibility of finding analytical solutions for an interacting QW in 1D lattices for a wide class of interactions. This may seem a toy model if we look at the phenomenological aspects of the problem, but it allows us to understand which may be the technical issues to face in the perspective of a more complex model, both in the geometry of the lattice and on the side of internal degrees of freedom.
A lot of work is yet to be done: in particular, it can be interesting exploiting the classification made in order to study interactions in a 3D lattice. Furthermore, we can increase the number of particles evolved by the walk and study also the interactions with 6-linear and 8-linear terms. A problem in this direction is the cumbersomeness of the calculations which can require the employment of a numerical approach at the expense of exact results, which can be instead provided with an analytical approach.

APPENDIX A

PYTHON CODES: THE "FERMIONS" MODULE

The problem of establishing an ordering for operators arises from the fact that in this work we have encountered many polynomials of Fermionic operators in our calculations and treating them *by hand* was not feasible in a short time. Luckily, there exists a Python module called *sympy* that allows us to handle symbolic mathematics and thus potentially even Fermionic algebra. Further problems arised when, even if there exists a sub-module dedicated to Fermions, it was not practical for our purposes and in particular lacked of operators handling in second quantization.
Moreover, even if we inserted in our code the "rules" to handle these operators, expressions like $a_{u_1}a^\dagger_{u_2}a_{u_2}a_{d_2}$ and $a_{d_2}a^\dagger_{u_2}a_{u_2}a_{u_1}$ were treated as different expressions even if they are equivalent modulo anticommutation rules.
We thus needed to "expand" sympy and write our custom module, which will be presented in this appendix.

1. ORDERING WITHOUT POSITIONAL DEGREE OF FREEDOM

We start from solving the problem of ordering Fermionic operators *locally*, i.e. without considering the positional degree of Freedom.
The central idea of the algorithm is reducing every expression of the form $f_1^{d_1}f_2^{d_2}...f_n^{d_n}$, where f_i is a Fermionic operator and d_i an additional index that indicates if it is taken as a or $a^\dagger$, to an equivalent operator such that the internals degrees of freedom follow the ordering

$$a^\dagger_{u_1}|a_{u_1}|a^\dagger_{d_1}|a_{d_1}|a^\dagger_{u_2}|a_{u_2}|a^\dagger_{d_2}|a_{d_2}. \tag{A.1}$$

This means that, as an example, a monomial like $a^\dagger_{u_2} a_{u_1}$ is converted in $-a_{u_1} a^\dagger_{u_2}$ according to the CAR and to the ordering "priority scale" (A.1) and an expression like $a^\dagger_{u_2} a_{u_1} + a_{u_1} a^\dagger_{u_2}$ is correctly evaluated as zero.
We underline that the algorithm is designed for the internal degrees of freedom used in the Dirac QCA, thus only u_1, d_1, u_2, d_2, but is theoretically adjustable for other scenarios.

The code

At the beginning we import the modules from which we need to inherit functions or classes. In this case `sympy` and others submodules designed for physics. `init_printing(use_unicode = True)` and `from IPython.display import display, Math` are used for printing results in LaTeX- style.

```
from sympy import *
init_printing(use_unicode = True)
from sympy.physics.secondquant import *
from IPython.display import display, Math
from sympy.physics.quantum import *
```

We then define symbols and lists designed for the notation used in this work for Fermionic operators:

```
fu1 = symbols('a_{u_1}', commutative=False)
fdu1 = symbols('a_{u_1}^\dagger', commutative=False)
fd1 = symbols('a_{d_1}', commutative=False)
fdd1 = symbols('a_{d_1}^\dagger', commutative=False)
fu2 = symbols('a_{u_2}', commutative=False)
fdu2 = symbols('a_{u_2}^\dagger', commutative=False)
fd2 = symbols('a_{d_2}', commutative=False)
fdd2 = symbols('a_{d_2}^\dagger', commutative=False)

fermi  = Matrix([fu1,fd1,fu2,fd2])
fermid = Matrix([fdu1,fdd1,fdu2,fdd2])
ops = [fdu1,fu1,fdd1,fd1,fdu2,fu2,fdd2,fd2]
```

The first function we define is called `dictionarize` and creates a list of lists of the form $[\alpha, \beta]$, where α is an operator or a numerical coefficient, while β acts as a "weight" assigning a position to α for the final sorting. For numbers or nilpotent operators (the input may contain expressions as f_i^n, but Fermionic operators are nilpotent) $\beta = 0$.

```
def dictionarize(strl):
    d = []
    counter = 0
    for i in strl:
        v = []
        if (i == fdu1) or (i == fu1):
            v.append(i)
            v.append(1+counter)
            d.append(v)
            counter = counter + 1
        elif (i == fdd1) or (i == fd1):
            v.append(i)
            v.append(100+counter)
            d.append(v)
            counter = counter + 1
        elif (i == fdu2) or (i == fu2):
            v.append(i)
            v.append(200+counter)
            d.append(v)
            counter = counter + 1
        elif (i == fdd2) or (i == fd2):
            v.append(i)
            v.append(300+counter)
            d.append(v)
            counter = counter + 1
        elif i not in ops:
            v.append(i)
            v.append(0)
            d.append(v) # for coefficients and powers of
                        # nilpotent operators
    return d
```

`bubble_sort` is the core of the code. It is based on the bubble sort algorithm, which is the most intuitive sorting algorithm. Despite not being the most efficient, it has the advantage of swapping nearest neighbours in a string, allowing us to keep track of the swaps made and thus to know when adding a minus sign for the CAR is needed.

```
def bubble_sort(strl):
    bubbles = dictionarize(strl)
```

```
    swapped = True
    asign = 1
    while swapped:
        swapped = False
```

The sorting is made according to the weights returned from `dictionarize`, but when two operators related to different internal degrees of freedom are swapped a minus sign is added according to the CAR. Notice that the weights in `dictionarize` are designed in order not to swap operators with the same internal degree of freedom, thus the CAR $\{a_i, a_i^\dagger\} = I$ is not considered at this level.

```
        for i in range(len(bubbles)-1):
            if bubbles[i][1] > bubbles[i+1][1]:
                bubbles[i], bubbles[i+1] = \
                bubbles[i+1], bubbles[i]
                                # Updated sign due to CAR
                asign = asign * (-1)
                swapped = True
        strl.clear()
    for i in bubbles:
        strl.append(i[0]) # for coefficients

    strl.append(asign)
    return strl
```

We define also subd, a function which, given an expression, substitutes 0 to nilpotent operators and $a_i^\dagger a_i$ to $a_i^\dagger a_i a_i^\dagger a_i$. A bit of redundance is added in order to make subd effective also with longer strings.

```
def subd(expr):
    return expr.subs({
        fu1*fu1 : 0,
        fdu1*fdu1 : 0,
        fd1*fd1 : 0,
        fdd1*fdd1 : 0,
        fu2*fu2 : 0,
        fdu2*fdu2 : 0,
        fd2*fd2 : 0,
        fdd2*fdd2 : 0
    }).subs({
        fdu1*fu1*fdu1*fu1 : fdu1*fu1,
        fdd1*fd1*fdd1*fd1 : fdd1*fd1,
```

```
        fdu2*fu2*fdu2*fu2 : fdu2*fu2,
        fdd2*fd2*fdd2*fd2 : fdd2*fd2,
    }).subs({
        fdu1*fu1*fdu1*fu1 : fdu1*fu1,
        fdd1*fd1*fdd1*fd1 : fdd1*fd1,
        fdu2*fu2*fdu2*fu2 : fdu2*fu2,
        fdd2*fd2*fdd2*fd2 : fdd2*fd2,
    }).subs({
        fdu1*fu1*fdu1*fu1 : fdu1*fu1,
        fdd1*fd1*fdd1*fd1 : fdd1*fd1,
        fdu2*fu2*fdu2*fu2 : fdu2*fu2,
        fdd2*fd2*fdd2*fd2 : fdd2*fd2,
    })
```

As a final step, we merge all these functions in `fermionize`, which does the task required at the beginning decomposing a polynomial in the Fermionic operators into a list of monomial, each one furtherly decomposed into a list of single operators, ready to be sorted by our `bubble_sort` function. The expression is then restored as object of a class suitable for `sympy`'s algorithms.

```
def fermionize(expr):
    listexpr = \
    [x.as_ordered_factors() for x in expr.as_ordered_terms()]
    listprov = []
    for i in listexpr:
        listprov.append(bubble_sort(i))

    # builds expression with sorted terms
    exprout = 0
    for i in range(len(listprov)):
        prod = 1
        for j in range(len(listprov[i])):
            prod = prod*listprov[i][j]

        exprout = exprout + prod

    return subd(exprout)
```

2. Ordering with Positional Degree of Freedom

We have also developed a version of the algorithm presented in the previous section capable of handling also positional degrees of freedom. In this case, positions are sorted in alphabetical order and, for each set of operators with the same positional DoF, the ordering for internal DoF is the same of Eq. A.1.

The code

It is convenient defining a **class** `Fermion` which inherits from sympy's class `Symbol`. It's objects are printed following our notation for Fermionic operators with positional DoF, i.e. $a_i(x)$ and $a_i(x)^\dagger$, with i internal DoF and x position.

```
class Fermion(Symbol):

    def __new__(self, f, x):
        obj = \
        Symbol.__new__(self,f+'('+x+')',commutative=False)
        return obj

    def __init__(self, f, x):
        self.internal = f
        self.pos      = x
```

We then define a `bubble_sort_pos` function in order to sort operators according to the CAR for positional DoF. In this case we don't need a weight like for internal DoF since positions are stored as characters and they can be sorted in alphabetical order.

```
def bubble_sort_pos(strl):

    bubbles = [i for i in strl if i.__class__.__name__== \
    Fermion('a','x').__class__.__name__]
    coeffs = [i for i in strl if i.__class__.__name__!= \
    Fermion('a','x').__class__.__name__]
    # Check on monomials of the kind a(x)^n
    coeffs2 = [0 if
    (i.__class__.__name__==(fu1*fu1).__class__.__name__ and
     i.is_commutative==False) else i for i in coeffs]
```

```
    swapped = True
    asign = 1
    while swapped:
        swapped = False
        for i in range(len(bubbles)-1):
            if bubbles[i].pos > bubbles[i+1].pos:
                bubbles[i], bubbles[i+1] = \
                bubbles[i+1], bubbles[i]
                # Updated sign due to CAR
                asign = asign * (-1)
                swapped = True
    bubbles += coeffs2
    bubbles.append(asign)
    return bubbles
```

We then define `fermionize_def` which performs the ordering task in n steps:

First, the polynomial to sort is decomposed into list of monomials, furtherly decomposed into lists of operators

```
def fermionize_def(expr):
    strl = \
    [x.as_ordered_factors() for x in expr.as_ordered_terms()]

    bubbled_pos = [bubble_sort_pos(k) for k in strl]
```

then it is extracted the list of the positions appearing in the initial expression sorted in alphabetical order:

```
    list_pos = \
    sorted(list(set(item.pos \
    for j in bubbled_pos \
    for item in j \
    if (item.__class__.__name__== \
    Fermion('a','x').__class__.__name__) )))
```

Each term is then divided into operators separated with respect to the position DoF. Also coefficients are taken into account and stored in lists with a weight, returned from `bubbled_pos`, which can be ± 1, depending on the even or odd number of swaps made by `bubbled_pos`.

```
resort = []
for j in bubbled_pos:
    park = []
    for x in list_pos:
        park.append([item for item in j \
        if (item.__class__.__name__== \
        Fermion('a','x').__class__.__name__ ) \
        if item.pos == x ] + [1])

    park.append([item for item in j \
     if (item.__class__.__name__!= \
      Fermion('a','x').__class__.__name__)])

    resort.append(park)
```

The expression is now reordered with respect to internal DoF. For this purpose, `fermionize` is invoked and the results are decomposed into single Fermionic operators and stored in `resort2`

```
resort2 = []
for i in resort:
    park = []

    for j in i:
        pos = [j[0].pos if \
         (j[0].__class__.__name__== \
         Fermion('a','x').__class__.__name__) else 1][0]

        internals = [symbols(k.internal, commutative=False) \
         if (k.__class__.__name__== \
         Fermion('a','x').__class__.__name__) \
         else k for k in j]

        prod_int_ferm = [ fermionize(prod(internals)) \
        if (prod(internals).__class__.__name__== \
        prod(ops).__class__.__name__ \
        or prod(internals).__class__.__name__== \
        (fu1*fu1).__class__.__name__) \
        else prod(internals) ][0]
```

```
            prod_int_ferm_pos = []

            if prod_int_ferm.__class__.__name__== \
            prod(ops).__class__.__name__ \
            or (prod_int_ferm.__class__.__name__== \
            fu1.__class__.__name__ \
            and prod_int_ferm.is_commutative==False):
                prod_int_ferm_pos.append([ Fermion(str(k),pos) \
                 if (k.__class__.__name__== \
                 fu1.__class__.__name__ \
                 and k.is_commutative==False) \
                 else k \
                 for k in prod_int_ferm.as_ordered_factors() ])
            else:
                prod_int_ferm_pos.append(prod_int_ferm)

            park.append(prod_int_ferm_pos[0])
        resort2.append(park)
```

The expression is thus reassembled in an object of a class suitable for sympy’s expression manipulation algorithms.

```
    resort3 = [[prod(k) \
    if  (k.__class__.__name__== ops.__class__.__name__) \
    else k for k in i] for i in resort2 ]

    polyend = sum([prod(k) for k in resort3])

    return polyend
```

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