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Exact Solution of the Weyl and Dirac Quantum Cellular Automata

Soluzione esatta degli Automi Cellulari Quantistici di Weyl e Dirac

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Sommario

In questa tesi viene affrontato lo studio di un modello dinamico discreto, gli *Automi Cellulari Quantistici*, che costituiscono l'estensione quantistica dei corrispettivi classici, gli *Automi Cellulari*. Gli automi cellulari quantistici sono costituiti da una collezione di sistemi quantistici collocati nei siti di un reticolo; in più si richiede che questi sistemi quantistici interagiscano localmente con un certo numero (finito) di loro vicini, che vanno a formare l'intorno di ogni cella. Inoltre si impone l'omogeneità delle interazioni in base al principio dell'universalità della *legge fisica*.

In questo lavoro vengono considerati gli automi di Dirac e Weyl nel settore di particella singola in una e due dimensioni spaziali rispettivamente. L'obiettivo che ci si era prefissi era applicare a questo caso l'approccio a *path-integral* discreto, riducendo quindi l'evoluzione a N passi dell'automa a una somma combinatoria su tutti i possibili cammini che connettono due punti del reticolo su cui esso stesso è definito.

Come risultato di questa analisi, si è ottenuta un'espressione analitica per la soluzione della dinamica degli automi nei due casi considerati. Specificatamente, fissando una coppia di punti sul reticolo si può cercare la matrice di transizione complessiva che descrive l'evoluzione dello stato del grado di libertà interno tra i due punti. La soluzione ottenuta consiste quindi nell'espressione esplicita dei coefficienti delle matrici di transizione associate a ciascuna possibile traslazione del reticolo.

CONTENTS

LIST OF FIGURES

1 INTRODUCTION

In this work we study the properties and features of a model of discrete dynamics which is called *Quantum Cellular Automaton* (QCA) and it is the extension to the quantum world of classical *Cellular Automata* (CA).

A QCA describes the discrete-time evolution of a lattice of finite-dimensional quantum systems. The characteristic traits of this model are a strict notion of locality, requiring that each quantum system interacts with a finite number of neighbours, and translational invariance. The inherent simplicity of these models is overcome by the surprising complexity of their emergent behaviours. The CA paradigm was introduced by John von Neumann [65] and, apart an initial skepticism and lack of attention, it has received during the years more and more contributions. QCAs have been a subject of investigation in the fields of *Computer Science* and *Quantum Information*, where they found a rigorous mathematical formalisation and an extensive study of their general features [3, 7, 9, 37, 45, 60].

The interest in this models was also motivated by their application in designing efficient *quantum algorithms*. Indeed, QCAs are proved to provide polynomial speedups for a number of relevant problems [6, 30, 52] and Childs et al. [18] have shown how QCAs allow an exponential speedup for an oracular problem.

Recently, discrete-dynamics models similar to cellular automata have been considered with the aim to describe the evolution of a relativistic particle, hence evolving according to the Klein-Gordon or the Dirac equations. We can mention some examples of these approaches like the quantum lattice Boltzmann [63], the quantum lattice gases [54] and the QCA framework [11, 62, 73]. Such a perspective was at the core of the considerations of R. P. Feynman and J. A. Wheeler [39] regarding the connections between *Physics* and *information processing*.

This is also the spirit of the recent research program of D'Ariano [20, 21, 23, 24] in the scope of giving fully informational foundations to *Quantum Theory* [19]. The successful results of these ideas opened the way to give informational premises also to *Quantum Field Theory*, which is the most fundamental and successful theoretical framework for present physics. In a recent paper [22], D'Ariano and Perinotti were able to derive a QCA from four postulates which gives, in the large-scale limit, the Weyl and Dirac equations.

In the literature one can find two different approaches to analyse the evolution of an automaton. A first way consists in the study of the automaton in the momentum space, providing both exact analytical solutions and approximate solutions in the asymptotic limit of very long times. The other one employs the discrete version of the path-integral formulation, consisting in expressing the probability amplitude for the transition between states of two systems located at two different

sites of the lattice as a combinatorial sum over all possible paths connecting the two sites.

The authors in [22] have already given the analytic solution in the momentum space. In the present work we will focus instead on the second approach, obtaining an analytic solution in the position representation for the Dirac and Weyl automata in one and two spatial dimensions respectively. For the one dimensional case, we can mention other analytical results as the one for the Hadamard walk by Ambainis et al. [7], that for the generalised Hadamard walk and for the disordered quantum walks by Konno [49, 48] and the one for the finite-differences Dirac equation obtained by Kauffman and Pierre Noyes [42]. The mono-dimensional automaton model considered in this thesis, derived in [12, 13] or in the aforementioned paper of D'Ariano and Perinotti [22], is different from these previous models and the analytic solution we have obtained for the Weyl automaton in two spatial dimensions constitutes one of the few examples of exactly solved models in dimension greater than one. Furthermore, these results will be very useful in analysing the large-scale behaviour of these automata. In particular, one can study how the isotropy of the causal cone is recovered thanks to the interference of the quantum paths.

2 CELLULAR AUTOMATA

Model of discrete-dynamics, the *Cellular Automaton* (CA) paradigm is very fascinating, showing high emergent complexity, arising from simple rules. Originally this model was introduced and studied by Stanislaw Ulam and John von Neumann when they were colleagues at the *Los Alamos National Laboratory* in the 1940*s*. Ulam was studying models of crystal growth, while von Neumann was committed to devising and developing *self-replicating systems* [65]. The results of this pioneering research were eventually systematised in [56].

The CA*s* are models describing a discrete dynamics (in time and space) based on local interactions between adjacent *sites* (or *cells*) of a n-dimensional lattice or more generally between sites belonging to a specified (finite) neighbourhood. Moreover, to each cell is associated a certain (finite) number of states (*e. g.* dead or alive) and an update rule which gives the new state of the cell, depending on the state of the other cells in the neighbourhood. For an example of different schemes see figure 1.

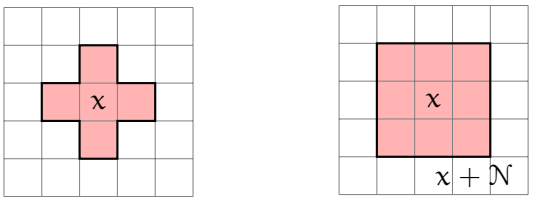
It was only when the John Conway's *Game of Life* was presented by Gardner [34] in 1970 that the CA paradigm obtained wide notoriety. The *Game of Life* is a very simple automaton characterised by an infinite 2-dimensional grid of square cells which can assume only two states: *dead* or *alive*. The update rules for this automaton are:

(i) any live cell with fewer than two live neighbours dies, as if caused by underpopulation;

(ii) any live cell with two or three live neighbours lives on to the next generation;

(iii) any live cell with more than three live neighbours dies, as if by overcrowding;

(iv) any dead cell with exactly three live neighbours becomes a live cell, as if by reproduction.



(a) *von Neumann neighbourhood.* **(b)** *Moore neighbourhood.*

Figure 1: Two examples of neighbourhood schemes for a cell x.

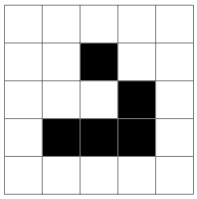


Figure 2: The Game of Life so called *glider*.

Surprisingly, such elementary rules give origin to very interesting behaviours, depending on the initial configuration. Very simple patterns can show complex global behaviours, such as systems of alive cells moving coherently on the grid, stationary configurations and oscillators. Among these peculiar patterns, we can cite the *gliders* as in figure 2. This particular pattern exhibits a surprising behaviour. Its evolution has a period of 4 generations to regain its original shape, meanwhile translating on the grid. The glider is the simplest propagating entity of the Game of Life. One can also build guns to periodically emit such gliders.

It was only with the paper by physicist Stephen Wolfram [70] that the CAs received a deep analysis and the first serious formalisation. As models of discrete dynamics the CAs resemble the evolution of physical systems as long as they can be described in the scope of *Classical Mechanics*. This fact was a limitation to the spread of the study of the automata in connection with *Theoretical Physics*. There were various attempts to overcome such limitations, extending the concept of CA to the *quantum world* as first suggested by Richard Phillips Feynman in his seminal paper [31]. Such extensions go by the name of *Quantum Cellular Automata* (QCAs) and are the main object of study of this work of thesis.

In relation to CAs there are other models of discrete dynamics which are called *Random Walks* (RWs) and *Quantum Walks* (QWs), first introduced by Aharonov, Davidovich, and Zagury [2]. These models simulate a single-particle evolution on a discrete lattice, while, on the contrary, the automata can accommodate many particles in local interaction. We can say that the one-particle sector of a QCA is, actually, a QW.

There were several attempts to extend the notion of classical CAs to the quantum case. For a brief review of some notions of QCA one can see the paper of Wiesner [67], where she highlights the differences between the various meaning of such quantum extensions to the classical automata. The study of QCAs began with Grössing and Zeilinger in [38] where they first coined the term. Later, there were other studies that led to many results in the field of *Quantum Information* with the works in [9, 37, 60], regarding the theory of QCAs. For QWs we can mention the references in [3, 7, 45]. The theory we are studying here is based on the notion of *Quantum Cellular Automaton* as defined by Reinhard F. Werner in the aforementioned paper [60].

2.1 CLASSICAL CELLULAR AUTOMATA

We have introduced above the concept of CA and QCA giving some intuition about the features of these models. Here we will rigorously formalise the ideas we have exposed.

Let us now begin giving the formal definition of a cellular automaton. Here we will consider only cubic infinite lattices, even in the quantum case, keeping in mind that in the literature one can find more general approaches, resorting to aspects of *Graph Theory* and connections with *Geometric Group Theory*, as one can notice from [8, 22, 53, 72].

Definition 2.1 (Lattice translation maps)**.** Let $D^{\mathbb{Z}^d}$ be a set of functions defined on the lattice with values in a set D. Then we can define *translations* τ_x of these functions as:

$$\begin{array}{rccc} \tau_x\colon & D^{\mathbb{Z}^d} & \longrightarrow & D^{\mathbb{Z}^d} \\ & c & \longmapsto & \tau_x[c] \end{array}$$

with

$$\tau_x[c](y) \coloneqq c(y-x),\ \forall\, y \in \mathbb{Z}^d.$$

Definition 2.2 (Cellular Automaton)**.** A (classical) *Cellular Automaton* (CA) is a 4-tuple $(L, A, \mathcal{N}, T)$ consisting in:

(i) a d-dimensional cubic lattice $L = \mathbb{Z}^d$ of cells (or sites);

(ii) a (finite) alphabet of symbols A, which constitutes the set of cell states;

(iii) a finite *neighbourhood scheme* $\mathcal{N} \subset L$;

(iv) a *local transition rule* $T\colon A^{\mathcal{N}} \to A$.

The cardinality $|A|$ is called the (local) *cell dimension*. The functions $c \in A^L$ are the (classical) *configurations* of the cells, assigning to each lattice site a symbol of the alphabet. Moreover, supposing that the configuration at time t is c_t, then the new configuration at time $t+1$ can be obtained as:

$$c_{t+1}(x) = T\left[\tau_{-x}[c_t]\big|_{\mathcal{N}}\right],\ \forall\, x \in L.$$

Remark 2.1 (Global transition map). It is apparent how the local transition rule induces a global, parallel transition of all the lattice sites:

$$\begin{array}{rccc} \mathcal{T}\colon & A^L & \longrightarrow & A^L \\ & c & \longmapsto & \mathcal{T}[c] \end{array}$$

defined as:

$$\mathcal{T}[c](x) \coloneqq T\left[\tau_{-x}[c]\big|_{\mathcal{N}}\right],\ \forall\, x \in L.$$

2.2 QUANTUM CELLULAR AUTOMATA

We present here the extension of the concept of cellular automata to the quantum world. Intuitively, we can imagine that such an extension is characterised by some lattice where in each site there is a quantum system in local unitary interaction with its neighbours. A naive implementation of these ideas would clearly follow such lines of thought.

In practice, one can assume that each cell x of the lattice is equipped with a *Hilbert space* $\mathcal{H}_x$, identical to the others, replacing the alphabet A of symbols of the classical case. Then one could think that the quantum systems located in each site interact between each other via a unitary operator U, requiring such interactions to be local. This means that this operator would be defined on the infinite tensor product $\bigotimes_{x\in L}\mathcal{H}_x$. Unfortunately, the resulting space would not be in general a Hilbert space.

To overcome these limitations it is effective to work in the Heisenberg picture rather than in the Schrödinger one. So, following the authors in [60] we will give an algebraic definition of a QCA.

Instead of associating to each site an Hilbert space, we associate to them the observable algebra $\mathcal{A}_x$, denoted the *cell structure*. These algebras are all isomorphic to the algebra $\mathcal{M}_s(\mathbb{C})$, *i. e.* the algebra of $s \times s$ complex matrices. If we consider a finite subset $\Lambda \subset L$, the associated algebra is the tensor product $\mathcal{A}(\Lambda) = \bigoplus_{x\in\Lambda}\mathcal{A}_x$. Whenever $\Lambda_1 \subset \Lambda_2 \subset L$, we can consider the natural injection $\mathcal{A}(\Lambda_1) \hookrightarrow \mathcal{A}(\Lambda_2)$, by tensoring with unit operators, so that we can regard $\mathcal{A}(\Lambda_1)$ as a subalgebra of $\mathcal{A}(\Lambda_2)$. With these identifications, are well defined the products AB of observable belonging to algebras located at different sites of the lattice. Moreover, since tensoring with the identity does not change the norm, we obtain a normed algebra of *local observables*, whose extension and completion Werner and Schumacher denote as the *quasi-local algebra* $\mathcal{A}(L)$.

Remark 2.2 (Lattice translations operators). Here the translations τ_x are isomorphisms of the local-observable algebras:

$$\begin{array}{rccc} \tau_x\colon & \mathcal{A}(\Lambda) & \longrightarrow & \mathcal{A}(\Lambda + x) \\ & A & \longmapsto & \tau_x(A). \end{array}$$

Definition 2.3 (Quantum Cellular Automaton)**.** A *Quantum Cellular Automaton* (QCA) is a 4-tuple $(L, \mathcal{A}, \mathcal{N}, \mathcal{T})$ consisting in:

(i) a d-dimensional cubic lattice $L = \mathbb{Z}^d$ of quantum systems;

(ii) an algebra $\mathcal{A}$ of local observables, which constitutes for every site the cell structure;

(iii) a finite neighbourhood scheme $\mathcal{N} \subset L$;

(iv) a unital homomorphism $\mathcal{T}\colon \mathcal{A}(L) \to \mathcal{A}(L)$ of the quasi-local algebra $\mathcal{A}(L)$ generated by $\mathcal{A}$.

The homomorphism $\mathcal{T}$ satisfies the following properties:

(i) it *commutes* with the lattice translations τ_x, $\forall\, x \in L$;

(ii) it satisfies the *locality condition*: $\mathcal{T}(\mathcal{A}(\Lambda)) \subset \mathcal{A}(\Lambda + \mathcal{N})$, $\forall\, \Lambda \subset L$, $|\Lambda| \in \mathbb{N}^+$.

Remark 2.3 (Local transition rule). The *local transition rule* is the homomorphism obtained restricting the action of $\mathcal{T}$ to the one-site algebra $\mathcal{A} \equiv \mathcal{A}_0$:

$$T \coloneqq \mathcal{T}\big|_{\mathcal{A}} \colon \mathcal{A} \to \mathcal{A}(\mathcal{N}).$$

Conversely, if one is given a local transition rule $T \colon \mathcal{A} \to \mathcal{A}(\mathcal{N})$, then the global homomorphism can be recovered from its homomorphism property:

$$\mathcal{T}\left(\bigotimes_{x\in\Lambda} A_x\right) = \prod_{x\in\Lambda} T_x(A_x),\ \forall\, \Lambda \subset L,\ |\Lambda| \in \mathbb{N}^+,$$

where T_x is the homomorphism defined by:

$$\begin{array}{rccl} T_x \colon & \mathcal{A}_x & \longrightarrow & \mathcal{A}(x + \mathcal{N}) \\ & A_x & \longmapsto & T_x(A_x) \coloneqq (\tau_x \circ T \circ \tau_{-x})(A_x). \end{array}$$

In the equations above we have made use of the identification between local observables of $\mathcal{A}$ and their injections into larger algebras, tensoring with identity operators. The proof of these facts can be found in the aforementioned paper of Schumacher and Werner [60].

2.3 QUANTUM WALKS

Among the discrete evolution models we can mention also the *Random Walks* (RWs) in the classical case and the *Quantum Random Walks* (QWs) for their quantum extension. Intuitively, a classical RW is the description of a particle moving in discrete time steps over neighbouring points of a lattice with certain probabilities.

A quantum version of such a model was first introduced in [2] where was considered a 1 dimensional lattice and measurements of the z-component of the spin of a $\frac{1}{2}$-spin particle decide whether it moves to the right or to the left. Subsequently, the measurements were substituted by specifying an evolution operator of the internal degree of freedom, which is called *coin* system. Rigorous analysis of QWs can be found in [1, 7, 43, 55].

For a QW the global space associated to the lattice of quantum systems is

$$\mathcal{H} = \bigoplus_{x\in L} \mathcal{H}_x,$$

*i. e.*the direct sum of the single site Hilbert spaces $\mathcal{H}_x$, rather than the tensor product. Each $\mathcal{H}_x$ is then the *cell structure* of the QW. So, now we can give the following definition.

Definition 2.4 (Quantum Random Walk)**.** A *Quantum Random Walk* (QW) is a 4-tuple $(L, \mathcal{C}, \mathcal{N}, U)$ consisting in:

(i) an infinite lattice $L \subseteq \mathbb{Z}^d$;

(ii) a finite Hilbert space $\mathcal{C}$, denoted the *cell structure* of the QW;

(iii) a finite *neighbourhood scheme* $\mathcal{N} \subset L$;

(iv) a unitary operator

$$\begin{aligned} U\colon \ \mathcal{H} &\longrightarrow \mathcal{H} \\ |\psi\rangle &\longmapsto U|\psi\rangle, \end{aligned}$$

where $\mathcal{H}$ is the total Hilbert space $\mathcal{H} = \bigoplus_x \mathcal{H}_x$ and $\mathcal{H}_x \simeq \mathcal{C}$.

Moreover, the action of U has to satisfy the locality requirement:

$$U|\psi\rangle \in \bigoplus_{x \in \mathcal{N}_x} \mathcal{H}_x, \forall\, |\psi\rangle \in \mathcal{H}_x,$$

where $\mathcal{N}_x = x + \mathcal{N}$.

Remark 2.4. If we consider the case in which $\mathcal{H}_x \simeq \mathbb{C}^n$ and $L = \mathbb{Z}^d$, then the total Hilbert space of the QW is

$$\mathcal{H} \simeq l^2\left(\mathbb{Z}^d\right) \otimes \mathbb{C}^d.$$

2.3.1 Quantum Walks versus Quantum Cellular Automata

As we have seen from the definitions we have given thus far, the two notions of QWs and QCAs are not in general not coincident. One way to see this fact is thinking of the classical case. A RW is the description of the discrete evolution of a single particle moving on a lattice, whereas a CA can describe, in general, a many-particle system. Intuitively, as long as the particles do not collide the CA can be regarded really as a RW.

In the quantum case, there exists a correspondent analogy. In fact, if we require the automaton unitary operator U to be linear and if we add the notion of a *vacuum state*, the resulting dynamics can be regarded as the dynamics of a single particle moving on the lattice. In this way we can identify the QCA with a QW. Conversely, as pointed out by Schumacher and Werner [60], one could "second quantise" a QW, obtaining a QCA whose single-particle sector is the given QW. In this work, we have studied only the single-particle sectors of the Weyl and Dirac QCAs.

2.4 THE DIRAC QUANTUM CELLULAR AUTOMATON

Numerical methods has been widely used as tools to obtain approximated results from physical theories, permitting phenomenological predictions, where analytical and exact calculations are not affordable. In order to make theoretical entities computationally tractable, one has to provide some way to discretise the underlying physical law.

This led, in the framework of *Quantum Field Theory*, to approaches like *Lattice Gauge Theory* [46, 47] adopted to provide approximations of the underlying continuous dynamics of quantum fields. Subsequently, some authors have proposed to apply the paradigm of QCAs to quantum fields. For example, we can mention the pioneering paper of Bialynicki-Birula [11], where the automaton describes a discrete classical-field dynamics, from which the Weyl and Dirac equations can be recovered in the continuum limit. Similar models, describing classical relativistic fields, were developed also in the context of *lattice-gas* simulations by Meyer [54] and Yepez [73].

All these approaches are considered only as discrete approximations of an underlying, more fundamental, dynamics. Only classical cellular automata have been contemplated as microscopic mechanisms, following the ideas of Feynman and Wheeler [39] in considering *Physcics* as *information processing*. For example, we can mention the works of 't Hooft [64] and Wolfram [69]. Recently, also *quantum cellular automata* have been considered by G. M. D'Ariano [20, 21, 23, 24] as a possibility for a microscopic fundamental description of physical processes. The large scale dynamics is then recovered in the continuum limit.

We have already presented the QCA on an infinite cubic lattice, but in principle it is possible to extend the concept to more general graphs with arguments of *Geometric Group Theory* as has been done by D'Ariano and Perinotti [22] in deriving the Weyl and Dirac automata. Specifically, the authors considered the family of *Bravais lattices*. Then in their derivation, they show how basic physical requirements on the geometric properties of the automaton select only the *cubic lattice* (in $(2+1)$-dimensions) and the *body centred* one (in $(3+1)$-dimensions).

Let us briefly summarise here the postulates from which they were able to derive the Weyl and Dirac automata:

(I) *unitarity* of the evolution;

(II) *locality* of the interactions;

(III) *homogeneity* of the interaction topology;

(IV) *isotropy* under lattice symmetries.

Moreover, they have selected the automaton with minimal complexity, that is the minimal dimension of the Hilbert space associated to the internal degree of freedom. Under such assumptions Paolo Perinotti and Giacomo Mauro D'Ariano were able to derive the unique automaton (modulo discrete symmetries) which describes, in the large scale limit, the Weyl equation. Then, coupling two such automata in the only possible way to respect these assumptions, one obtains the unique automaton (again modulo symmetries) which describes the Dirac equa-

tion. This automaton can be characterised in its QW sector with a unitary operator U over the space $l^2(L) \otimes \mathbb{C}^s$, which can be written as:

$$U = \sum_{h \in \Omega} T_h \otimes A_h, \tag{1}$$

where Ω is the set of generators of the group whose *Cayley's graph* is the lattice L over which the QCA is defined. Here the operators T_h are the *lattice translations* acting over elements of $l^2(L)$ as:

$$T_h |n\rangle = |n + h\rangle \, , \, \forall \, |n\rangle \in l^2(L).$$

The complex matrices A_h are the transition matrices acting on the internal degree of freedom of the lattice sites. As pointed out by the authors in [22], the unitarity condition is particularly restrictive in selecting the possible forms these matrices can assume. Now we want to briefly report the two specific cases we have studied in this work. Namely, the Dirac automaton in 1 spatial dimension and the Weyl automaton in 2 spatial dimensions. In the next chapters we will give some more insights on the properties of these automata along with an explicit expression for their evolution at arbitrary discrete times.

2.4.1 Dirac automaton in $(1+1)$-dimensions

Retaining the expression of the full unitary operator in equation (1), we can give here the explicit expression for the transition matrices in this case. The minimal internal dimension for the present case is $s = 2$. Since the spatial lattice is the linear graph $\mathbb{Z}$, we have only two generators for the lattice translations, namely a particle can move to the right or to the left. Furthermore, as this automaton has mass, in order to describe the Dirac field in the continuum limit, we have to consider a matrix associated to the identity element of the group $\mathbb{Z}$. That is, we have to allow the particle to remain still in a lattice site; the only effect in this case is a change in the state of the internal degree of freedom. So, we have the three matrices:

$$A_R = \begin{pmatrix} n & 0 \\ 0 & 0 \end{pmatrix}, \quad A_L = \begin{pmatrix} 0 & 0 \\ 0 & n \end{pmatrix}, \quad A_M = \begin{pmatrix} 0 & im \\ im & 0 \end{pmatrix}, \tag{2}$$

where the unitarity constraint requires that $n^2 + m^2 = 1$, $n > 0$, $m > 0$.

2.4.2 Weyl automaton in $(2+1)$-dimensions

For the 2 spatial dimensions, we have considered only the Weyl automaton, that is, an automaton describing the Weyl mass-less field in the large scale limit. Moreover, since in this case the *spin* reduces to the *helicity* states, the internal dimension is still $s = 2$. In this case the lattice is the square lattice $\mathbb{Z}^2$, therefore the possible

translations are 4 and so are the transition matrices (we have not to consider the mass term):

$$\begin{aligned} A_R &= \begin{pmatrix} 1 & 0 \\ -\nu & 0 \end{pmatrix}, \quad A_U = \begin{pmatrix} 1 & 0 \\ \nu & 0 \end{pmatrix}, \\ A_L &= \begin{pmatrix} 0 & \nu^* \\ 0 & 1 \end{pmatrix}, \quad A_D = \begin{pmatrix} 0 & -\nu^* \\ 0 & 1 \end{pmatrix}, \end{aligned} \tag{3}$$

where the unitarity imposes that $|\nu| = 1$.

2.4.3 Symmetries

The isotropy property for these automata is expressed, in general terms, by the *covariance* of the automaton U under the action of some group G of symmetries of the lattice:

$$g \cdot U = \sum_{h \in \Omega} g \cdot (T_h \otimes A_h) = \sum_{h \in \Omega} T_{g \cdot h} \otimes V_g A_h V_g^\dagger = U, \forall\, g \in G, \tag{4}$$

where $g \cdot (\cdot)$ denotes the action of the group G and V_g is an its (unitary) representation. In the specific case of the Weyl automaton in 2 spatial dimensions, as pointed out by Perinotti and D'Ariano in their paper, the actual symmetries are given by the rotations of $\frac{\pi}{2}$ on the lattice.

3 SUM OVER HISTORIES

Based on ideas of Paul Adrien Maurice Dirac [27, 28], Richard Phillips Feynman presented in his remarkable paper [32] the space-time formulation of Quantum Mechanics, using functional methods which are called *path integrals*. Later, this different approach to Quantum Mechanics was developed in collaboration with Hibbs in [33].

Today this approach has become a fundamental tool in characterising Quantum Field Theories [4, 25, 36, 41, 58]. Although it has such successful applications, it suffers from mathematical difficulties. The main issue with a naive implementation of the ideas of the path integral as originally formulated by Feynman is the fact that there not exist an infinite dimensional Lebesgue measure on the space of continuous functions, besides the trivial one [40]; stated in other words, every (translation-invariant) measure that is not identically 0 assigns an infinite measure to every open subset of the space of paths. Motivated by these considerations, during the years there were several attempts to give a precise meaning to the concept of an integral – *i. e.*, an infinite sum – over such a space of paths [4, 5, 17, 26].

3.1 FEYNMAN'S PATH INTEGRAL

The aim of the *path integral* formulation of Quantum Mechanics is to generalise the Hamilton's principle of Classical Mechanics. The *Principle of Stationary Action* in the Hamilton sense says that a classical system described by a Lagrangian L defined on the tangent bundle of the configuration space of the system TC takes those paths which make the action functional stationary:

$$\mathcal{S}[q] \coloneqq \int_{t_1}^{t_2} L(q(t), \dot{q}(t); t)\, dt.$$

More precisely, assuming that this functional is Fréchet-differentiable and considering proper variations of a given curve

$$(t, \varepsilon) \mapsto q_\varepsilon(t) = q(t) + \varepsilon h(t),$$

namely (differentiable) curves with fixed endpoints, the statement is that the *Gâteaux derivative* of the action vanishes for all such variations:

$$\mathcal{D}\mathcal{S}[q] \circ h = 0,\ \forall\, h \in \mathfrak{X}(C),\ h(t_1) = h(t_2) = 0,$$

where $\mathfrak{X}(C)$ is the set of smooth vector fields. It can be proved [44, 57] that in this way one obtains the *Euler-Lagrange* equations of motion:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0.$$

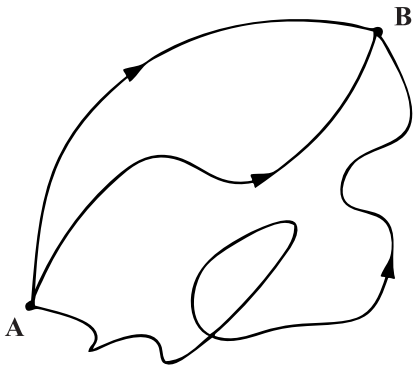


Figure 3: Paths connecting two points A and B.

So we see that the path, given some initial conditions, a classical particle actually follows is obtained as an extremum of a suitable functional.

Instead, when we look at the Quantum World we can no more associate a path in the physical space to a quantum particle. The concept of a trajectory has no meaning according to the standard formulation of Quantum Mechanics. But the thoughts of Dirac were oriented towards the possibility of formulating an Action Principle even in the Quantum World. From earlier preliminary studies in his Ph.D. thesis with John Archibald Wheeler, Feynman developed a new different formulation of Quantum Mechanics which generalises the classical Action Principle.

In Quantum Mechanics, suppose we have a particle in an initial state $|x_0, t_0\rangle$, that is we know the particle at time t_0 is localised in x_0. Then we may ask what is the probability of finding the particle in x at a later time t. According to the *Born rule* this is given by the squared modulus of the probability amplitude:

$$\psi(x,t) = \langle x,t|x_0,t_0\rangle\,.$$

If we think classically for a moment, we may ask which path the particle has *actually* travelled. But, of course, there are $\aleph_1$-infinitely many paths connecting the two points (x_0,t_0) and (x,t) in space-time; for example we can consider the case sketched in figure 3 (the image is taken from Wikipedia.org [68]).

So, now comes the basic idea of path-integrals: we have to sum (integrate) all these contributions, according to the principles of Quantum Mechanics [61, 29]. The next step is to work out how each path contributes to the total amplitude. According to Feynman each path contributes equally in magnitude and the phase factor is given by:

$$\exp\left(\frac{i}{\hbar}\mathcal{S}[q;t_1,t_2]\right),$$

where $\mathcal{S}$ is the classical action computed on a path q. Then using the *stationary phase approximation* [71], we can see that the paths which will give the more significant contributions to the sum are the classical ones, preserving in this way the correct classical limit.

3.2 PATH INTEGRAL FOR QUANTUM WALKS

In the previous section we have given some sketches of the concept of the path integral, which is, in practice, a sum over all the histories of a physical system. Now we will focus on discrete quantum systems and we will see in more details how the idea of a sum over histories applies in this case. An example of this model is due to Feynman in his *Checkerboard Model* for a relativistic electron [33].

3.2.1 Basic ideas

Let us imagine a world in which one can go only through discrete steps. That is, one is allowed to go from one point (or site) of this world to another and there are no halfway pit stops. There are clearly many ways to define a set of rules according to which one can move through such a world. In general such a construction gives origin to a *graph* [14, 66]. The points in this world are the vertices (or nodes) of the graph and the possible connections – we will also call them *transitions* – are its edges. The rules we define determine the type of the graph and the properties of its edges, characterising in this way its topology. A general approach to such a construction of graphs can be found in the scope of *geometric group theory* [16, 50].

Let us now focus on the case of our interest. That is, a graph which can be embedded in the plane generating a square lattice. Suppose we start in a point A of the lattice. Then we have four choices we can take. If, moreover, we assume that each way is equivalent to the others, then we can toss an appropriate coin which tells us in which direction to go. In this way we define a *Random Walk* [1, 2, 43, 51].

After N steps on this graph one reaches some point B. Then one may ask us what is the probability to go from A to B, considering all the possible ways to reach B.

As we can see from figure 4 on the following page, in order to compute the probability $p(B|A;N)$ to go from A to B in N steps we have to sum up all the probabilities for each sequence of points connecting A with B:

$$p(B|A;N) = \sum_{i_1,\dots,i_{N-1}} p\big(B|x_{i_{N-1}}|\dots|x_{i_1}|A\big), \tag{5}$$

This is basically the idea behind the concept of *summing over histories*. From equation (5) we see that what we have to know are the single probabilities associated to each path defined by a sequence $\chi = (x_0, \dots, x_n)$. We can immediately notice

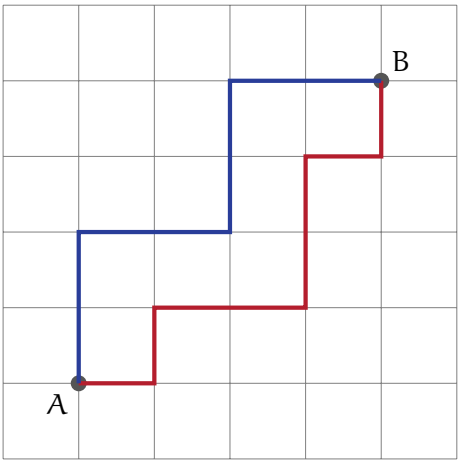


Figure 4: Paths connecting A and B in a square lattice.

a first thing. The probability associated to a path χ is certainly 0 if the length $l(\chi) = n$ is greater than the requested number of steps N. This means that the set of points reached by paths of length N define the set of points *causally* related to a given initial point, that is its (future) *causal cone* – or improperly the *light cone*.

Remark 3.1. Regarding the example we have exposed here, we can encode the paths into strings of bits; specifically, each step can be encoded with two bits and therefore a sequence χ of length N can be uniquely associated to a binary string Ξ of length 2N. Since we have supposed that each direction is equivalent to the others, then all the paths Ξ are equally probable with probability $p(\Xi) = \frac{1}{2^{2N}}$. Then the probability we are looking for is given by:

$$p(B|A;N) = \frac{\mathcal{N}(A,B;N)}{2^{2N}},$$

where $\mathcal{N}(A,B;N)$ is the number of paths connecting A and B of length N. We can give an explicit expression for this probability. In order to achieve this result, given a binary string Ξ of length 2N we can think of it as made by a pair (α,β) of strings. As a convention we denote here an element of α as a_i and an element of β as b_i; then we have the relation $a_i = x_{2i-1}$ and $b_i = x_{2i}$ with $i = 1,\dots,N$ and x_j an element of Ξ. Moreover, we can define the *bit count* of a binary string as:

$$\hat{\alpha} := \sum_{i=1}^{N} a_i.$$

Now, if we label the points of the square lattice with some coordinates (x,y), associating $A \equiv (0,0)$, we have the following relation between coordinates and bit counts:

$$\begin{cases} \hat{\alpha} \equiv K_1 = \frac{N-x+y}{2}, \\ \hat{\beta} \equiv K_2 = \frac{N-x-y}{2}. \end{cases}$$

We shall give the proof of this fact in chapter 5 on page 25. Now we are able to compute the counting function $\mathcal{N}$. In fact, the condition above tells us that we can permute the two strings α and β *independently* and therefore we have simply:

$$\mathcal{N}(K_1, K_2) = \binom{N}{K_1}\binom{N}{K_2}. \tag{6}$$

The ideas we have expressed thus far are perfectly suited to deal with *classical* random walks. One may wonder where the quantum effects appear in this world. All the problems arise from equation (5) on page 15. The definition we have given is inappropriate in the quantum case. The crucial point is that we have implicitly assumed that a particle travelling from A to B actually is in a specific point x between them. Instead, a quantum particle can exist in a superposition of states corresponding to different positions. This means that we can not associate at each step a definite position to the particle. As a consequence, a quantum particle can show interference patterns. What we have to do is to change the description of the particle not directly in terms of probabilities but instead in terms of probability *amplitudes*. In practice, we can retain the definitions we have given so far, simply substituting $p \rightsquigarrow \varphi$, where φ is complex-valued. The relation between the two is: $p(E) = |\varphi(E)|^2$, where E is the event we are considering. Clearly, the results given in remark 3.1 have to be modified to take into account the different interferences of the various paths. We shall give the full solution of this problem in the next chapters, in the case of Weyl and Dirac automata.

3.2.2 General formulation

In the previous paragraphs we have exposed some ideas concerning the path integral. Here we want to show a more systematic way to obtain the path sum, adopting a slightly different approach. Let us suppose we are given a Quantum Cellular Automaton – in this case it is actually a Quantum Walk, as pointed out in section 2.3.1 on page 8 – which can be represented as a unitary operator over the space $l^2(Z) \otimes \mathbb{C}^s$, where Z is the associated graph:

$$U = \sum_{h \in \Omega} T_h \otimes A_h. \tag{7}$$

Moreover suppose that, in a group-theoretical language, Ω is the set of generators of an abelian group G whose Cayley graph is Z. From the definition we can notice that the transition matrices $\{A_h\}_{h\in\Omega}$ are uniquely associated to the colours defining the translations on the graph. This fact permits us to describe a path as a sequence of transitions; more precisely there is a one to one correspondence between the sequences of translations and sequences of transition matrices. Since the paths are in correspondence to suitable binary strings Ξ, we will always identify such sequences of transitions with these binary strings.

In order to simplify a bit the derivation of the solutions that we will give in the next chapters, we can ask ourselves which is the transition matrix associated

to a point B if we started from A. Then we can compute the components of the resulting field $\psi(x, N)$ in x at time $t = N$, given the values of the field $\psi(y, 0)$ at time $t = 0$, for all lattice sites y in the past causal cone. From the definition of the automaton given in equation (7) we can write the N steps evolution as:

$$U^N = \sum_{\Xi \in \Omega^N} T_{h_1} \cdots T_{h_N} \otimes A_{h_1} \cdots A_{h_N} \tag{8}$$

We will write the product of transition matrices as $\mathcal{A}(\Xi)$. Then, since a translation operator T_h acts on an element $|g\rangle$ of $l^2(Z)$ as

$$T_h |g\rangle = |g + h\rangle ,$$

the position state associated to a path Ξ will be:

$$T_{h_1 + \cdots + h_N} |g\rangle = |g + h_1 + \cdots + h_N\rangle .$$

Associating the initial point A to the identity element of the group, we can label it with coordinates $(0, 0, \ldots, 0)$ with the final point B of the path Ξ corresponding to the state $|h_1 + \cdots + h_N\rangle$. Now we want to find out which is the transition matrix to arrive at a point x after N steps of evolution:

$$\begin{aligned} \tau(x; N) &= (\langle x| \otimes I)\, U^N\, (|0\rangle \otimes I) \\ &= \sum_{\Xi} \langle x \,|\, h_1 + \cdots + h_N \rangle\, \mathcal{A}(\Xi) \\ &= \sum_{\Xi} \delta(x, \Xi) \mathcal{A}(\Xi), \end{aligned} \tag{9}$$

where δ is a function that assures a given point x can be reached by a path Ξ:

$$\delta(x, \Xi) \coloneqq \begin{cases} 1, & \text{if } \Xi \text{ leads to } x, \\ 0, & \text{otherwise.} \end{cases}$$

4 DIRAC SOLUTION IN 1-DIMENSION

In this chapter we will expose the solution for the Dirac quantum cellular automaton in one spatial dimension that we have introduced in section 2.4.1 on page 10. Let us recall here the evolution operator in this case:

$$U = T_R \otimes A_R + T_L \otimes A_L + T_M \otimes A_M, \tag{10}$$

where $T_{R,L}$ are the lattice-translation operators defined over sequences $f \in l^2(\mathbb{Z})$:

$$(T_R f)(x) := f(x-1),$$
$$(T_L f)(x) := f(x+1).$$

Here T_M is the identity operator over $l^2(\mathbb{Z})$. In this context the transition matrices are:

$$A_R = \begin{pmatrix} a & 0 \\ 0 & 0 \end{pmatrix}, \quad A_L = \begin{pmatrix} 0 & 0 \\ 0 & a \end{pmatrix}, \quad A_M = \begin{pmatrix} 0 & ib \\ ib & 0 \end{pmatrix}, \tag{11}$$

where the labelling specifies the transition type and $a, b \in \mathbb{R}^+$, $a^2 + b^2 = 1$.

In this work we focus on the path-integral approach to give an explicit expression for the evolution of the automaton. As mentioned in chapter 3 a first scheme attempting to formulate the path-integral in a discrete context was given by Feynman in his Chessboard Model. In this chapter we want to exploit this approach in order to solve the problem of giving an explicit expression for the evolution of the Dirac automaton in one spatial dimension. Let us recall the expression for the sum over histories we have previously found in a general context in equation (9) on page 18:

$$\tau(x; N) = \sum_{\Xi \in \Omega^N} \delta(x, \Xi) \mathcal{A}(\Xi). \tag{12}$$

In order to obtain an explicit formula for the sum above, we have first to analyse the algebraic properties of the transition matrices of the one dimensional case. A first thing one can notice is that anyhow we multiply these matrices between them we can always extract a factor that gives the amplitude for that product. This amplitude can be written in the form:

$$\alpha(f) := (ib)^f a^{N-f} \tag{13}$$

where f counts the number of times a flip occurs (*i. e.* the number of mass terms). So, we can drop the coefficients and use the following set of matrices:

$$A_R = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad A_L = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad A_M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{14}$$

Moreover it is easily seen that at each point one is allowed to choose from two of the three possible steps. For example, if we begin in the left mode, then we can either go to the left or switch to the right mode, analogously if we began in the right mode. Furthermore we can notice that the matrix A_M contributes only with one of its non null elements. This means that adopting a suitable binary encoding such that $R = 00$, $L = 11$, we can write each product using the set of matrices:

$$\begin{aligned} A_{00} &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad A_{11} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \\ A_{10} &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad A_{01} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \end{aligned} \tag{15}$$

considering that the mass transition matrix can be written as:

$$A_M = A_{10} + A_{01}.$$

Then it can be easily seen that each product of two of these matrices vanishes if the internal bits are different and the result depends only on the first and the last bit of the sequence. More precisely, we have the following lemma.

Lemma 4.1. *The product of two matrices of the set* (15) *on this page is given by:*

$$A_{ab}A_{cd} = \frac{1 + (-1)^{b \oplus c}}{2} A_{ad}.$$

As a consequence of this algebraic property we have the following rules for the products concerning the mass matrix.

Corollary 4.1. *The matrix* A_M *satisfies the following rules:*

$$\begin{aligned} A_M^2 &= I, \\ A_{aa}A_M &= A_{ab}, \\ A_M A_{aa} &= A_{ba}, \\ A_M A_{ab} &= A_{bb}, \\ A_{ab}A_M &= A_{aa}, \end{aligned}$$

with $a \neq b$.

With these results in mind we can go back to the general expression for the transition matrix after N steps in equation (12) on page 19. Now we want to count how many paths there are which give each matrix. Our purpose here is to find out an expression like:

$$\tau(x; N) \rightsquigarrow c_N^R R + c_N^L L + c_N^M M,$$

where the coefficients counts the number of strings Ξ which result in each matrix. We might expect to obtain such an expression since the set (15) on this page is closed under matrix multiplication, eventually adding the null matrix and the

identity. Moreover, given that the matrices 10 and 01 appear together in the mass matrix, we can expect that they would contribute equally in the result – indeed, they do as we will see soon.

Equation (13) on page 19 suggests us to parameterise the sum over histories with the number of flips f which in general run over the set $\{0, \dots, N\}$. So we can write:

$$\tau(x; N) = \sum_{f=0}^{N} \alpha(f) \sum_{\Xi_f} \delta(x, \Xi_f) \mathcal{A}(\Xi_f), \tag{16}$$

where $\{\Xi_f\}$ are the strings with exactly f mass terms. Let us denote the total number of steps as $N = r + l + f$, where r is the number of right steps and l is the number of left steps. Now we would like to relate somehow these three parameters to the final point x.

Lemma 4.2. *Fixing the number of flips f we have:*

$$\begin{cases} r = \frac{N+x-f}{2}, \\ l = \frac{N-x-f}{2}. \end{cases}$$

Proof. The result follows immediately from the fact that $r - l = x$. □

Corollary 4.2. *f is even if and only if $N + x$ is even.*

Let us now consider strings Ξ_f. Then from the rules in lemma 4.1 and corollary 4.1 on page 20 it is apparent that the strings which give a non null result are those in which the matrices R and L alternate each other between the swap matrices M. In fact if a matrix $a\,a$ is followed by an M, then the next can only be either another mass or a $b\,b$, with $a \neq b$. Therefore, the allowed strings (*i. e.* non null) show patterns like:

$$\Xi = \mathtt{RRRMLLM\ MLMRRMLLL}, \tag{17}$$

and, considering that we can always collapse repetitions of an R or an L, the sequence in equation (17) has the same transition matrix of

$$\Xi = \mathtt{RMLM\ MLMRML}. \tag{18}$$

So we can see that a given number of flips f determines $f + 1$ slots where we have to arrange the right- and left-steps.

Lemma 4.3. *Let Ξ be a string with f swaps. Then, we can assert what follows.*

$$f < N \implies \mathcal{A}(\Xi) = \begin{cases} A_{a\,a}, & \text{if } f \text{ is even}, \\ A_{a\,b}, & \text{if } f \text{ is odd}, \end{cases}$$

where $a\,a$ refers to the matrices in the odd slots and $b \neq a$. Furthermore,

$$f = N \implies \mathcal{A}(\Xi) = \begin{cases} I, & \text{if } N \text{ is even}, \\ A_M, & \text{if } N \text{ is odd}. \end{cases}$$

Proof. In order to prove the statement we split the two case where f is even or odd.

- $f < N$, f even. We can proceed by induction over N. For $N = 1$ the statement is clearly true. Then, for $N > 1$, assuming $\mathcal{A}(\Xi) = A_{aa}$, we can add one more A_M so that the result is A_{ab}.
- $f < N$, f odd. Analogously we can add one more mass term and obtain A_{aa}.
- $f = N$. Just consider that $A_M^2 = I$. □

We can say, in other words, that the result is determined only by the first step and the parity of the number of swaps.

Now we have only to count the number of times each result appears.

Theorem 4.1. *Let* $N \in \mathbb{N}^+$, $-N < x < N$ *and* $0 \leqslant f \leqslant \min\{N - x, N + x\}$. *Then, if* f *is even,*

$$c_N^R(x, f) = \binom{\frac{N+x}{2}}{\frac{f}{2}} \binom{\frac{N-x}{2} - 1}{\frac{f}{2} - 1},$$
$$c_N^L(x, f) = \binom{\frac{N-x}{2}}{\frac{f}{2}} \binom{\frac{N+x}{2} - 1}{\frac{f}{2} - 1};$$

if f *is odd,*

$$c_N^M(x, f) = \binom{\frac{N+x-1}{2}}{\frac{f-1}{2}} \binom{\frac{N-x-1}{2}}{\frac{f-1}{2}}.$$

Proof. Let $N > 0$, $-N < x < N$, $x \neq 0$, $0 < f \leqslant \min\{N - x, N + x\}$ and consider strings Ξ_f. Then we can think of placing first the mass terms and then distributing the remaining objects in the $f + 1$ slots. From lemma 4.2 on page 21 we know we have to distribute r R-steps and l L-steps. From the conditions on the parameters we have that r and l are never both 0 nor they can be equal to N. From the algebraic properties of the matrices we have analysed above, we know that the resulting matrix is determined once we have chosen to place a given type of steps in the odd slots. Then we can permute the objects in the odd and even slots independently. This fact implies that we will have a product of two terms. For each factor we can follow the same reasoning. The situation can be formulated as follows. We have, say, n distinguishable slots in which to arrange k identical objects. These arrangements can be viewed as combinations with repetitions [see for example 10], which are counted with the multi-choose coefficients:

$$w(n, k) = \left(\!\!\binom{n}{k}\!\!\right) = \binom{n + k - 1}{k}.$$

Then we have to count the number of odd and even slots separately:

$$n_{\text{odd}} = \left\lceil \frac{f + 1}{2} \right\rceil, \quad n_{\text{even}} = \left\lfloor \frac{f + 1}{2} \right\rfloor.$$

Therefore, we have the following cases.

- f even. In this case $n_{\text{odd}} = \frac{f}{2} + 1$ and $n_{\text{even}} = \frac{f}{2}$; therefore:

$$\begin{aligned} c_N^R &= \binom{\frac{f}{2}+r}{r}\binom{\frac{f}{2}+l-1}{l} \\ &= \binom{\frac{N+x}{2}}{\frac{N+x-f}{2}}\binom{\frac{N-x}{2}-1}{\frac{N-x-f}{2}} \\ &= \binom{\frac{N+x}{2}}{\frac{f}{2}}\binom{\frac{N-x}{2}-1}{\frac{f}{2}-1}; \end{aligned}$$

$$\begin{aligned} c_N^L &= \binom{\frac{f}{2}+l}{l}\binom{\frac{f}{2}+r-1}{r} \\ &= \binom{\frac{N-x}{2}}{\frac{N-x-f}{2}}\binom{\frac{N+x}{2}-1}{\frac{N+x-f}{2}} \\ &= \binom{\frac{N-x}{2}}{\frac{f}{2}}\binom{\frac{N+x}{2}-1}{\frac{f}{2}-1}. \end{aligned}$$

- f odd. Now $n_{\text{odd}} = n_{\text{even}} = \frac{f+1}{2}$. Therefore we have that $c_N^{10} = c_N^{01} = c_N^M$ and the coefficient for this case is:

$$\begin{aligned} c_N^M &= \binom{\frac{f+1}{2}+r-1}{r}\binom{\frac{f+1}{2}+l-1}{l} \\ &= \binom{\frac{N+x-1}{2}}{\frac{N+x-f}{2}}\binom{\frac{N-x-1}{2}}{\frac{N-x-f}{2}} \\ &= \binom{\frac{N+x-1}{2}}{\frac{f-1}{2}}\binom{\frac{N-x-1}{2}}{\frac{f-1}{2}}. \end{aligned}$$

- $f = N$. In this case $r = l = 0 \wedge x = 0$ and therefore the resulting matrix would be either the identity or M depending on the parity of N. As a matter of fact, we can reuse the expressions above since they reduce to 1 in this case, which is the correct result.

- $f = 0$. If $|x| < N$ then both the coefficients c_N^R and c_N^L are 0. Otherwise, if $x = N$, then $c_N^R = 1$ and $c_N^L = 0$; else if $x = -N$, then $c_N^R = 0$ and $c_N^L = 1$. Therefore, again, we can use the general formulae since the binomial $\binom{n}{k} = 0$ if $k > n$. □

To end the considerations about the solution of the Dirac automaton in one spatial dimension, we can rewrite equation (16) on page 21, splitting the two cases:

- if $N + x$ is even we have to sum over even fs:

$$\tau(x; N) = \sum_{k=0}^{k_{\max}^{\text{even}}} \alpha(2k)\left[c_N^R(x, 2k)A_R + c_N^L(x, 2k)A_L\right], \tag{19}$$

where $k_{\max}^{\text{even}} = \min\left\{\frac{N-x}{2}, \frac{N+x}{2}\right\}$;

- if $N + x$ is odd we have the other case:

$$\tau(x; N) = \sum_{k=0}^{k_{max}^{odd}} \alpha(2k+1) c_N^M(x, 2k+1) A_M, \tag{20}$$

where $k_{max}^{odd} = \min\left\{ \frac{N-x-1}{2}, \frac{N+x-1}{2} \right\}$.

5 WEYL SOLUTION IN 2-DIMENSIONS

Analogously to the one dimensional case, we can express the evolution of the Weyl automaton in 2 spatial dimensions, introduced in section 2.4.2 on page 10, as the sum:

$$\tau(x, y; N) = \frac{1}{2^N} \sum_{\Xi \in \Omega^N} \delta(x, y, \Xi) \mathcal{A}(\Xi). \tag{21}$$

5.1 PRELIMINARY ANALYSES

Here the transition matrices are:

$$\begin{aligned} A_R &= \begin{pmatrix} 1 & 0 \\ -\nu & 0 \end{pmatrix}, \quad A_U = \begin{pmatrix} 1 & 0 \\ \nu & 0 \end{pmatrix}, \\ A_L &= \begin{pmatrix} 0 & \nu^* \\ 0 & 1 \end{pmatrix}, \quad A_D = \begin{pmatrix} 0 & -\nu^* \\ 0 & 1 \end{pmatrix}, \end{aligned} \tag{22}$$

with $|\nu| = 1$.

5.1.1 Basic properties

Now letting $h, k \in \{1, 2\}$, we can obtain some algebraic properties of this set of matrices.

Lemma 5.1. *The set of matrices in (22) has the following product rules:*

$$A_{\pm h}^2 = A_{\pm h}, \tag{23a}$$
$$A_{\pm h} A_{\mp h} = -A_{\mp k}, \tag{23b}$$
$$A_{\pm h} A_{\pm k} = A_{\pm h}, \tag{23c}$$
$$A_{\pm h} A_{\mp k} = A_{\mp k}, \tag{23d}$$

with $k \neq h$. Moreover these matrices sum up to the identity:

$$\sum_{h \in \Omega} A_h = 2I. \tag{24}$$

Corollary 5.1. *Upon encoding the matrices in (22) onto a boolean algebra, with* R $= 00$, L $= 10$, U $= 01$, D $= 11$, *the product rules in lemma 5.1 become:*

$$A_{a,b} A_{c,d} = (-1)^{(a \oplus c)(b \oplus d \oplus 1)} A_{c, a \oplus b \oplus c}. \tag{25}$$

Proof. From the products in equations (23a) to (23d) we can see that the sign part of the encoding is always that of the second term in the product. The direction part of the encoding is the same as that of the first term, unless the signs were opposite. The sign of the product is -1 if and only if the directions are the same and the signs are opposite. □

Now, for a sequence $\Xi \equiv (\alpha, \beta)$, with $\alpha, \beta \in \{0,1\}^N$, we can express the function $\mathcal{A}$ as

$$\mathcal{A}(\alpha,\beta) = (-1)^{\varphi(\alpha,\beta)} A_{\mu(\alpha,\beta)},$$

where the function $\mu\colon \{0,1\}^{2N} \to \{0,1\}^2$ returns the corresponding matrix and $\varphi\colon \{0,1\}^{2N} \to \{0,1\}$ gives the phase associated to the path; the circle notation emphasises the fact that the phase is cyclic, as will be apparent from the following lemmata.

Lemma 5.2. *Given $\alpha^N, \beta^N \in \{0,1\}^N$ and expressing the result as*

$$\mu(\alpha^N,\beta^N) = \big(\mathfrak{a}(\alpha^N,\beta^N), \mathfrak{b}(\alpha^N,\beta^N)\big), \tag{26}$$

the transition matrix is given by

$$\begin{aligned} \mathfrak{a}(\alpha^N,\beta^N) &= a_N, \\ \mathfrak{b}(\alpha^N,\beta^N) &= \mathfrak{b}(\alpha^{N-1},\beta^{N-1}) \oplus \mathfrak{a}(\alpha^{N-1},\beta^{N-1}) \oplus a_N \\ &= a_1 \oplus b_1 \oplus a_N, \end{aligned} \tag{27}$$

where, in α^{N-1}, we have dropped the last element of α^N.

Proof. In the following we will assume this notation convention: $f^N \equiv f(\alpha^N,\beta^N)$. Now using the associativity of the matrix product we can establish a recursive relation for $\mathfrak{a}$:

$$\mathfrak{a}^N = \mathfrak{a}(\mathfrak{a}^{N-1}a_N, \mathfrak{b}^{N-1}b_N).$$

From corollary 5.1 we have immediately that

$$\mathfrak{a}^N = a_N.$$

Analogously, for the encoding part we have the recursion:

$$\begin{aligned} \mathfrak{b}^N &= \mathfrak{b}(\mathfrak{a}^{N-1}a_N, \mathfrak{b}^{N-1}b_N) \\ &= \mathfrak{b}^{N-1} \oplus \mathfrak{a}^{N-1} \oplus a_N. \end{aligned}$$

Now, assuming $\mathfrak{b}^N = a_1 \oplus b_1 \oplus a_N$, the expression above becomes

$$\begin{aligned} \mathfrak{b}^{N+1} &= \mathfrak{b}^N \oplus \mathfrak{a}^N \oplus a_{N+1} \\ &= a_1 \oplus b_1 \oplus a_N \oplus a_N \oplus a_{N+1} \\ &= a_1 \oplus b_1 \oplus a_{N+1}. \end{aligned}$$

□

In order to obtain a similar result for the phase it is worth introducing a different encoding for the matrices, simplifying in this way the results.

Definition 5.1 (Matrix encoding)**.** Let us define the following transformation of the bit strings

$$\begin{aligned} f(\alpha^N, \beta^N) &:= (\beta^N, \alpha^N \oplus \beta^N), \\ f^{-1}(\alpha^N, \beta^N) &= (\alpha^N \oplus \beta^N, \alpha^N), \end{aligned} \tag{28}$$

where the XOR operator in the definition acts component-wise on the strings. In this encoding the association with the letters is: R = 00, L = 11, U = 10, D = 01.

Lemma 5.3. *In the encoding defined by equations* (28)*, the matrix resulting from* (α^N, β^N) *is*

$$\mu(\alpha^N, \beta^N) = (a_1, b_N). \tag{29}$$

Proof. Denoting the function μ in the new encoding as

$$\mu'(\alpha^N, \beta^N) = f^{-1}(\mu(f(\alpha^N, \beta^N))),$$

we can write

$$\begin{aligned} \mu'(\alpha^N, \beta^N) &= f^{-1}(\mathbf{a}(\beta^N, \alpha^N \oplus \beta^N), \mathbf{b}(\beta^N, \alpha^N \oplus \beta^N)) \\ &= f^{-1}(b_N, a_1 \oplus b_1 \oplus b_1 \oplus b_N) \\ &= f^{-1}(b_N, a_1 \oplus b_N) \\ &= (b_N \oplus a_1 \oplus b_N, b_N) \\ &= (a_1, b_N). \end{aligned}$$

□

From now on we will always use this encoding. Now we are able to give a simple expression for the phase function.

Theorem 5.1. *The phase associated to the pair* $(\alpha^N, \beta^N) \in \{0, 1\}^{2N}$ *is given by:*

$$\begin{aligned} \varphi(\alpha^N, \beta^N) &= \varphi(\alpha^{N-1}, \beta^{N-1}) \oplus (a_1 \oplus a_N)(b_{N-1} \oplus b_N) \\ &= \bigoplus_{j \in \mathbb{Z}_N} a_j (b_{j-1} \oplus b_j) \\ &= \bigoplus_{j \in \mathbb{Z}_N} (a_j \oplus a_{j+1}) b_j, \end{aligned} \tag{30}$$

where $\mathbb{Z}_N$ *is the cyclic group with* N *elements and* $\varphi^0 = \varphi^1 = 0$.

Proof. From corollary 5.1 we can write the recursion:

$$\varphi^N = \varphi^{N-1} \oplus (\mathbf{a}^{N-1} \oplus a_N)(\mathbf{b}^{N-1} \oplus b_N \oplus 1).$$

Then, adopting the encoding in definition 5.1 the expression above becomes:

$$\begin{aligned} \varphi'^N &= \varphi'^{N-1} \oplus (b_{N-1} \oplus b_N)(a_1 \oplus b_{N-1} \oplus a_N \oplus b_N \oplus 1) \\ &= \varphi'^{N-1} \oplus (b_{N-1} \oplus b_N)(a_1 \oplus b_{N-1} \oplus a_N \oplus b_N \oplus b_{N-1} \oplus b_N) \\ &= \varphi'^{N-1} \oplus (b_{N-1} \oplus b_N)(a_1 \oplus a_N), \end{aligned}$$

proving the first part of the thesis. Now supposing that

$$\varphi'^{N} = \bigoplus_{j=1}^{N} a_j \left(b_{j-1} \oplus b_j \right),$$

the next step is:

$$\begin{aligned}
\varphi'^{N+1} &= \bigoplus_{j=1}^{N} a_j \left(b_{j-1} \oplus b_j \right) \oplus (a_1 \oplus a_{N+1})(b_N \oplus b_{N+1}) \\
&= a_1 (b_N \oplus b_1) \oplus \bigoplus_{j=2}^{N} (\dots) \oplus (a_1 \oplus a_{N+1})(b_N \oplus b_{N+1}) \\
&= a_1 (b_{N+1} \oplus b_1) \oplus \bigoplus_{j=2}^{N+1} a_j \left(b_{j-1} \oplus b_j \right) \\
&= \bigoplus_{j=1}^{N+1} a_j \left(b_{j-1} \oplus b_j \right).
\end{aligned}$$

The last expression in equation (30) can be deduced in a similar way. □

5.1.2 Directed paths

We will focus here on paths with only two types of steps allowed. The first preliminary result will be about the specific case where these two steps alternate each other. Although this might seem a restriction, we will see that this condition can cover more general situations. This fact follows from the idempotence of the transition matrices as defined in equation (22) on page 25. Now we can state the following result.

Theorem 5.2. *Let* $\Xi = \left(\alpha^N, \beta^N \right) \in \Omega^{2N}$. *Suppose that the sequence* Ξ *satisfies the condition*

$$\begin{cases} a_j = a_{j+2}, \\ b_j = b_{j+2}, \end{cases} \tag{31}$$

$\forall\, j \in \mathbb{Z}_N : j + 2 \leqslant N$. *Then we have that*

$$\varphi^{4K} = 0, \tag{32a}$$
$$\varphi^{4K+1} = 0, \tag{32b}$$
$$\varphi^{4K+2} = (a_1 \oplus a_2)(b_1 \oplus b_2), \tag{32c}$$
$$\varphi^{4K+3} = (a_1 \oplus a_2)(b_1 \oplus b_2). \tag{32d}$$

Proof. We begin proving the case $N = 4K$ in equation (32a). From theorem 5.1 on page 27 we can write:

$$\begin{aligned}\varphi^{4K} &= \sum_{j=1}^{4K} a_j \left(b_{j-1} \oplus b_j\right) \\ &= \sum_{j=0}^{K-1} \sum_{l=1}^{4} a_{4j+l} \left(b_{4j+l-1} \oplus b_{4j+l}\right).\end{aligned}$$

Then the inner sum evaluates to:

$$\begin{aligned}\varphi^{4K} = \sum_{j=0}^{K-1} \big[&a_{4j+1} \left(b_{4j} \oplus b_{4j+1}\right) \oplus a_{4j+2} \left(b_{4j+1} \oplus b_{4j+2}\right) \oplus \\ &\oplus a_{4j+3} \left(b_{4j+2} \oplus b_{4j+3}\right) \oplus a_{4j+4} \left(b_{4j+3} \oplus b_{4j+4}\right) \big] .\end{aligned}$$

Now, using the condition (31) the sum becomes:

$$\begin{aligned}\varphi^{4K} &= \sum_{j=0}^{K-1} \left[\left(a_{4j} \oplus a_{4j+1}\right) \left(b_{4j} \oplus b_{4j+1}\right) \oplus \left(a_{4j} \oplus a_{4j+1}\right) \left(b_{4j} \oplus b_{4j+1}\right) \right] \\ &= 0.\end{aligned}$$

The next step is to prove the case $N = 4K + 1$, for which we have:

$$\begin{aligned}\varphi^{4K+1} &= \varphi^{4K} \oplus (a_1 \oplus a_{4K+1})(b_{4K} \oplus b_{4K+1}) \\ &= (a_1 \oplus a_1)(b_2 \oplus b_1) \\ &= 0.\end{aligned}$$

Now, for $N = 4K + 2$, we can write:

$$\begin{aligned}\varphi^{4K+2} &= \varphi^{4K+1} \oplus (a_1 \oplus a_{4K+2})(b_{4K+1} \oplus b_{4K+2}) \\ &= (a_1 \oplus a_2)(b_1 \oplus b_2).\end{aligned}$$

Finally for $N = 4K + 3$, we have that:

$$\begin{aligned}\varphi^{4K+3} &= \varphi^{4K+2} \oplus (a_1 \oplus a_{4K+3})(b_{4K+2} \oplus b_{4K+3}) \\ &= (a_1 \oplus a_2)(b_1 \oplus b_2) \oplus (a_1 \oplus a_1)(b_2 \oplus b_1) \\ &= (a_1 \oplus a_2)(b_1 \oplus b_2).\end{aligned}$$

□

The study of paths with only two kind of steps allowed can be exploited to analyse the case of *directed paths*. We have just seen that, in general, the phase takes values according to the remainder classes of 4 of the number of steps. But, whenever we consider paths in which $a_1 = a_2$ or $b_1 = b_2$, *i. e.* directed paths, the phase always vanishes and the paths interfere constructively. Such directed paths lead always to the nappes of the (future) causal cone, to which we will refer as *causal front*, defined by the condition $|x| + |y| = N$. In this case we can give in a very straightforward way the explicit expression of the coefficients of the transition matrices. Without loss of generality, we will focus on the points (x, y) of the first quadrant, *i. e.* $x, y \geqslant 0$, considering that for the other quadrants we can follow a similar reasoning.

Proposition 5.1 (Causal front). *Let* $N \in \mathbb{N}^+$ *and* $x, y \geqslant 0$ *with* $x + y = N$. *Then, the non-vanishing coefficients are:*

$$c_N^R = \binom{N-1}{x-1} = \binom{N-1}{y},$$
$$c_N^U = \binom{N-1}{y-1} = \binom{N-1}{x}.$$

Proof. Let $N \in \mathbb{N}^+$ and $x, y \geqslant 0$. The total number of steps N can be written as $N = r + l + u + d$ with $r - l = x$ and $u - d = y$. Therefore, $l + d = 0$ and $l = d = 0$. So $c_N^L = c_N^D = 0$. Having only right- or up-steps, this is precisely the case for which the phase always vanishes. So, the paths reaching the causal front, as one may expect, interfere always constructively. Then we have only to distinguish the resulting matrix. This is achieved by fixing the first and the last step and permuting the intermediate steps. So we have to count the permutations with repetitions of $r + u$ objects:

$$c(r, u) = \frac{(r+u)!}{r!u!} = \binom{r+u}{r}.$$

Then, considering that $N = r + u$ and $r = x$, $u = y$, fixing the first and the last step, we have four sub-cases:

$$c_N^{RR}(x, y) = \binom{N-2}{x-2}, \qquad c_N^{UR}(x, y) = \binom{N-2}{y-1},$$
$$c_N^{RU}(x, y) = \binom{N-2}{x-1}, \qquad c_N^{UU}(x, y) = \binom{N-2}{y-2},$$

where the superscript IJ corresponds to paths where the first step is of type I and the last is of type J. Now, putting together the first two and likewise the last two, we have:

$$c_N^R(x, y) = \binom{N-2}{x-2} + \binom{N-2}{x-1} = \binom{N-1}{x-1} = \binom{N-1}{y},$$
$$c_N^U(x, y) = \binom{N-2}{y-1} + \binom{N-2}{y-2} = \binom{N-1}{y-1} = \binom{N-1}{x}. \qquad \square$$

5.1.3 Recurrence relations

From the expression in equation (21) on page 25, we can obtain a recurrence expression for the coefficients of each matrix in the resulting transition matrix. Let us now redefine the matrix sum as:

Definition 5.2 (Transition matrix function)**.**

$$F_N(x, y) := \sum_{\Xi \in \Omega^N} \delta(x, y, \Xi) \mathcal{A}(\Xi).$$

From the expression above we have a first result, giving a recurrence for F_N.

Lemma 5.4.

$$F_N(x,y) = A_R F_{N-1}(x-1,y) + A_L F_{N-1}(x+1,y) + \\ + A_U F_{N-1}(x,y-1) + A_D F_{N-1}(x,y+1).$$

Proof. From definition 5.2 on page 30 we have:

$$F_N(x,y) = \sum_h \sum_{\Xi'} \delta(x,y,h,\Xi')\mathcal{A}(h,\Xi') \\ = \sum_h A_h \sum_{\Xi'} \delta(x,y,h,\Xi')\mathcal{A}(\Xi'),$$

with $h \in \Omega$ and $\Xi' \in \Omega^{N-1}$. So, we see we have a recursive relation for F_N:

$$F_N(x,y) = A_R F_{N-1}(x-1,y) + A_L F_{N-1}(x+1,y) + \\ + A_U F_{N-1}(x,y-1) + A_D F_{N-1}(x,y+1). \qquad \square$$

Now we are able to give a recursive expression for the coefficients. Let us suppose we know the expression for F_N at step N:

$$F_N(x,y) = c_N^R A_R + c_N^L A_L + c_N^U A_U + c_N^D A_D. \tag{33}$$

Then we can deduce the recursive expression for the c_Ns.

Theorem 5.3 (Recursive coefficients)**.** *The coefficients in equation* (33) *satisfy the relation:*

$$c_N^R(x,y) = c_{N-1}^{R+U}(x-1,y) + c_{N-1}^{R-U}(x,y+1), \\ c_N^L(x,y) = c_{N-1}^{L+D}(x+1,y) + c_{N-1}^{L-D}(x,y-1), \\ c_N^U(x,y) = c_{N-1}^{U+R}(x,y-1) + c_{N-1}^{U-R}(x+1,y), \\ c_N^D(x,y) = c_{N-1}^{D+L}(x,y+1) + c_{N-1}^{D-L}(x-1,y),$$

where

$$c_N^{\alpha X+\beta Y} = \alpha c_N^X + \beta c_N^Y.$$

Proof. From equation (33) we have:

$$A_R F_N(x,y) = c_N^R A_R - c_N^L A_D + c_N^U A_R + c_N^D A_D \\ = c_N^{R+U} A_R + c_N^{D-L} A_D, \\ A_L F_N(x,y) = -c_N^R A_U + c_N^L A_L + c_N^U A_U + c_N^D A_L \\ = c_N^{L+D} A_L + c_N^{U-R} A_U, \\ A_U F_N(x,y) = c_N^R A_U + c_N^L A_L + c_N^U A_U - c_N^D A_L \\ = c_N^{L-D} A_L + c_N^{U+R} A_U, \\ A_D F_N(x,y) = c_N^R A_R + c_N^L A_D - c_N^U A_R + c_N^D A_D \\ = c_N^{R-U} A_R + c_N^{D+L} A_D.$$

Now using lemma 5.4 on page 31 we can write:

$$\begin{aligned} F_{N+1}(x,y) = \quad & c_N^{R+U}(x-1,y)A_R + c_N^{D-L}(x-1,y)A_D + \\ & + c_N^{L+D}(x+1,y)A_L + c_N^{U-R}(x+1,y)A_U + \\ & + c_N^{L-D}(x,y-1)A_L + c_N^{U+R}(x,y-1)A_U + \\ & + c_N^{R-U}(x,y+1)A_R + c_N^{D+L}(x,y+1)A_D. \end{aligned} \tag{34}$$

Then, collecting the terms with the same matrices, we obtain:

$$\begin{aligned} F_{N+1}(x,y) = \quad & \left[c_N^{R+U}(x-1,y) + c_N^{R-U}(x,y+1)\right]A_R + \\ & + \left[c_N^{L+D}(x+1,y) + c_N^{L-D}(x,y-1)\right]A_L + \\ & + \left[c_N^{U+R}(x,y-1) + c_N^{U-R}(x+1,y)\right]A_U + \\ & + \left[c_N^{D+L}(x,y+1) + c_N^{D-L}(x-1,y)\right]A_D. \end{aligned}$$

□

As a first consequence of theorem 5.3 on page 31 we can show how the result given in proposition 5.1 on page 30 for the causal front can also be proved by induction, solving the corresponding recurrence relation.

Corollary 5.2 (Causal front). *Let* $x, y \geqslant 0$ *and* $x + y = N$. *Then the coefficients for the transition matrices are:*

$$c_N^R(x,y) = \binom{N-1}{y}, \tag{35a}$$

$$c_N^U(x,y) = \binom{N-1}{x}. \tag{35b}$$

Proof. Let us identify the points of the causal front as $(N-i, i)$, $i \in \{0, \ldots, N\}$. Then the coefficients are:

$$\begin{aligned} c_N^R(N-i,i) &= c_{N-1}^R(N-i-1,i) + c_{N-1}^U(N-i-1,i), \\ c_N^U(N-i,i) &= c_{N-1}^U(N-i,i-1) + c_{N-1}^R(N-i,i-1), \end{aligned}$$

where we have dropped the null ones, corresponding to a distance greater than the number of steps. Now supposing that

$$\begin{aligned} c_{N-1}^R(N-i-1,i) &= \binom{N-2}{i}, \\ c_{N-1}^U(N-i-1,i) &= \binom{N-2}{N-i-1} = \binom{N-2}{i-1}, \end{aligned}$$

we obtain for the next step the expressions:

$$c_N^R(N-i,i) = \binom{N-2}{i} + \binom{N-2}{i-1} = \binom{N-1}{i}.$$

The other case can be proved analogously. □

Now we are able to find the coefficients in other two cases. In the first case we compute the coefficients for the points $(N-2, 0)$ and in the second those for the points $(N-3, 1)$. These points lie on the second front, immediately preceding the causal front, at distance $N-2$.

Corollary 5.3 (Points $(N-2,0)$)**.** *We have that* $\forall\, N \geqslant 2$ *the coefficients are*

$$\begin{aligned}
c^{R}_{N}(N-2,0) &= (N-3)^2 - 2,\\
c^{L}_{N}(N-2,0) &= -1,\\
c^{U}_{N}(N-2,0) &= N-3,\\
c^{D}_{N}(N-2,0) &= N-3.
\end{aligned}$$

Proof. From theorem 5.3 on page 31 we can write, dropping the null coefficients:

$$\begin{aligned}
c^{R}_{N}(N-2,0) &= c^{R+U}_{N-1}(N-3,0) + \binom{N-2}{N-3} - \binom{N-2}{0},\\
c^{L}_{N}(N-2,0) &= -\binom{N-1}{0},\\
c^{U}_{N}(N-2,0) &= \binom{N-2}{N-3} - \binom{N-2}{N-2},\\
c^{D}_{N}(N-2,0) &= c^{D}_{N-1}(N-3,0) - c^{L}_{N-1}(N-3,0).
\end{aligned}$$

Now we have immediately that $c^{L}_{N} = -1$ and $c^{U}_{N} = N-2-1 = N-3$. Then for D we have the recursion $c^{D}_{N}(N-2,0) = c^{D}_{N-1}(N-3,0) + 1$. This can be easily solved, but we can also consider that on the x-axes, for the symmetries of the automaton (see section 2.4.3 on page 11), the coefficients of U and D must be the same. So $c^{D}_{N}(N-2,0) = c^{U}_{N}(N-2,0) = N-3$. Now, for R we have:

$$\begin{aligned}
c^{R}_{N}(N-2,0) &= c^{R}_{N-1}(N-3,0) + N - 4 + N - 3\\
&= c^{R}_{N-1}(N-3,0) + 2N - 7.
\end{aligned}$$

So, we have to solve the recurrence:

$$\begin{cases}
a_2 &= -1,\\
a_{n+1} &= a_n + 2(n+1) - 7, \forall\, n \geqslant 2.
\end{cases}$$

We can solve this recursion considering the fact that the sum of odd numbers is the square of the number of elements summed. Or, we can simply verify it by induction. In fact, supposing that $a_n = (n-3)^2 - 2$, we have

$$\begin{aligned}
a_{n+1} &= (n-3)^2 + 2n - 7\\
&= n^2 - 6n + 9 + 2n - 7\\
&= n^2 - 4n + 4 - 2\\
&= (n+1-3)^2 - 2.
\end{aligned}$$

□

Corollary 5.4 (Points $(N-3,1)$)**.** *We have that* $\forall\, N \geqslant 2$ *the coefficients are*

$$\begin{aligned}
c^{R}_{N}(N-3,1) &= \frac{(N-2)(N-3)(N-7)}{2},\\
c^{L}_{N}(N-3,1) &= -(N-3),\\
c^{U}_{N}(N-3,1) &= (N-4)^2 - 3,\\
c^{D}_{N}(N-3,1) &= \frac{(N-2)(N-5)}{2}.
\end{aligned}$$

Proof. We begin with L:

$$\begin{aligned} c^{L}_{N}(N-3,1) &= c^{L-D}_{N-1}(N-3,0) \\ &= -1-(N-4) \\ &= -(N-3). \end{aligned}$$

Then for U we have:

$$\begin{aligned} c^{U}_{N}(N-3,1) &= c^{U+R}_{N-1}(N-3,0) + c^{U-R}_{N-1}(N-2,1) \\ &= (N-4) + (N-4)^2 - 2 + \binom{N-2}{0} - \binom{N-2}{N-3} \\ &= (N-4)(N-4+1) - 2 + 1 - (N-2) \\ &= (N-3)(N-4) - (N-1). \end{aligned}$$

Now, for D we can write:

$$\begin{aligned} c^{D}_{N}(N-3,1) &= c^{D-L}_{N-1}(N-4,1) \\ &= c^{D}_{N-1}(N-4,1) + (N-4) \\ &= \frac{(N-3)(N-6)}{2} + (N-3) - 1 \\ &= (N-3)\left[\frac{N-6}{2} + 1\right] - 1 \\ &= \frac{(N-3)(N-4)}{2} - 1 \\ &= \frac{N^2 - 7N + 10}{2} \\ &= \frac{(N-2)(N-5)}{2}. \end{aligned}$$

Finally we can solve the recurrence for R:

$$\begin{aligned} c^{R}_{N}(N-3,1) &= c^{R+U}_{N-1}(N-4,1) + c^{R-U}_{N-1}(N-3,2) \\ &= c^{R+U}_{N-1}(N-4,1) + \binom{N-2}{N-4} - \binom{N-2}{1} \\ &= c^{R+U}_{N-1}(N-4,1) + \frac{(N-2)(N-3)}{2} - (N-2) \\ &= c^{R+U}_{N-1}(N-4,1) + \frac{(N-2)(N-5)}{2} \\ &= c^{R}_{N-1}(N-4,1) + (N-4)(N-5) - (N-3) - 1 + \\ &\quad + \frac{(N-2)(N-5)}{2} \\ &= c^{R}_{N-1}(N-4,1) + \frac{3}{2}(N-3)(N-6). \end{aligned}$$

Finally we can substitute the induction hypothesis to obtain:

$$\begin{aligned} c^{R}_{N}(N-3,1) &= \frac{(N-3)(N-4)(N-8)}{2} + \frac{3}{2}(N-3)(N-6) \\ &= \frac{N-3}{2}[(N-4)(N-8)+3(N-6)] \\ &= \frac{N-3}{2}\left(N^2-9N+14\right) \\ &= \frac{(N-2)(N-3)(N-7)}{2}. \end{aligned}$$

□

5.2 GENERAL CASE SOLUTION

Thus far we have given some insights of the properties on the phase function, considering how it affects the paths of the underlying graph. Now we want to find a general method in order to better exploit the *path-integral* approach we have studied in this work.

5.2.1 Fundamental result

In the one dimensional case, an effective way to solve the path count problem is to make, in practice, a kind of *change of lattice coordinates*. Instead of using the pair (x,t) we can adopt the pair (r,l) which directly characterises the path count. The effect of the mass term is only to add a new parameter f. In the present context, a problem which arises studying the path count is that we have to properly characterise those paths which keep fixed the ending point. As in the one dimensional case, here we will show that there exists a necessary and sufficient condition which can be regarded as a kind of change of coordinates. As a consequence, this condition allows us to formulate a method to obtain a general expression for the path count.

Theorem 5.4 (Necessary and sufficient condition for fixed endpoints paths)**.** *A path (α,β) reaches the point (x,y) in N steps if and only if $N-|x|-|y|$ is even and nonnegative and it holds that*

$$\begin{cases} K_1 \equiv \hat{\alpha} = \frac{N-x+y}{2}, \\ K_2 \equiv \hat{\beta} = \frac{N-x-y}{2}, \end{cases} \tag{36}$$

where $\hat{\alpha} := \sum_{i=1}^{N} a_i$ and $\hat{\beta} := \sum_{i=1}^{N} b_i$ are the bit count of α and β respectively.

Proof. Let us first prove the necessity of the condition above. If a path (α,β) leads to the point (x,y) in N steps, then it is formed by a certain number of steps in each direction: $N = r+l+u+d$. The distance constraints read: $r-l = x$, $u-d = y$. Let us now recall the encoding for each step type: `R` $=$ `00`, `L` $=$ `11`, `U` $=$ `10`, `D` $=$ `01`. For the string α, we can see that the only steps contributing to

the bit count are L and U and so $K_1 = l + u$. What remains is the number of 0*s*: $N - K_1 = r + d$. For β we can follow a similar reasoning and get $K_2 = l + d$ and $N - K_2 = r + u$. So we have immediately that $K_1 - K_2 = y$. Then we have $(N - K_1 + N - K_2) - (K_1 + K_2) = 2x$. Therefore we obtain the system:

$$\begin{cases} x = N - K_1 - K_2, \\ y = K_1 - K_2, \end{cases} \tag{37}$$

which can be easily inverted to obtain the expression for K_1 and K_2. Now we want to prove the sufficiency. Let us choose a N steps path (α, β) with $\hat{\alpha} = K_1$ and $\hat{\beta} = K_2$. Then it reaches the point (x', y') given by the system (37). Therefore if we choose K_1 and K_2 as in (36) we have $x' = x$ and $y' = y$. □

Remark 5.1. Theorem 5.4 shows us that there exists a necessary and sufficient condition so that a path reaches a given point (x, y). Moreover we can notice that this condition applies independently to the strings α and β. This means that we can permute these strings *ad libitum*. This is precisely what we need to be able to count the paths according to their phase, as we will see in the following.

5.2.2 Counting techniques

Since the technique we are going to explain here derives directly from the definition of the phase, let us recall its expression:

$$\varphi = \bigoplus_{j \in \mathbb{Z}_N} (a_j \oplus a_{j+1})\, b_j. \tag{38}$$

It is now apparent which operations do not change the phase, considering that we can deal with α and β independently. In fact, we can at first look up which strings α have some fixed number of pairs with different bits, cyclically. That is, considering for example $\dot{0}\bar{0}\bar{1}\dot{0}\dot{1}\bar{1}$, it has four pairs with different bits, denoted by bars (over the first bit of the pair), and the last pair is cyclic. The pairs in which the bits are equal are denoted by dots. Then, fixed the number of pairs, the role of β is that of choosing a certain number of these pairs; more precisely the bit count of β is the number of pairs chosen. Therefore it is clear that the phase is 1 if and only if $\hat{\beta}$ is odd. This means that we have found a way to select the paths with the same phase. Moreover, counting the number of strings with a fixed number of pairs is independent from the number of ways we can select a certain number of them; this fact is the consequence of theorem 5.4. So, firstly, we solve the pairs problem and then the pairs-selection one.

Now we want to find a way to keep fixed the number of pairs (with different bits) in a string. From the example above, we can see that the pairs appear exactly twice the number of slots of 1-bits, considering the last cyclically. Then we have to count in how many ways we can distribute the 1-bits in these slots. But, for every arrangement of 1*s* we can arrange in all possible ways the 0*s*. So, we will have a product of two terms.

Let us first consider the arrangements of 1-bits. Suppose we have $K > 0$ of them to distribute in $p \geqslant 1$ slots. This is equivalent to consider the integer compositions of K with p parts. In fact a given arrangement can be seen as a p-tuple $(k_1, \ldots, k_p)$ with the property $\sum_{l=1}^{p} k_l = K$. We have to consider compositions instead of partitions because a different ordering generates a distinct path. The compositions and partitions of integers are broadly analysed in the literature: see for example Benjamin and Quinn [10] and Brualdi [15] for a general treatise on combinatorics and related topics.

Theorem 5.5. *The number of p-compositions of K are given by*

$$w_p(K) = \binom{K-1}{p-1}. \tag{39}$$

Proof. A composition of K can be seen as an arrangement of K indistinguishable objects into p distinguishable slots, where at least 1 object has to be left in each slot. That is, we have to specify that there are p slots. So, we are left with $K - p$ objects to distribute in p slots, now freely. We can think of distributing objects as choosing each slot a certain number of times, even 0. These are precisely the multi-combinations of a set with p elements. Therefore we have:

$$\begin{aligned} w_p(K) &= \left(\!\!\binom{p}{K-p}\!\!\right) \\ &= \binom{p+K-p-1}{K-p} \\ &= \binom{K-1}{p-1}. \end{aligned}$$

□

Using this result we know that we have $w_p(K)$ ways to arrange the K 1-bits. Now we are left with $N - K$ 0-bits to distribute in the remaining slots. In order to do this, we have to consider distinct sub cases: *i. e.* we have to fix the first and last bit.

Lemma 5.5. *The number of strings α of length N such that $\hat{\alpha} = K > 0$ and with $p \geqslant 1$ parts is given by:*

$$\begin{aligned} n_p(0,0) &= \binom{K-1}{p-1}\binom{N-K-1}{p}, \\ n_p(1,1) &= \binom{K-1}{p-1}\binom{N-K-1}{p-2}, \\ n_p(1,0) &= \binom{K-1}{p-1}\binom{N-K-1}{p-1}, \\ n_p(0,1) &= \binom{K-1}{p-1}\binom{N-K-1}{p-1}, \end{aligned} \tag{40}$$

where $n_p(i,j)$ denotes the number of strings with $a_1 = i$ and $a_N = j$.

Proof. As said before we have to distinguish four sub-cases, each corresponding the different ways a string can start and end. For all these cases the count of 1-bits arrangements is $w_p(K)$. All we have to do is to count the number of arrangements in which we can distribute the $N-K$ 0*s* between the 1*s*. With a similar reasoning as in theorem 5.5, the count is given by $w_{p'}(N-K)$, where p' has to be specified:

- case $(0,0)$: in this case the number of slots is $p' = p+1$, therefore $n_p(0,0) = w_p(K)w_{p+1}(N-K)$;
- cases $(0,1)$ and $(1,0)$: here the slots are $p' = p$ and then $n_p(0,1) = w_p(K)w_p(N-K)$;
- case $(1,1)$: the slots are $p' = p-1$ and therefore

$$n_p(1,1) = w_p(K)w_{p-1}(N-K). \qquad \square$$

Now we have to count the number of ways we can choose a given number of pairs. Firstly it has to be noticed that this can be done for each string with that number of pairs: here is were theorem 5.4 on page 35 comes into play. Then, since we have to count the paths for each matrix, we have to fix the first bit in α and the last in β. In principle, for each 1-bit in β we can have a selection, permuting them accordingly. So we will have a sum over each possible number of selections.

Lemma 5.6. *Let us consider binary strings α and β of length N such that $\hat{\beta} = K \geqslant 0$ and such that α has $p \geqslant 1$ parts. Then the number of ways of choosing k pairs is given by:*

$$c_{p,k}(000) = \binom{2p}{k}\binom{N-2p-1}{K-k}, \qquad c_{p,k}(001) = \binom{2p}{k}\binom{N-2p-1}{K-k-1},$$
$$c_{p,k}(110) = \binom{2p-2}{k}\binom{N-2p+1}{K-k}, \quad c_{p,k}(111) = \binom{2p-2}{k}\binom{N-2p+1}{K-k-1},$$
$$c_{p,k}(011) = \binom{2p-1}{k}\binom{N-2p}{K-k-1}, \qquad c_{p,k}(010) = \binom{2p-1}{k}\binom{N-2p}{K-k},$$
$$c_{p,k}(101) = \binom{2p-1}{k}\binom{N-2p}{K-k-1}, \qquad c_{p,k}(100) = \binom{2p-1}{k}\binom{N-2p}{K-k},$$

where $c_k(i,j,l)$ is the number of strings with $a_1 = i$, $a_N = j$, $b_N = l$ and with p parts.

Proof. In all of the cases we have to consider we can make the same reasoning. Disregarding in which way the strings can end, we can say that α has a fixed number of pairs, say p'. Then, we want to choose k of them, permuting β. This can be done in $\binom{p'}{k}$ ways. Finally, we have still to place $K-k$ objects in $N-p'$ boxes and this can be done in $\binom{N-p'}{K-k}$ ways. When we fix the endpoints of the strings, what we have to do is modify a little the considerations just done.

- Case 000: we have $2p$ internal pairs, so the count is exactly $\binom{2p}{k}$; the $(K-k)$ remaining 1-bits are to be placed in $N-2p-1$ boxes, since we have a 0 as the last bit in β, so the count is $\binom{N-2p-1}{K-k}$.

- Case `110`: here there are $2p-2$ pairs: so the count is $\binom{2p-2}{k}$; then we have to place $K-k$ ones in $N-(2p-2)-1$ boxes, since a slot is always fixed, then: $\binom{N-2p+1}{K-k}$.
- Cases `011` and `101`: here there are $2p$ pairs, but only $2p-1$ free, since the last is always chosen (the last bit of β is `0`); therefore the count is $\binom{2p-1}{k}$; then we are left with $K-k-1$ objects to place in $N-2p$ slots and this time we have $\binom{N-2p}{K-k-1}$.
- Case `001`: the pair selection gives $\binom{2p}{k}$; then we have $K-k-1$ objects (since one is fixed) to place in $N-2p-1$ boxes since one is already chosen and so the count is $\binom{N-2p-1}{K-k-1}$.
- Case `111`: here there are $2p-2$ pairs: $\binom{2p-2}{k}$; then we have $K-k-1$ objects to distribute in $N-(2p-2)-1$ slots: $\binom{N-2p+1}{K-k-1}$.
- Cases `010` and `100`: now there are $2p$ pairs, but one never chosen: $\binom{2p-1}{k}$; then we have to place $K-k$ objects in $N-2p$ slots: $\binom{N-2p}{K-k}$. □

Corollary 5.5. *Let us consider paths of length* N (α, β) *such that* α *has* $p \geqslant 1$ *parts and* $\hat{\beta} = K \geqslant 0$. *Then, permuting* β *and keeping* α *fixed, we have the following interference functions:*

$$
\begin{aligned}
c_p(\texttt{000}) &= \sum_{k=0}^{2p} (-1)^k c_{p,k}(\texttt{000}), & c_p(\texttt{001}) &= \sum_{k=0}^{2p} (-1)^k c_{p,k}(\texttt{001}),\\
c_p(\texttt{110}) &= \sum_{k=0}^{2p-2} (-1)^k c_{p,k}(\texttt{110}), & c_p(\texttt{111}) &= \sum_{k=0}^{2p-2} (-1)^k c_{p,k}(\texttt{111}),\\
c_p(\texttt{011}) &= \sum_{k=0}^{2p-1} (-1)^{k+1} c_{p,k}(\texttt{011}), & c_p(\texttt{010}) &= \sum_{k=0}^{2p-1} (-1)^k c_{p,k}(\texttt{010}),\\
c_p(\texttt{101}) &= \sum_{k=0}^{2p-1} (-1)^{k+1} c_{p,k}(\texttt{101}), & c_p(\texttt{100}) &= \sum_{k=0}^{2p-1} (-1)^k c_{p,k}(\texttt{100}).
\end{aligned}
$$

Proof. The signs for the cases `011` and `101` are reversed because we always choose at least one pair. □

Now we are able to give the general result.

Theorem 5.6 (General case)**.** *The coefficients of the resulting matrices for paths of length* N *characterised by the pair* (K_1, K_2) *can be expressed as:*

$$
c_N^{a,b}(K_1, K_2) = \sum_{p=\min\{1, K_1\}}^{K_1} \sum_{a'=0}^{1} n_p(a, a') c_p(a, a', b). \tag{41}
$$

Proof. The result follows directly from lemma 5.5 and corollary 5.5. □

Previously we have given two proof of the formula for the coefficients on the causal front. Now we want to show how the same result can be derived from the general expressions of theorem 5.6. As before we will assume that the points lie in the first quadrant $x, y > 0$ and $N = x + y$.

Corollary 5.6 (Causal front)**.** *The non vanishing coefficients of the transition matrices on the causal front are given by:*

$$\begin{aligned} c^{R}_{N} &= \binom{N-1}{y}, \\ c^{U}_{N} &= \binom{N-1}{x}. \end{aligned} \tag{42}$$

Proof. The causal front is characterised by the condition $x + y = N$. So the parameters of theorem 5.4 on page 35 become:

$$\begin{cases} K_1 = \frac{N-x+y}{2} = y, \\ K_2 = \frac{N-x-y}{2} = 0. \end{cases}$$

The coefficients now are:

$$\begin{aligned} c^{R}_{N} &= \sum_{p=1}^{y} (n_p(00)c_p(000) + n_p(01)c_p(010)), \\ c^{U}_{N} &= \sum_{p=1}^{y} (n_p(10)c_p(100) + n_p(11)c_p(110)), \\ c^{L}_{N} &= \sum_{p=1}^{y} (n_p(10)c_p(101) + n_p(11)c_p(111)), \\ c^{D}_{N} &= \sum_{p=1}^{y} (n_p(00)c_p(001) + n_p(01)c_p(011)). \end{aligned}$$

Then the pair-counts are:

$$\begin{aligned} n_p(0,0) &= \binom{y-1}{p-1}\binom{N-y-1}{p}, & n_p(1,1) &= \binom{y-1}{p-1}\binom{N-y-1}{p-2}, \\ n_p(0,1) &= \binom{y-1}{p-1}\binom{N-y-1}{p-1}, & n_p(1,0) &= \binom{y-1}{p-1}\binom{N-y-1}{p-1}. \end{aligned}$$

The counts for the pairs selection become:

$$\begin{aligned} c_{p,k}(000) &= \binom{2p}{k}\binom{N-2p-1}{-k}, & c_{p,k}(101) &= \binom{2p-1}{k}\binom{N-2p}{-k-1}, \\ c_{p,k}(010) &= \binom{2p-1}{k}\binom{N-2p}{-k}, & c_{p,k}(111) &= \binom{2p-2}{k}\binom{N-2p+1}{-k-1}, \\ c_{p,k}(100) &= \binom{2p-1}{k}\binom{N-2p}{-k}, & c_{p,k}(001) &= \binom{2p}{k}\binom{N-2p-1}{-k-1}, \\ c_{p,k}(110) &= \binom{2p-2}{k}\binom{N-2p+1}{-k}, & c_{p,k}(011) &= \binom{2p-1}{k}\binom{N-2p}{-k-1}. \end{aligned}$$

From the expressions above we can see immediately that the second column gives no contributions at all and therefore the corresponding coefficients vanish: $c^{L}_{N} = c^{D}_{N} = 0$. The counts in the first column give a non vanishing contribution only for $k = 0$. So we have that:

$$c^{R}_{N} = \sum_{p=1}^{y} \left[\binom{y-1}{p-1} \binom{N-y-1}{p} + \binom{y-1}{p-1} \binom{N-y-1}{p-1} \right],$$
$$c^{U}_{N} = \sum_{p=1}^{y} \left[\binom{y-1}{p-1} \binom{N-y-1}{p-1} + \binom{y-1}{p-1} \binom{N-y-1}{p-2} \right].$$

Now we can easily perform the sum in the two cases.

- Case R. Using the following identity for the binomials:

$$\binom{n}{k} = \binom{n-1}{k} + \binom{n-1}{k-1},$$

we can rewrite the sum as:

$$\begin{aligned} c^{R}_{N} &= \sum_{p=1}^{y} \binom{y-1}{p-1} \binom{N-y}{p} \\ &= \sum_{p=1}^{y} \binom{y}{p} \binom{N-y}{p} - \sum_{p=1}^{y} \binom{y-1}{p} \binom{N-y}{p}. \end{aligned}$$

Now, upon adding the contribution from $p = 0$ on both sums and considering that the contribution from $p = y$ in the second sum is 0, we can write:

$$c^{R}_{N} = \sum_{p=0}^{y} \binom{y}{p} \binom{N-y}{p} - \sum_{p=0}^{y-1} \binom{y-1}{p} \binom{(N-1)-(y-1)}{p}.$$

Then we can apply the identity [eq. 11 59, p. 616]:

$$\sum_{k=0}^{n} \binom{n}{k} \binom{m-n}{k} = \binom{m}{n}. \tag{43}$$

So we have:

$$\begin{aligned} c^{R}_{N} &= \binom{N}{y} - \binom{N-1}{y-1} \\ &= \binom{N-1}{y}. \end{aligned}$$

- Case U. We can follow similar steps. We begin now rewriting the sum using the identity (43):

$$\begin{aligned} c_N^U &= \sum_{p=1}^{y} \binom{y-1}{p-1}\binom{N-y}{p-1} \\ &= \sum_{p=0}^{y-1} \binom{y-1}{p}\binom{(N-1)-(y-1)}{p} \\ &= \binom{N-1}{y-1} \\ &= \binom{N-1}{x}. \end{aligned}$$

□

5.2.3 Cycles

Now we want to analyse the cycles of the automaton, that is, paths returning back to the starting point. We can assume that these paths always start at the origin $(0,0)$ and return at this point. First of all, we seek a way to enumerate all of them. We have already given this result in equation (6) on page 17 in general terms. Here we will show another way to obtain the same expression in the case of cycles. Firstly, considering that $x = 0 \implies r = l$ and $y = 0 \implies u = d$, then the number of steps is even: $N = 2r + 2u$, as one can notice also from the fact that $K_1 = K_2$ by theorem 5.4 on page 35.

Theorem 5.7 (Number of cycles)**.** *The number of* $(2K)$*-steps cycles is*

$$\mathcal{N} = \binom{2K}{K}^2. \tag{44}$$

Proof. Suppose a cycle consists of r, l, u, d steps such that $r + l + u + d = 2K$. Then, because the distance is 0, we have that $r = l$ and $u = d$ and therefore $r + u = K$. So we can iterate over $k = 0, \dots, K$, right steps (equivalently, up steps). The total number of paths is given by the number of possible permutations: $(2K)!$. But we have k steps to the right and equally k steps to the left. The same goes for up and down steps. This means that we have to count the number of permutations with repetitions.

$$\begin{aligned} \mathcal{N} &= \sum_{k=0}^{K} \frac{(2K)!}{k!^2(K-k)!^2} \\ &= \sum_{k=0}^{K} \frac{(2K)!}{K!^2}\left(\frac{K!}{k!(K-k)!}\right)^2 \\ &= \binom{2K}{K}\sum_{k=0}^{K}\binom{K}{k}^2, \end{aligned}$$

where the last sum is well known [see eq. 1 in 59, p. 616, or 35, p. 5]:

$$\sum_{k=0}^{K} \binom{K}{k}^2 = \binom{2K}{K}.$$

And so, finally, we obtain the expression we looked for:

$$\mathcal{N} = \binom{2K}{K}^2. \qquad \square$$

In order to obtain the coefficients of the transition matrices in this case, it is effective to introduce a slightly different convention on the way of counting the number of parts. That is, instead of counting the parts on a segment we can imagine to arrange the bits around a ring and count the part on it. This trick allows us to simplify the formulae of the general case. In fact using this convention the number of pairs with different bits is always $2p$, where p is the number of "cyclic" parts. Instead, the number of strings with a given number of parts has still to be counted as if we cut the ring somewhere. This is because the paths are actually not cyclic. Now we are able to give the following result.

Theorem 5.8 (Cycles coefficients)**.** *For cycles of* $N = 4K + Q$ *steps with* $Q \in \{0, 2\}$*, the coefficients of the transition matrices are all equal and read:*

$$c_{4K+Q} = (-1)^{\frac{Q}{2}} 2^{Q-2} \binom{2K}{K}^2. \tag{45}$$

Proof. The number of strings with p "cyclic" parts are given by the same equations of lemma 5.5 on page 37 with the only variation of $n_p(1,1)$. Let $N = 2n$:

$$n_p(1,1) = \binom{n-1}{p}\binom{2n-n-1}{p-1} = \frac{p(n-p)}{n^2}\binom{n}{p}^2,$$

since, in this case, if there are p parts then we have $p+1$ slots, with this convention. Now we have to compute c_p. In this convention there are always $2p$ pairs. Then, since the four coefficients are equal for the cycles (by the symmetries of the Weyl's automaton in 2D, presented in section 2.4.3 on page 11), it is no more necessary to fix the endpoints and the c_ps are all equal:

$$c_p = \sum_{k=0}^{2p} (-1)^k \binom{2p}{k}\binom{2n-2p}{n-k}.$$

This sum results to be [see eq. 20 in 59, p. 617]:

$$\begin{aligned} c_p &= (-1)^p \frac{\binom{n}{p}\binom{2n}{n}}{\binom{2n}{2p}} \\ &= (-1)^p \frac{(2p)!\,(2n-2p)!}{p!\,n!\,(n-p)!}. \end{aligned}$$

Now summing all the contributions from $n_p(a, a')$ we have:

$$\begin{aligned} n_p &:= \left[\frac{2p(n-p)}{n^2} + \frac{2p^2}{n^2}\right]\binom{n}{p}^2 \\ &= \frac{2p}{n}\binom{n}{p}^2. \end{aligned}$$

Finally, keeping in mind that the coefficients are $\frac{1}{4}$ of the total, the sum over p becomes:

$$\begin{aligned} c_{2n}(n,n) &= \frac{1}{4}\sum_{p=1}^{n}(-1)^p \frac{2p}{n}\frac{(n!)^2}{(p!)^2\,((n-p)!)^2}\frac{(2p)!\,(2n-2p)!}{p!\,n!\,(n-p)!} \\ &= \frac{1}{2}\sum_{p=1}^{n}(-1)^p \frac{p}{n}\binom{n}{p}\binom{2p}{p}\binom{2n-2p}{n-p} \\ &= \frac{1}{2}\sum_{p=1}^{n}(-1)^p \binom{n-1}{p-1}\binom{2p}{p}\binom{2n-2p}{n-p}. \end{aligned}$$

In order to obtain an explicit expression for this sum, we have to distinguish the two cases: $n = 2K$ and $n = 2K+1$.

- Case $n = 2K$. In this case using *Mathematica* we obtain:

$$c_{4K}(2K, 2K) = 4^{2K-1}\frac{\Gamma^2\left(\frac{1}{2}+K\right)}{\pi(K!)^2}.$$

  This expression can be simplified using the properties of the Gamma function:

$$\Gamma\left(\frac{1}{2}+n\right) = \frac{(2n)!}{4^n n!}\sqrt{\pi},$$

  then we have the result:

$$\begin{aligned} c_{4K}(2K,2K) &= \frac{4^{2K-1}}{\pi(K!)^2}\frac{((2K)!)^2}{4^{2K}(K!)^2}\pi \\ &= \frac{1}{4}\left(\frac{(2K)!}{K!\,K!}\right)^2 \\ &= \frac{1}{4}\binom{2K}{K}^2. \end{aligned}$$

- Case $n = 2K+1$. Now *Mathematica* gives:

$$c_{4K+2}(2K+1, 2K+1) = -4^{2K}\frac{\Gamma^2\left(\frac{1}{2}+K\right)}{\pi(K!)^2}.$$

Simplifying we have:

$$\begin{aligned} c_{4K+2}(2K+1, 2K+1) &= -\frac{4^{2K}}{\pi(K!)^2}\frac{((2K)!)^2}{4^{2K}(K!)^2}\pi \\ &= -\left(\frac{(2K)!}{K!\,K!}\right)^2 \\ &= -\binom{2K}{K}^2. \end{aligned}$$

□

6 CONCLUSIONS

The aim of this thesis was to study and analyse the properties and features of a model of discrete dynamics, which is called *Quantum Cellular Automaton* (QCA), consisting in a homogeneous lattice of finite-dimensional quantum systems in local interaction. The notion of QCA we have adopted here was presented by Schumacher and Werner [60], extending the classical notion of *Cellular Automata* first introduced by Von Neumann [65]. This dynamical model has been a subject of research in the scope of *Computer Science* and *Quantum Information* where it found a rigorous formalisation and further analysis [3, 7, 9, 37, 45, 60].

The present work have had origin within the recent research program of D'Ariano in the informational foundations of *Quantum Theory* [19]. The recent results opened the way to the program of giving informational premises also to *Quantum Field Theory* adopting as the microscopic mechanism a QCA; this approach was first proposed in the pioneering work of Bialynicki-Birula [11] and subsequently in the works of Strauch [62] and Yepez [73]. In the recent paper of D'Ariano and Perinotti [22] the authors show how a QCA can be derived from four basic postulates of physical nature: *unitarity*, *locality*, *homogeneity*, *isotropy*. Then they prove that this automaton gives the correct large-scale limit, recovering the Weyl and Dirac equations, giving also the analytic solution in the momentum space.

We have studied here the Dirac and Weyl automata in one and two spatial dimensions respectively in their single-particle sectors, which can be regarded as *Quantum Walks*, introduced by Aharonov, Davidovich, and Zagury [2] as an extension of the classical *Random Walks* [51]. We have analysed these automata employing the discrete path-integral approach, expressing the N-steps evolution of the automaton as a sum over all possible paths leading to a specified point of the lattice starting from some initial point.

We have been able to obtain an analytic solution for the problem of the representation of the automata in the position space in these two cases, giving the exact expression for the coefficients of the resulting transition matrices in the path-sum. For the one dimensional case, we can mention some other solved models as those considered by Kauffman and Pierre Noyes [42], Ambainis et al. [7], and Konno [49, 48]. However, the result we have found for the two-dimensional Weyl QCA is somewhat surprising since it is a rare example of an analytically-solved quantum model in two dimensions.

The results we have found during the analysis of these automata are certainly of theoretic interest since we have been able to present an explicit analytic expression of the N-steps evolution. Moreover, these results permit the analysis of some large-scale behaviour of the automata, regarding the way the isotropy of the causal cone is recovered thanks to the interference of the quantum paths. Furthermore,

we can also highlight the possible applications of these results in a computational context. In fact, there could be a significative speedup of the algorithms used to simulate these automata.

6.0.4 Future perspectives

Beside these successful results in one and two dimensions there is still work to do. In the future, this work is directed toward the possibility of finding a solution also for the three-dimensional case, specifically for the Weyl automaton.

Furthermore, we have not considered here the Dirac automaton in dimensions greater than one for which there is still room for investigation. Finally, as we have seen in this presentation, we have studied the single-particle sectors of the considered automata, reducing them to quantum walks; so in the future there will certainly be a in-depth analysis also of the aspects concerning the full interacting automaton scenario.

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