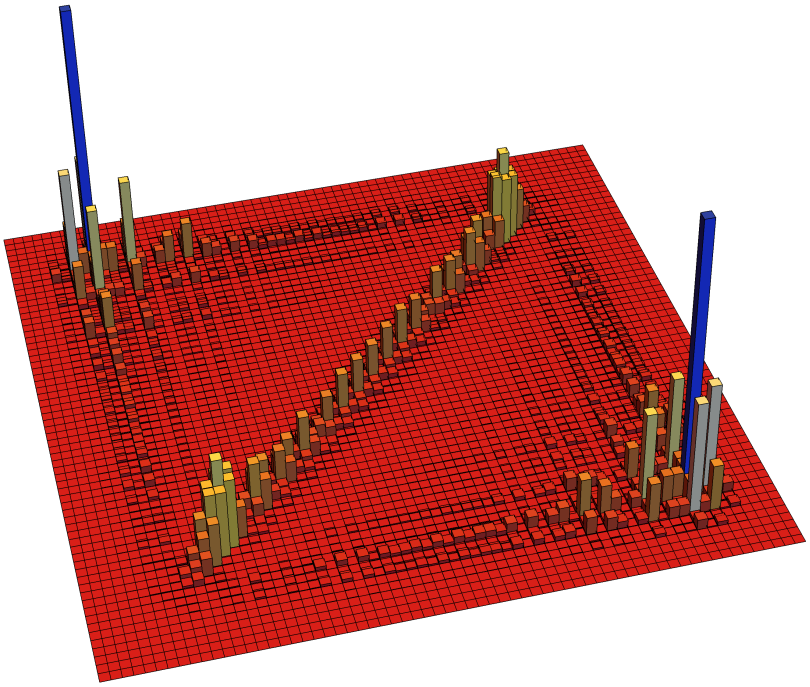
Università degli Studi di Pavia
Dottorato di Ricerca in Fisica – XXX Ciclo

Analytical Solutions of the Dirac Quantum Cellular Automata:

Path-sum Methods for the Solution of Quantum Walk Dynamics in Position Space

Nicola Mosco



Tesi per il Conseguimento del Titolo

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ANALYTICAL SOLUTIONS OF THE DIRAC QUANTUM CELLULAR AUTOMATA

Path-sum Methods for the Solution of Quantum Walk Dynamics in Position Space

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Probability distribution after $t = 32$ time-steps of a singlet state located at the origin, evolved according to the Thirring Quantum Cellular Automaton with mass $m = 0.6$ and coupling constant $\chi = \pi/2$.

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ACRONYMS

CA Cellular Automaton

QCA Quantum Cellular Automaton

RW Random Walk

QW Quantum Walk

BCC Body-Centred Cubic

QT Quantum Theory

QM Quantum Mechanics

IT Information Theory

QI Quantum Information

QIT Quantum Information Theory

QFT Quantum Field Theory

FT Fourier Transform

FFT Fast Fourier Transform

DFT Discrete Fourier Transform

DTFT Discrete-Time Fourier Transform

1 INTRODUCTION

The concept of information is tightly related to that of knowledge in the sense that it quantifies how many questions one should ask in order to understand a concept or otherwise to become "informed" of something. For example, suppose that there are two parties and the first one has to send a message to the other one. This message contains some information that the other party should know. So, in order to convey this message one has to find a suitable representation for it, the simplest one being a binary encoding of the message. More generally, it is certainly possible to employ any alphabet. The aim of Information Theory (IT) is then the study of how such information can be stored and communicated efficiently, preserving the message from possible errors. The seminal work of Shannon [1] led to the development of the broad field of IT encompassing many applications from mathematics, physics and computer science to neurobiology and electrical engineering.

The many applications and the success of IT led to a profound reconsideration of the role that information could play in physics. Many aspects of the physical world can be formulated in terms of information. For instance, if we consider information as a quantification of the different configurations in which a system can be, we can interpret the entropy of the system as a quantification of our ignorance of the microscopic description of the system itself. So, in the words of Lewis [2], we can say that "a gain in entropy always means loss of information, and nothing more". The notion of information comes into play also in other fields than physics: for example in biology, where a living system can be characterized by its ability of gathering and processing information. Such a broad appearance of the concept of information in various fields of human knowledge led to the development of the informational paradigm in physics.

For this reason, the informational paradigm is based on the idea that information plays, at a fundamental level, a crucial role in the description of natural phenomena. The hypothesis that the universe is in fact a huge computer has been originally proposed by Zuse [3], suggesting the idea that physics could actually be the result of the computation performed by a Cellular Automaton (CA). Along this view comes the motto of Wheeler *it from bit* [4], encompassing the idea that "every *it*—every particle, every field of force, even the space-time continuum itself—derives its function, its meaning, its very existence entirely—even if in some contexts indirectly—from the apparatus-elicited answers to yes-or-no questions, binary choices, bits". According to Wheeler's view information lies at the core of the phys-

ical phenomena which become just an emergent expression of "the registering of equipment-evoked responses".

What kind of information? is the question that arises following the line of thoughts of Wheeler. Being Quantum Field Theory (QFT) our best—to our knowledge—theoretical description of the elementary physical processes, it is natural to consider Quantum Information (QI) as the fundamental context in which we should develop the informational paradigm. Therefore, as Feynman pointed out [5], not a *classical* CA, rather a Quantum Cellular Automaton (QCA) should be considered as the theoretical tool underlying the informational approach to physics. According to this approach, hence, physics is the result of the processing of information, while Quantum Theory (QT) is the theoretical framework asserting which information-theoretic tasks can or can not be performed.

Analogously to classical IT, Quantum Information Theory (QIT) studies the properties of information in the quantum world. The research in the field of QIT has been successful in providing deep insights on the basic concepts and features of QT. The results in the framework of QIT led to important applications from quantum computation to quantum cryptography drawing a path that eventually could lead to the exploitation of the bizarre features of the quantum world in every-day life. In the past years, thus, QIT has played a major role in the comprehension of the basic notions and features of the quantum world, such as *entanglement* and *non-locality*. Therefore it has been considered also as a guide in the investigation of the foundations of Quantum Mechanics (QM), believing that information could play a significant role in the study of a physical theory. Under this view, thus, we start our investigation from basic notions of informational nature characterizing the physical theory.

The foundational investigation of physics should start from fundamental postulates regarding the mathematical structure of the theory. In the literature there are various attempt to give QT an operational axiomatization. In the field of Quantum Logic, initiated by von Neumann and Birkhoff [6], we can mention the axiom system of Mackey [7] and the attempts of Piron [8] and Ludwig [9]. These axiomatization programs, however, were not fully successful in deriving all the features of QT from purely operational axioms. In the following years, the prominent results of QIT suggested that QT, at its core, could be regarded as a theory of information, providing a fertile ground to study the foundational problems of QT in this scenario [10, 11]. In this perspective the work of D'Ariano, Perinotti, and Chiribella provided a complete axiomatization of finite dimensional QT based on principles of informational nature [12].

QT is a theory of systems and does not provide any mechanical notion. From this point of view, QFT is also a theory of systems, but provides also the mechanical part such as the quantization rules and the equations governing the evolution of the physical systems. So we need to find an

extension of the theory that includes dynamics from an informational perspective. To this end, on the one hand the quantum algorithm that describes the physical evolution—the universal *physical law* that we aim to describe—should be of finite computational complexity and, hence, the quantum systems in this theory should have minimal Hilbert-space dimension. Furthermore, there should be finitely many systems that interact with a given one. On the other hand, the universality of the *physical law* entails that the quantum algorithm should perform in the same way for each system. This means that the interaction network should be topologically *homogeneous*. Therefore, the investigation starts from a collection of finite dimensional quantum systems in mutual interaction. We then pose the basic principles that this interaction network should satisfy: *unitarity*, *linearity*, *locality*, *homogeneity*, and *isotropy*. Unitarity endows the conservation of the probabilities. The linearity requirement means that the one-step update of the cell state is given by a linear combination of the states of the neighbouring cells. The locality assumption entails that the cell evolution is affected only by a finite number of neighbours. Homogeneity means that each cell is treated in the same way and that there should not exist any discrimination procedure that allows one to distinguish one cell from another. Finally, the *isotropy* assumption encompasses the idea that every direction is equivalent. The structure emerging from such assumptions is actually a QCA defined on the Cayley graph of a group, describing precisely the unitary evolution of a denumerable collection of finite dimensional quantum systems interacting with a finite number of neighbours.

The automaton theory, hence, draws a different path with respect to other discrete descriptions of relativistic fields where usually one is interested in a discrete approximation of continuous dynamics that can be implemented numerically. In a Lattice Gauge Theory context [13], for instance, one has a relativistic action of a gauge theory from which a finite difference version of it is derived that can then be used to study numerically the non-perturbative regime of the theory, as in *e.g.* Quantum Chromodynamics. In this respect, the discrete theory focuses not on foundational questions, but rather on the development of effective tools that can be used to make predictions for the continuum theory. On the contrary, from the foundational perspective, we are interested in assuming the discrete theory as fundamental and in recovering the continuum theory as an effective theory.

A linear QCA can be regarded as the second quantization of a Quantum Walk (QW) [14], which is another model of discrete evolution describing the motion of a particle hopping through the sites of a lattice. A QW is the quantum version of a classical Random Walk (RW). In the seminal work of Ref. [15] Aharonov presented the first notion of a QW where the motion of a spin-1/2 particle is determined by the measurement of the z-component of its spin. Subsequently, the concept of a QW was general-

ized to encompass arbitrary unitary operators acting on the so-called *coin space*, representing the internal degree of freedom, leading to the notion of a *coined* QW [16, 17]. The generalization to arbitrary graphs was formalized in the works of Refs. [16–18].

In recent years, the increasing interest in the QW theory is twofold. On the one hand, it gained attention in computer science for the computational speedup that it provides with respect to the classical counterpart in solving certain classes of problems. We can mention amongst the successful applications oracular problems, element distinctness problem, the triangle finding problem, and also Grover's search algorithm [19–25]. On the other hand, the idea that relativistic dynamics can emerge from a discrete fundamental mechanism has been thoroughly investigated in the literature [26–42]. The relation between the walk dynamics and the relativistic one given by the Dirac equation has been studied also in presence of external fields, providing a tool to simulate discrete gauge theories [43, 44]. Furthermore, introducing a dependence on time and space, one can show that in the continuum limit the evolution of a discrete-time QW describes the propagation of the massless Dirac field in presence of an arbitrary gravitational field [45].

Aside from the theoretical interest, physical realizations of QWs have been considered as quantum simulators of physical systems with the aim to harness the computational speedup provided by quantum algorithms [46, 47]. Experimental implementations of discrete-time QWs have been realized for the one-dimensional case in a number of physical systems: *e.g.* neutral atoms in spin-dependent optical lattices [48–51], ions in a linear ion trap [52], photons in waveguide lattices [53, 54], and optical fibre network loops [55, 56]. The major obstacle to the implementation of multidimensional QWs is due to the decoherence effects, requiring huge technological efforts. Nevertheless, there are recent realizations of multidimensional QWs with an optical fibre network [57]. Furthermore, the effects of homogeneous electric fields have been also studied both from a theoretical point of view [58] and in an experimental realization employing optical lattices [59], showing how the evolution of the walk strongly depends on whether the electric field is rational or irrational.

Assuming the Planck scale as the hypothetical scale at which the QCA operates, the usual particle physics should be recovered, in some way, as a continuum-limit approximation of the discrete evolution [40, 42, 60, 61]. The discreteness of the interaction graph has also the consequence of breaking the continuum symmetries, in particular the Lorentz covariance. Spacetime itself is an emergent concept in this scenario. We need, thus, to introduce a corresponding notion of reference frame, without resorting to physical space or time. An effective way to do so is by resorting to the mathematical notion of representation of the dynamics applied on the one-step update rule of the automaton. We can reformulate the relativity principle by saying

that the *inertial representation* is the representation that preserves the mathematical form of the one-step update rule [62, 63]. In this way we obtain new transformations—which are deformed Lorentz transformations—that recover the usual Lorentz ones on a scale much larger than a fundamental reference scale, say the Planck scale [64, 65].

The informational paradigm, thus, provides an alternative, consistent framework where we can address the open problems that we face in contemporary physics, especially the physics beyond the Standard Model of particle physics. Although QFT has been proven to be one of the most successful physical theories in the description of natural phenomena, there is still a tension between *General Relativity* and QFT. In this regard, QFT should be an effective theory of a more fundamental one, encompassing also a quantum theory of gravity.

The present thesis focuses in the first part on the solution of the Dirac QW in one spatial dimension and of the Weyl QWs in two and three spatial dimensions via a discrete path-integral approach (a path-sum). The first example of application of this approach to discrete physics models is the Feynman *checkerboard problem* [66]. The idea behind the Feynman checkerboard is to describe the evolution of a Dirac particle in $1+1$ dimensions on a lattice, providing an effective way to solve a finite-difference equation. The probability amplitude to go from one lattice point to another—as for the path-integral formulation of QM—can be expressed as a sum over all the paths joining the two points. The problem is thus translated into a combinatorial problem for the lattice paths. Early attempts to this problem [67, 68] were improved by the work of Kauffman and Noyes [69]. The same Jacobson and Foster provided also a generalization to $3+1$ dimensions [70]. Although such approaches provide an effective way to solve the finite-difference Dirac equation, there is not an equivalent description, in our context, in terms of a QW. This is due, in general, to the failure of unitarity in the evolution provided by finite-difference equations. This fact motivates to consider the path-sum approach in the context of QWs.

In general, a QW is described by some transition matrices representing the transition amplitudes between two neighbouring sites of the lattice. The matrices of the Weyl and Dirac QWs manifest peculiar algebraic properties that can be exploited to aid the calculation of the propagator: specifically, they generate a finite semigroup (up to phases and rescaling). Another key ingredient that considerably simplifies the derivation of the solution is the binary encoding of lattice paths. In this way one can translate the topological properties of the paths into algebraic properties of binary strings. Once we obtained a classification of all the binary strings that correspond to the set of paths contributing with the same transition matrix, the computation of the propagator amounts to solve a simplified combinatorial problem involving these binary strings.

In the second part of the thesis we present a non-linear QCA representing the local interaction of particles. The particles on lattice feel the interaction only when they are in the same lattice site. We give a briefly review of the analytical solution for the problem restricted to the two-particle sector. Furthermore, we present the results of the numerical evaluation of the walk in the case of perfectly localized states, that can give us an insight on the diffusion properties showing the appearance of bound states. We also provide the graphical representation of a peculiar kind of bound states that are spatially localized on few sites. Then we present the basics of the perturbative approach to this interacting theory, computing the tree-level Feynman diagrams. We also provide a numerical evaluation of the free Dirac QW for the classes of perfectly localized states and of gaussian states, featuring the *Zitterbewegung* effect.

1.1 OUTLINE OF THE THESIS

In Chapter 2 we are going to present the framework and the background of the QCA theory [14, 27, 28, 71]. The general setting is that of QCAs on Cayley graphs, the graph links representing the interactions between a denumerable collection of finite dimensional quantum systems. We show how, from some basic assumptions characterizing the propagation of information through the causal network of quantum systems, the emergent structure of the net is that of a Cayley graph. In the same chapter we introduce the concept of a QW, which can be regarded as a special kind of QCA [14], providing the evolution of a single particle on a graph. Restricting to the case of Cayley graphs of Abelian groups that are embeddable in the Euclidean space, we present the unique QCAs satisfying the assumptions of *unitarity*, *linearity*, *homogeneity*, *locality*, and *isotropy*, derived in Ref. [40]. The QCAs derived under these assumptions can be shown to reproduce the usual evolution provided by the Dirac equation in the relativistic limit of small wave-vectors and of small masses. We can say that if we take the Planck scale as reference scale for the automaton, then at the scale of particle physics the description in terms of QCA is indistinguishable from the usual one given by the Dirac equation: the two theories coincide where the discreteness can not be probed.

In Chapter 3 we provide an insight into the properties of the Dirac QW in dimension $d = 1$ and $d = 3$ by the numerical evaluation of the walk for two classes of states. On the one hand we discuss the evolution of smooth wave packets, say Gaussian states, for which the evolution resembles the one given by the Dirac equation. On the other hand, in the QW scenario, one can have highly localized states whose evolution will be very different from the usual relativistic one, since the effects of the discreteness are prominent.

In Chapter 4 we review the solution in position space in terms of sum over paths derived in Ref. [72] for the Dirac QW in dimension $d = 1$. A QW can be described either in terms of a unitary operator acting on the Hilbert space associated to the graph or in terms of a set of so-called *transition matrices* constituting the one-step update of the walk. Remarkably, the transition matrices of the Dirac walk generate a (finite) semigroup structure allowing for the exploitation of the path-sum method. Moreover, the overall matrix associated to a path depends only on the first and last step of the path.

In Chapter 5 we review the analytical derivation of the propagator for the Weyl QW in dimension $d = 2$ based in the exploitation of the semigroup properties of the transition matrices and the binary encoding of lattice paths. The solution is based on the derivation provided in Ref. [73]. In this case the binary encoding of paths provides a considerable aid in the solution of the combinatorial problem that one has to solve in order to count the number of paths contributing with the same resulting matrix.

In Chapter 6 we provide the analytic solution of the Weyl QW in dimension $d = 3$ derived in Ref. [74] as an extension of the solution given in Chapter 5. This extension is possible since the transition matrices have a similar composition rule.

In Chapter 7 we present the Thirring QCA for which the linearity assumption is dropped allowing for an interaction between particles to be present. We review the analytical solution of Ref. [75] for two particles. The restriction to a fixed number of particles allows one to describe the automaton in terms of a QW. This is possible since the interaction employed preserves the number of particles. We also show the results of the numerical evaluation of the walk for perfectly localized states. In the same chapter we give a sketch of the perturbation theory of this walk by computing the vertex diagrams at first order in the perturbation expansion.

In Chapter 8 we draw our conclusions giving some future perspectives on the possible continuation of the study of the QCA framework as a fundamental mechanism underlying QFT.

2 QUANTUM CELLULAR AUTOMATA

A CA is a discrete model characterized by simple rules governing its evolution, and yet it shows a complex emergent dynamics. This feature makes CAs very promising since they can be adopted to describe physical systems, as Wheeler suggested with its motto "it form bit" [4, 76]. Originally, CAs were introduced by Ulam and von Neumann when they were colleagues at the *Los Alamos National Laboratory* in the 1940*s*. A CA consists in a collection of cells—for example arranged in a two-dimensional grid—which can assume a finite number of states. The evolution of the whole grid is then specified by providing a local update rule, which involves, for any given cell, only a finite number of neighbouring cells. There are many ways to specify a *neighbourhood scheme*. For instance, in Fig. 1 are represented two well-known schemes: the Moore neighbourhood and the von Neumann neighbourhood. In principle, one can provide a different update rule for each cell and for each time-step. However, we are interested in a description that is the same everywhere: in other words, all the sites should be treated in the same way and it should not be possible to distinguish one cell from another thanks to the dynamical evolution. Therefore, the basic requirement is that the local update rule should be the same for each site. A thorough formalization and classification of classical CAs ha been provided by Wolfram in Ref. [77].

2.1 JOHN CONWAY'S GAME OF LIFE

One of the most known instances of CA is Conway's *Game of Life*. It is characterized by an infinite two-dimensional grid of cells each of which can assume only the two values black and white (a black cell is said to be *dead* and a white cell is said to be *alive*). The neighbourhood of this CA is usually the Moore neighbourhood and the update rule goes as follows:

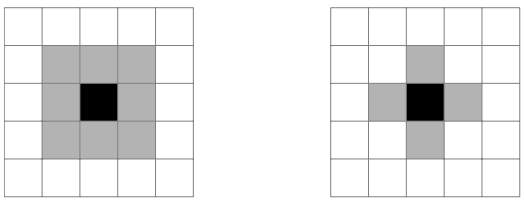


Figure 1.: On the left is represented the Moore neighbourhood and on the right the von Neumann neighbourhood.

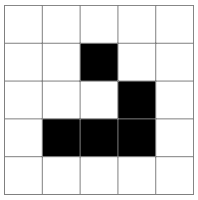


Figure 2.: Glider: the simplest moving object of Game of Life.

1. a dead cell becomes alive if it has exactly three live neighbours;
2. any live cell with fewer than two or more than three live neighbours dies;
3. the state remains unchanged in the other cases.

It is remarkable that from such simple rules arise complex patterns showing non-trivial global behaviours: *e.g.* steady configurations, periodic patterns or even systems of live cells moving coherently on the lattice. Amongts the simplest moving objects there is the so called *glider*, depicted in Fig. 2. From the elementary building blocks one can construct also other "ships" and generators ("guns") producing such objects: *e.g.* in Fig. 3 it is shown Gosper's glider gun which continuously emits new gliders in a period of 30 steps.

The Game of Life is an example of a *classical* CA for which the states are classical states. In 1982, Feynman suggested the idea that physics, being inherently quantum, should be simulated by a quantum computer [5], the appropriate model of computation being a quantum version of a CA. After the seminal paper of Feynman, the concept of a QCA has been developed and studied in the literature of Computer Science and QI, receiving increasing attention during the years [71, 78]. The general framework we adopt in the present work has been provided by Werner and Schumacher with the definition of a reversible QCA [14].

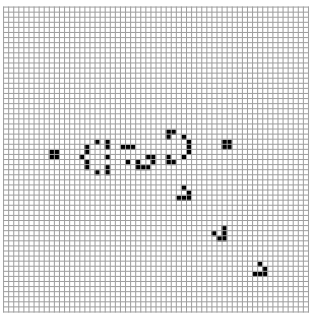


Figure 3.: Gosper's glider gun.

2.2 QUANTUM CELLULAR AUTOMATA BACKGROUND

The interest in the community of QI on QCAs is motivated by the connection between QI and foundations of QM, as the study of quantum protocols, such as teleportation and tomography, provided a fertile ground to deepen the understanding of *entanglement* and *nonlocality*. The fundamental idea is that QT can be regarded as a theory of information, stating the properties of the basic tasks of information-processing. The reformulation of QT as a theory of information inspired numerous works regarding the operational axiomatization [8–11, 79–83]. A complete derivation of finite dimensional QT was achieved by Chiribella, D'Ariano and Perinotti [12] starting from six principles of informational nature. However, in this scenario, QT is a theory of systems without any reference to mechanical notions, such as particles and quantization rules. The mechanical part is provided by QFT, which is nowadays the best description of the elementary processes in particle physics. The aim of the informational approach is, therefore, to provide a theoretical framework based on informational principles from which we can derive also the dynamical features encompassed by QFT.

The idea that at a fundamental level there should be an upper bound on the amount of information that can be stored in a finite region of space [84–86] requires our fundamental description to involve a countable set of finite dimensional quantum systems. The theoretical framework in which we should develop such a description of natural phenomena is thus that of QCAs [5], since they represents precisely the unitary evolution of countably-many quantum systems in local interaction.

The QCA framework encompasses also another model of discrete evolution of a particle hopping through the sites of a lattice. Classically this model is known as a RW: at each time-step, a particle moves from one lattice site to the neighbouring lattice sites according to some probability. RWs have been studied extensively in several fields from mathematics and physics to economics [87–89]. A first attempt to obtain a *quantization* of a classical RW—which would be called then QW—was provided by Aharonov [15]. In this seminal work, the motion of a spin-1/2 particle on the line is determined by measuring the z-component of its spin, whose outcome decides whether the particle moves to the right or to the left. The concept of a QW was generalized replacing the measurement with a unitary operator acting on the internal degree of freedom, know as *coin* space, leading to the notion of *coined* QW [16, 17]. In the computer science literature the study of coined QWs was motivated by the computational speedup over classical RWs in solving a number of problems: *e.g.* oracular problems and search algorithms, such as Grover's search algorithm, as well as the element distinctness problem and the triangle finding problem [19–25]. The rigorous formalization of the concept of a QW was provided in Refs. [16–18] both for a QW on the line and for QWs on general graphs.

Analogously to the classical case, a QCA describes the dynamics of many particles systems in interaction, whereas a QW can be seen as the restriction to the one-particle sector of a given QCA. Conversely, a QCA can be considered the *second-quantization* of a QW [14]. Assuming the QW description, we explore the possible emergent dynamics, namely we study the *free* evolution of a particle on a lattice. Such a program has been successful in proving that QCAs (and QWs) can actually be employed as discrete quantum simulators of free relativistic particle physics [26–33, 35–42]. As one can expect the discreteness of the interaction network necessarily breaks the continuum symmetries: in particular, the Lorentz symmetry is distorted at the Planck scale. If we insist on the QCA microscopic description, the usual relativistic dynamics can be recovered in the limit of small wave vectors (small with respect to the Planck scale), where the effects of discreteness can not be probed [40, 42, 61]. Since the QCA description does not have any reference to space-time, we need to formulate the concept of *inertial frame* in this context. We identify the notion of a *reference frame* with that of *representation* of the dynamics: the relativity principle is then expressed by defining the *inertial representation* as the representation for which the physical law is invariant, *i.e.* it has the same mathematical form. As a consequence we end up with modified Lorentz transformations and the usual ones are recovered on a scale much larger than the underlying microscopic scale [64, 65].

2.3 QUANTUM CELLULAR AUTOMATA ON CAYLEY GRAPHS

The path we draw in the present work follows from the necessity of giving to QFT a foundational basis that resorts to principles of informational nature [62, 63]. As we already mentioned, the general setting is that of a denumerable set G of quantum systems in mutual interaction. Let us see now how the QCA structure emerges from basic assumptions on the interaction network. Since we are interested in a possible description of QFT emerging from this framework, we assume each cell of G to be associated to a quantum field. The discreteness assumption follows from the idea—as already expressed by Feynman [5]—that the amount of information that can be stored in finite volume of space can not be infinite: as such, the quantum fields should obey the Fermi statistics. Such a requirement is not restrictive since systems obeying the Bose–Einstein statistics can be retrieved from many Fermionic modes [61]. From a computational perspective it has been proven that a theory based on Fermionic systems is computationally equivalent to one based on qubits [90–92].

The investigation of the QCA framework proceeds by adding a specific structure on the interaction network, in order to obtain the one-step update rule of the automaton. This structure is based on the following assumptions: *unitarity*, *linearity*, *homogeneity*, *locality* and *isotropy*. Let us see what are the consequences of these principles on the interaction network. So starting from unitarity—a reasonable requirement since we want probabilities to be conserved during evolution—the one-step update rule is provided by a unitary map applied in discrete identical steps to a countable set G of quantum systems. Each quantum system, labeled by $g \in G$, is described by a C*-algebra generated by $s_g < \infty$ Fermionic modes $\psi_{g,l}$, with $l = 1, \dots, s_g$, obeying the canonical anti-commutation relations:

$$\{\psi_{g,l}, \psi_{g',l'}\} = 0, \qquad \{\psi_{g,l}, \psi^\dagger_{g',l'}\} = \delta_{g,g'}\delta_{l,l'}.$$

Unitarity of the evolution implies that the field $\psi_g(t)$ is updated via a unitary operator U as

$$\psi_g(t+1) = U\psi_g(t)U^\dagger.$$

The linearity assumption entails that the previous equation can be expressed in terms of linear combinations of field operators:

$$\psi_g(t+1) = \sum_{g' \in G} A_{g,g'}\psi_{g'}(t), \tag{1}$$

where $A_{g,g'}$ is an $s_g \times s_{g'}$ complex matrix called *transition matrix*. In this way, the QCA is described by a unitary evolution on the Hilbert space $\mathscr{H} = \bigoplus_{g \in G} \mathscr{H}_g$, with $\mathscr{H}_g = \mathrm{Span}\{\psi_{g,l}\}_{l=1}^{s_g}$. In this case the QCA is called QW and the system corresponds to the single-particle sector of the corresponding Fock space. The description in terms of QWs is also possible for any fixed number of particles by enlarging, essentially, the coin space and by considering a lattice in higher dimensions.

From Eq. (1), it is apparent that the set of transition matrices endows the set G with a directed graph structure $\Gamma(G, E)$, with vertex set G and edge set is $E = \{(g, g') \in G \times G \mid A_{g,g'} \neq 0\}$. We will denote by $\mathcal{N}_g := \{g' \in G \mid A_{g,g'} \neq 0\}$ the *neighbourhood* of g. The locality assumption amounts to the requirement that $\mathcal{N}_g$ is finite for every $g \in G$ and uniformly bounded: *i.e.* there exists $M > 0$ such that $|\mathcal{N}_g| < M$ for all $g \in G$. The homogeneity requirement amounts to consider the cells to be indistinguishable from each other. So, on the one hand, each system should interact with the same number of neighbours, so that $s_g = s_{g'} = s$ for every $g, g' \in G$. On the other hand, the set of transition matrices should be the same for each and every cell: in practice, this means that there should exist a reference set $\mathcal{S} \subseteq G$ and a set of $s \times s$ complex matrices $\{A_h\}_{h \in \mathcal{S}}$ such that, for each $g, g' \in G$, $A_{g,g'} = A_h$ for some $h \in \mathcal{S}$. As such, each edge (g, g') is labeled with an element $h \in \mathcal{S}$, and so the graph $\Gamma(G, E)$ becomes a coloured directed graph. Select now an element $g \in G$. Starting from it, each neighbour $g' \in \mathcal{N}_g$ can

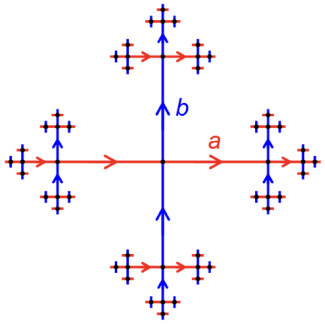
be identified with a colour $h \in \mathcal{S}$. Selecting subsequent neighbours, we can trace a path on the graph, determined by the sequence of colours of each step. One can also view the set $\mathcal{S}$ as an alphabet and, thus, each path corresponds to a *word* (or *string*) over this alphabet [93]. The set $\mathcal{S}^\star$ of all the words over the alphabet $\mathcal{S}$ carries a natural composition operation: two words $w = h_1 \dots h_n$ and $w' = h'_1 \dots h'_{n'}$ can be concatenated to form a new word $ww' \coloneqq h_1 \dots h_n h'_1 \dots h'_{n'}$. This operation makes $\mathcal{S}^\star$ a monoid with identity the empty string (denoted here as ε).

Consider now a path $r = h_1 \cdots h_n$ such that the starting and final points coincide, namely a *closed path*: we denote the set of all closed paths as R. The homogeneity principle further requires that, if a path r is closed starting from the vertex g, it is closed also starting from every other vertex of the graph. If $gh = g' \in G$ then we assume that there exist an element denoted h^{-1} so that we can formally write $g'h^{-1} = g$ and the colour set can be split as $\mathcal{S} = \mathcal{S}_+ \cup \mathcal{S}_-$ with $\mathcal{S}_- \coloneqq \mathcal{S}_+^{-1}$. Therefore, the set $\mathcal{S}^\star$ results to be enriched with a group structure, called the *free group* F with generators $\mathcal{S}_+$. The set of closed paths R generates a normal subgroup N_R of F and hence the quotient F/N_R is also a group, with elements corresponding to those of G. The homogeneity constraint thus implies that the set G is a group that can be finitely presented as $G = \langle \mathcal{S}_+ | R \rangle$ and the graph $\Gamma(G, E) \equiv \Gamma(G, \mathcal{S}_+)$ is called the *Cayley graph* of the group G corresponding to that presentation [40, 63]. In the language of geometric group theory, the elements of $\mathcal{S}_+$ are called *generators* and the elements of R are called *relators*. For convenience of the reader we recall the definition of Cayley graph.

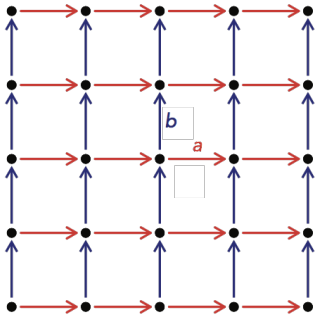
Definition 2.3.1 (Cayley Graph)**.** Let G be a group and let $\langle \mathcal{S}_+ | R \rangle$ be a presentation of G. Then the *Cayley graph of* G corresponding to the presentation $\langle \mathcal{S}_+ | R \rangle$, denoted $\Gamma(G, \mathcal{S}_+)$, is the coloured directed graph $(G, E, \mathcal{S})$, such that the vertex set is G, the edge set is $E = \{(g, gh) \mid g \in G, h \in \mathcal{S}\}$ and each $h \in \mathcal{S}$ has a colour assigned to it. If a generator $h \in \mathcal{S}_+$ is of order 2, namely $h^{-1} = h$, then the corresponding arc on the graph is conventionally drawn without the arrowhead.

In Fig. 4 we report some examples of Cayley graphs. The first image in Fig. 4a, shows the Cayley graph of the free group (*i.e.* it does not have any relator) with two generators $\langle a, b \rangle$; the second graph in Fig. 4b represents the group $\mathbb{Z}^2$, *i.e.* the free Abelian group with two generators presented as $\langle a, b \mid a^{-1}b^{-1}ab \rangle$; the one in Fig. 4c is the Cayley graph of the Fuchsian group $\langle a, b \mid a^4, b^4, (ab)^3 \rangle$; and, finally, in Fig. 4d is represented the graph of the dihedral group $D_4 = \langle a, b \mid a^2, b^4, (ab)^2 \rangle$.

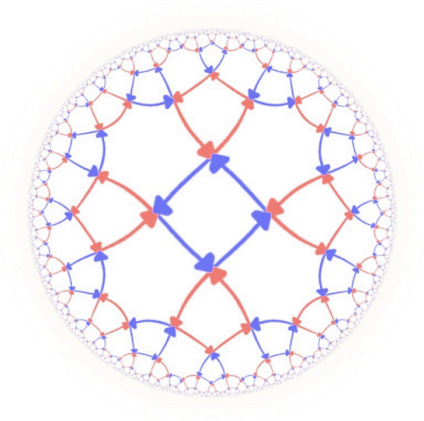
We have seen so far how the assumptions that we made impose a special structure on the interaction network that turns out to be associated to a group structure. The automaton is actually represented by a unitary oper-



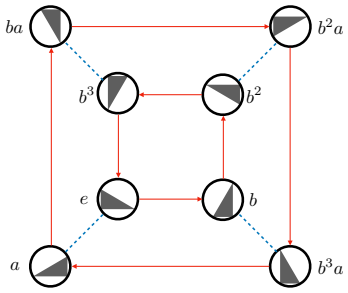
(a) $\langle a, b\rangle$



(b) $\langle a, b \mid a^{-1}b^{-1}ab\rangle$



(c) $\langle a, b \mid a^4, b^4, (ab)^3\rangle$



(d) $\langle a, b \mid a^2, b^4, (ab)^2\rangle$

Figure 4.: Cayley graphs of some groups: in Fig. 4a is depicted the Cayley graph of the free group on two generators presented as $\langle a, b\rangle$; in Fig. 4b is depicted the Cayley graph of the free Abelian group on two generators (*i.e.* $\mathbb{Z}^2$) presented as $\langle a, b \mid a^{-1}b^{-1}ab\rangle$; in Fig. 4c is depicted the Cayley graph of the Fuchsian group $\langle a, b \mid a^4, b^4, (ab)^3\rangle$; finally, in Fig. 4d is depicted the Cayley graph of the dihedral group D_4 whose presentation is $\langle a, b \mid a^2, b^4, (ab)^2\rangle$, where e denotes the identity element of the group, a is represented by a dashed blue line, and b is represented by a red arrow.

ator W acting on the Hilbert space $\mathscr{H} = \bigoplus_{g\in G} \mathscr{H}_g \cong \ell^2(G) \otimes \mathbb{C}^s$ and, in terms of the transition matrices, it can be written as:

$$\begin{aligned} W &= \sum_{g,g'\in G} |g\rangle\langle g'| \otimes A_{g,g'} \\ &= \sum_{h\in S}\sum_{g\in G} |gh^{-1}\rangle\langle g| \otimes A_h \\ &= \sum_{h\in S} T_h \otimes A_h, \end{aligned}$$

where T is the *right-regular* representation of G on $\mathscr{H}$ acting as $T_g|g'\rangle = |g'g^{-1}\rangle$, that is T_g represents a translation on the graph $\Gamma(G, S_+)$.

We still have to implement the isotropy requirement. The notion of *isotropy* encompasses the idea that *all directions are equivalent to one another*. This notion is applied to a QCA or QW by saying that there should exist a group L of automorphisms of $\Gamma(G, \mathcal{S}_+)$ such that the evolution operator W is L-covariant [94]. Roughly speaking, this means that a permutation of the vertices of the graph that leaves the link structure unaffected acts unitarily on the set of transition matrices by a permutation of the colour set $\mathcal{S}_+$:

$$A_{\lambda(h)} = U_l A_h U_l^\dagger, \quad \forall l \in L, \ \forall h \in \mathcal{S}_+,$$

where λ is a permutation of $\mathcal{S}_+$ and U_l is a unitary matrix on $\mathbb{C}^s$.

2.3.1 Quantum Walks on free Abelian groups

The main focus of the present dissertation is on QWs defined on Cayley graphs $\Gamma(G, S_+)$ of the Abelian group $\mathbb{Z}^d$, for $d = 1, 2, 3$. The more general scenario of non-Abelian groups, in particular virtually-Abelian groups, is also investigated in the literature [62, 63, 94–96]. The study of QWs on non-Abelian groups is motivated by the fact that coin-less QWs (so-called *scalar* QWs) are trivial for Cayley graphs of infinite Abelian groups, whereas in the non-Abelian case it is possible to construct non-trivial *scalar* QWs [28, 95, 97]. Nevertheless, for finite Abelian groups one can show that scalar QWs actually exist [97].

In the Abelian case, since we study the group $\mathbb{Z}^d$, we will employ the vector notation $\mathbf{x} \in \mathbb{Z}^d$ to denote its elements; furthermore, we also adopt the additive notation for the group composition operation. The *right-regular* representation of $\mathbb{Z}^d$ on $\ell^2(\mathbb{Z}^d)$ is thus expressed as

$$T_h |\mathbf{x}\rangle = |\mathbf{x} - \mathbf{h}\rangle$$

and, being the group Abelian, it is diagonal in the Fourier representation:

$$T_h |\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{h}} |\mathbf{k}\rangle, \qquad |\mathbf{k}\rangle \coloneqq \frac{1}{\sqrt{|B|}} \sum_{\mathbf{x}\in\mathbb{Z}^d} e^{i\mathbf{k}\cdot\mathbf{x}} |\mathbf{x}\rangle, \quad \mathbf{k} \in B,$$

where B denotes the *first Brillouin zone* of the lattice. In this way, the walk unitary operator W can be block-diagonalized in the Fourier basis:

$$W = \int_B d\mathbf{k} \ |\mathbf{k}\rangle\langle\mathbf{k}| \otimes W_\mathbf{k}, \qquad W_\mathbf{k} \coloneqq \sum_{h\in\mathcal{S}} e^{i\mathbf{k}\cdot\mathbf{h}} A_h, \tag{2}$$

where $W_\mathbf{k}$ is a unitary matrix for every $\mathbf{k} \in B$. The matrix $W_\mathbf{k}$ can be diagonalized as

$$W_\mathbf{k} |u_i(\mathbf{k})\rangle = e^{-i\omega_i(\mathbf{k})} |u_i(\mathbf{k})\rangle, \tag{3}$$

where $|u_i(\mathbf{k})\rangle$ are the eigenvectors and $\{e^{-i\omega_i(\mathbf{k})}\}$ denotes the spectrum of the walk. In particular, the functions $\omega_i(\mathbf{k})$ are called *dispersion relations* and provide a fundamental tool to study the walk dynamics.

2.3.2 Coined Quantum Walks

A *coined* QW is a particular case of the QW model considered in this manuscript [16]. Such a walk is described by an operator $W = TC$ on $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z})$[1], consisting in a coin-flip operator C and a translation operator T. As an example, let us consider the well-known Hadamard walk described by the operator $W_H = TC$, where

$$T = \begin{pmatrix} S & 0 \\ 0 & S^\dagger \end{pmatrix},$$

S being the right shift $S|x\rangle \coloneqq |x+1\rangle$, and

$$C = H \otimes I, \qquad H \coloneqq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

In terms of the transition matrices the Hadamard walk can be written as

$$W_H = A_R \otimes S + A_L \otimes S^\dagger,$$

with

$$A_R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \qquad A_L = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ 1 & -1 \end{pmatrix}.$$

The momentum representation of the Hadamard walk is thus

$$W_{H,k} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{ik} & e^{ik} \\ e^{-ik} & -e^{-ik} \end{pmatrix},$$

with the off-diagonal matrix elements depending on the momentum k.

2.4 THE DIRAC QUANTUM WALK

In this section, we present and review the Dirac QW on $\mathbb{Z}^d$ for $d = 1, 2, 3$; the complete derivation can be found in Ref. [40]. From the assumptions of Section 2.3 one derives a QW that in the limit of small wave vectors simulates the Weyl equation, so we say that it is a *massless* walk. As we shall see in the following, the local coupling of two Weyl QWs can be

1 For a generalization of coined Quantum Walks on general graphs see Ref. [16].

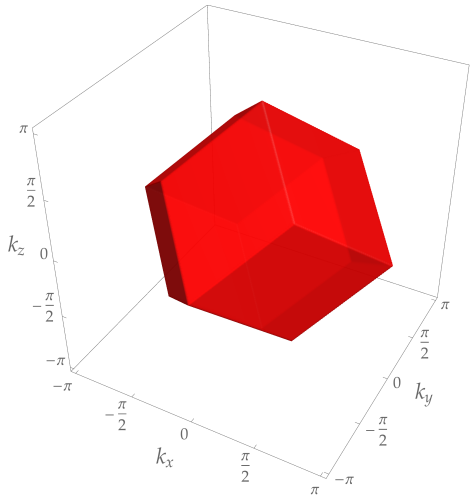


Figure 5.: First Brillouin zone B of the BCC lattice, which is a rhombic dodecahedron.

shown to simulate the Dirac equation, interpreting *a posteriori* the coupling parameter as the mass of the Dirac field. The correspondence is obtained for small values of the wave vector and of the mass parameter.

2.4.1 The massless case

The Weyl QW of Ref. [40] in dimension $d = 3$ is the only unitary quantum walk satisfying the principles introduced in Section 2.3 of locality, homogeneity, and isotropy, with minimal computational complexity, that can be embedded in the three-dimensional Euclidean space [40, 65, 94]. The unitarity condition selects a specific Cayley graph of the group $\mathbb{Z}^3$; in fact, the solution exists only for the Body-Centred Cubic (BCC) lattice $\Gamma(G, \mathcal{S}_+)$, with vertex set $G = 2\mathbb{Z}^3 \cup (2\mathbb{Z}^3 + (1,1,1))$ and generating set $\mathcal{S}_+ \coloneqq \{\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \mathbf{h}_4\}$ where

$$\mathbf{h}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{h}_2 = \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix}, \quad \mathbf{h}_3 = \begin{pmatrix} -1 \\ 1 \\ -1 \end{pmatrix}, \quad \mathbf{h}_4 = \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}.$$

The first Brillouin zone B of the BCC lattice, depicted in Fig. 5, is the set of inequivalent wave vectors $\mathbf{k}$ defined in cartesian coordinates as

$$B \coloneqq \left\{ (k_x, k_y, k_z) \in \mathbb{R}^3 \;\middle|\; -\pi \leqslant k_i \pm k_j \leqslant \pi,\ i \neq j,\ i,j \in \{x,y,z\} \right\}.$$

In the Fourier representation, the unique solutions existing on the BCC are denoted $V_{\mathbf{k}}^{\pm}$ and have the form:

$$V_{\mathbf{k}}^{\pm} = I \cos \omega_{\mathbf{k}}^{\pm} - i\, \boldsymbol{\sigma} \cdot \mathbf{n}_{\mathbf{k}}^{\pm},$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices and

$$\omega_{\mathbf{k}}^{\pm} = \arccos(c_x c_y c_z \mp s_x s_y s_z) \tag{4}$$

with $c_i \coloneqq \cos k_i$ and $s_i \coloneqq \sin k_i$, and the vector $\mathbf{n}_{\mathbf{k}}^{\pm}$ given by

$$\mathbf{n}_{\mathbf{k}}^{\pm} \coloneqq \begin{pmatrix} -s_x c_y c_z \mp c_x s_y s_z \\ -c_x s_y c_z \pm s_x c_y s_z \\ -c_x c_y s_z \mp s_x s_y c_z \end{pmatrix}.$$

The two admissible solutions existing on the BCC are related to one another by a CPT symmetry. The spectrum of $V_{\mathbf{k}}^{\pm}$ is $\{e^{-i\omega_{\mathbf{k}}^{\pm}}, e^{i\omega_{\mathbf{k}}^{\pm}}\}$ with dispersion relation $\omega_{\mathbf{k}}^{\pm}$ and group velocity given by $\boldsymbol{\nu}_{\mathbf{k}}^{\pm} \coloneqq \nabla_{\mathbf{k}} \omega_{\mathbf{k}}^{\pm}$ that represents the speed of a wave packet centred around the wave vector $\mathbf{k}$. For later convenience, we write the matrix $V_{\mathbf{k}}^{\pm}$ as follows:

$$V_{\mathbf{k}}^{\pm} = \begin{pmatrix} z_{\mathbf{k}} & -w_{\mathbf{k}}^* \\ w_{\mathbf{k}} & z_{\mathbf{k}}^* \end{pmatrix},$$

so that $\mathbf{n}_{\mathbf{k}}^{\pm} = (-\operatorname{Im} w_{\mathbf{k}}, \operatorname{Re} w_{\mathbf{k}}, -\operatorname{Im} z_{\mathbf{k}})$ and $\omega_{\mathbf{k}}^{\pm} = \arccos(\operatorname{Re} z_{\mathbf{k}})$.

In dimension $d = 2$ the assumptions of Section 2.3 impose that the only lattice admitting a non-trivial evolution is the square lattice, which is the Cayley graph of $\mathbb{Z}^2$ on two generators $\mathbf{h}_1 = (1, 0)$ and $\mathbf{h}_2 = (0, 1)$. Upon defining $k_i \coloneqq \mathbf{k} \cdot \mathbf{h}_i$, for $i \in \{1, 2\}$, and $k_x \coloneqq \frac{k_1 + k_2}{2}$, $k_y \coloneqq \frac{k_1 - k_2}{2}$, the first Brillouin zone B in this case is given by

$$B \coloneqq \left\{ \mathbf{k} \in \mathbb{R}^2 \;\middle|\; -\pi \leqslant k_l \leqslant \pi,\ l \in \{x, y\} \right\}.$$

The walk unitary matrix in the Fourier representation can be written in a similar form as in the $d = 3$ case as

$$V_{\mathbf{k}} = I \cos \omega_{\mathbf{k}} - i\, \boldsymbol{\sigma} \cdot \mathbf{n}_{\mathbf{k}} = \begin{pmatrix} z_{\mathbf{k}} & -w_{\mathbf{k}}^* \\ w_{\mathbf{k}} & z_{\mathbf{k}}^* \end{pmatrix}, \tag{5}$$

where $z_{\mathbf{k}} = c_x c_y - i s_x s_y$ and $w_{\mathbf{k}} = -s_x c_y - i c_x s_y$ with $c_l \coloneqq \cos k_l$, $s_l \coloneqq \sin k_l$ for $l \in \{x, y\}$.

Finally, we consider the case $d = 1$. Our requirements impose the choice of the one-dimensional lattice $\mathbb{Z}$, namely the free Abelian group on one generator with $S_+ = \{h\}$. The unique solution can be written in the Fourier representation as

$$V_k = I \cos k - i\, \boldsymbol{\sigma} \cdot \mathbf{n}_k = \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix}, \qquad \mathbf{n}_k \coloneqq \begin{pmatrix} 0 \\ 0 \\ -\sin k \end{pmatrix}, \tag{6}$$

whose dispersion relation is simply $\omega_k = k$.

In order to conclude the presentation of the Weyl QW, we summarize the solutions for $d = 1, 2, 3$. As we have seen, the general form of the (massless) walk can be written as

$$V_{\mathbf{k}} = \lambda_{\mathbf{k}} I - i\,\boldsymbol{\sigma} \cdot \mathbf{n}_{\mathbf{k}}, \tag{7}$$

once the functions $\lambda_{\mathbf{k}}$ and $\mathbf{n}_{\mathbf{k}}$ has been specified; the corresponding dispersion relation can be written in general as

$$\omega_{\mathbf{k}} \coloneqq \arccos \lambda_{\mathbf{k}}.$$

In each case, in the limit of small wave vectors the walk evolution is indistinguishable from the one given by the Weyl equation. In order to see this, one can extend the evolution to continuous times, introducing the interpolating Hamiltonian $H^W(\mathbf{k})$ such that $V_{\mathbf{k}} = e^{-iH^W(\mathbf{k})}$. In each dimension the interpolating Hamiltonian has the following form:

$$H^W(\mathbf{k}) = \operatorname{sinc}^{-1}(\omega_{\mathbf{k}})\, \boldsymbol{\sigma} \cdot \mathbf{n}_{\mathbf{k}}. \tag{8}$$

In order to see that we effectively can approximate the usual relativistic evolution, we consider the power expansion at the first order in $\mathbf{k}$, obtaining

$$H^W(\mathbf{k}) = \boldsymbol{\sigma} \cdot \mathbf{k} + \mathcal{O}(|\mathbf{k}|^2).$$

Interpreting $\mathbf{k}$ as the momentum of the relativistic particle, the first order term $\boldsymbol{\sigma} \cdot \mathbf{k}$ can be interpreted as the usual Weyl Hamiltonian, showing that the walk evolution and the relativistic evolution are indistinguishable for sufficiently small values of the wave vector.

We remark that the structure of the walk matrix in momentum space is independent of the dimension, allowing to express in general form the eigenvectors. The matrix $V_{\mathbf{k}}$ has the general form

$$V_{\mathbf{k}} = \begin{pmatrix} z_{\mathbf{k}} & -w_{\mathbf{k}}^* \\ w_{\mathbf{k}} & z_{\mathbf{k}}^* \end{pmatrix},$$

where $z_{\mathbf{k}}$ and $w_{\mathbf{k}}$ are functions of the wave vector defined by

$$\operatorname{Re}(z_{\mathbf{k}}) = \lambda_{\mathbf{k}},$$

and

$$\mathbf{n}_{\mathbf{k}} = (-\operatorname{Im}(w_{\mathbf{k}}), \operatorname{Re}(w_{\mathbf{k}}), -\operatorname{Im}(z_{\mathbf{k}})).$$

With this convention, the general solution of the eigenvalue problem for $V_{\mathbf{k}}$

$$V_{\mathbf{k}} |u_s^W(\mathbf{k})\rangle = e^{-is\omega_{\mathbf{k}}} |u_s^W(\mathbf{k})\rangle, \qquad s = \pm, \tag{9}$$

can be written in the following way:

$$|u_s^W(\mathbf{k})\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 - s\nu_{\mathbf{k}}^W} \\ -se^{i\varphi}\sqrt{1 + s\nu_{\mathbf{k}}^W} \end{pmatrix}, \qquad \nu_{\mathbf{k}}^W := \frac{\mathrm{Im}(z_{\mathbf{k}})}{\sqrt{1 - \lambda_{\mathbf{k}}^2}}, \tag{10}$$

where $\varphi = \mathrm{Arg}\, w_{\mathbf{k}} - \frac{\pi}{2}$.

2.4.2 The massive case

We have seen how the assumptions of Section 2.3 restrict the kind of dynamics that emerge in our discrete scenario. The premisses that we have made entail that the emergent dynamics corresponds to massless particles in the relativistic limit. In order to add a mass to the walk evolution we can ask ourselves which is the minimal extension that allows us to do so. One can show that, starting from the local coupling of two Weyl QWs satisfying the principles of Section 2.3, there is only one way to locally couple two Weyl QWs and the resulting evolution approximates that of the Dirac equation. If $V_{\mathbf{k}}$ denotes the Weyl QW in dimension d, the unique coupling (modulo unitary conjugation) has the form[2]

$$D_{\mathbf{k}} = \begin{pmatrix} nV_{\mathbf{k}} & -im \\ -im & nV_{\mathbf{k}}^\dagger \end{pmatrix}, \quad n, m > 0, \quad n^2 + m^2 = 1.$$

Such a construction holds in any spatial dimension $d = 1, 2, 3$; in dimension $d = 1$, however, the walk decouples into two massive QWs with smaller coin dimension $s = 2$ [40, 42], providing the same physics. With a simple change of basis the resulting walk can be written in block-diagonal form as

$$\begin{pmatrix} ne^{ik} & -im & 0 & 0 \\ -im & ne^{-ik} & 0 & 0 \\ 0 & 0 & ne^{-ik} & -im \\ 0 & 0 & -im & ne^{ik} \end{pmatrix}.$$

Accordingly, we consider only the walk on the smaller coin space:

$$D_{\mathbf{k}} = \begin{pmatrix} ne^{ik} & -im \\ -im & ne^{-ik} \end{pmatrix}, \tag{11}$$

with dispersion relation

$$\omega_{\mathbf{k}} = \arccos(n \cos k).$$

2 We remark that, in contrast with the coined Quantum Walk shown in Section 2.3.2, as a result of this coupling the off-diagonal matrix elements do not depend on the momentum.

This is in agreement with the fact that the Dirac equation in dimension $d = 1$ is described by a two-component field.

The unitary matrix D_k of the Dirac QW in dimension d can be written in a convenient form in terms of the gamma matrices in the chiral representation:

$$D_k = n\lambda_k I - i\, n\gamma_0 \boldsymbol{\gamma} \cdot \mathbf{n}_k - im\gamma_0, \tag{12}$$

where λ_k and $\mathbf{n}_k$ are the functions characterizing the Weyl QWs of Section 2.4.1. The dispersion relation for the Dirac walks described by Eq. (12) is simply given by

$$\omega_k = \arccos(n\lambda_k). \tag{13}$$

Also in this case the relativistic limit of small wave vectors is obtained by power-expanding the interpolating Hamiltonian $H^D(\mathbf{k})$

$$H^D(\mathbf{k}) = \frac{\omega_k}{\sin \omega_k}(n\gamma_0 \boldsymbol{\gamma} \cdot \mathbf{n}_k - m\gamma_0), \tag{14}$$

which at the first order in $\mathbf{k}$ and m recovers the expression of the Dirac Hamiltonian

$$H^D(\mathbf{k}) = \gamma_0 \boldsymbol{\gamma} \cdot \mathbf{k} + m\gamma_0 + \mathcal{O}(m^2) + \mathcal{O}(|\mathbf{k}|^2). \tag{15}$$

In order to conclude the presentation of the massive case, let us write the general expression for the eigenvectors of D_k. The eigenvalue equation

$$D_k \left|u^D_{s,r}(\mathbf{k})\right\rangle = e^{-is\omega_k} \left|u^D_{s,r}(\mathbf{k})\right\rangle, \quad s, r = \pm, \tag{16}$$

has four solutions given by the vectors $|u^D_{s,r}(\mathbf{k})\rangle \in \mathbb{C}^4$:

$$|u^D_{s,r}(\mathbf{k})\rangle = \frac{1}{2} \begin{pmatrix} \sqrt{(1 - r\nu^W_k)(1 + s r \nu^D_k)} \\ -re^{i\varphi}\sqrt{(1 + r\nu^W_k)(1 + s r \nu^D_k)} \\ -s\sqrt{(1 - r\nu^W_k)(1 - s r \nu^D_k)} \\ sre^{i\varphi}\sqrt{(1 + r\nu^W_k)(1 - s r \nu^D_k)} \end{pmatrix}, \quad \nu^D_k = \frac{n\sqrt{1 - \lambda_k^2}}{\sqrt{1 - n^2\lambda_k^2}}, \tag{17}$$

where the functions λ_k and ν^W_k along with the phase φ are the same as those of the corresponding massless QWs of Eqs. (9) and (10). In the special case of $d = 1$, D_k is a 2×2 matrix (see Eq. (11)) and its eigenvectors are actually $\mathbb{C}^2$-vectors:

$$D_k \left|s, k\right\rangle = e^{-is\omega_k} \left|s, k\right\rangle, \quad \left|s, k\right\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 - s\nu_k} \\ s\sqrt{1 + s\nu_k} \end{pmatrix}, \quad s = \pm,$$

v_k being the group velocity, namely

$$v_k \coloneqq \frac{d\omega_k}{dk} = \frac{n \sin k}{E_k}, \qquad E_k \coloneqq \sin \omega_k = \sqrt{n^2 \sin^2 k + m^2}.$$

2.5 PATH-SUM FOR QUANTUM WALKS

The Abelian property of the lattice on which the Weyl and Dirac QWs are defined allow one to easily obtain the solutions of the walks in the Fourier representation. In this way one can analyse many properties of the dynamics of these walks. On the other hand, one may need to know the evolution directly in position space. To this end, we provide and review the solutions in position space for the QWs in dimension $d = 1, 2, 3$ of [72–74].

In the general setting of QWs on a Cayley graph $\Gamma(G, \mathcal{S}_+)$ of some group G, the goal is to find a solution of a walk described by the unitary operator W acting on the Hilbert space $\mathscr{H} = \ell^2(G) \otimes \mathbb{C}^s$. The state at time t located at the cell labeled $x \in G$ is denoted as $|\psi_x(t)\rangle \in \mathbb{C}^s$. Thus, $|\psi_x(t)\rangle$ is a solution of the walk W if it satisfies the one-step update equation

$$|\psi_x(t+1)\rangle = \sum_{h \in \mathcal{S}} A_h \, |\psi_{xh}(t)\rangle \,, \tag{18}$$

where $\{A_h\}_{h \in \mathcal{S}}$ denotes the set of transition matrices associated to the walk W. Notice that, according to our conventions, the matrix A_h is associated to the step h^{-1}. The set $\mathcal{S}$ in the massless case is defined as $\mathcal{S} \coloneqq \mathcal{S}_+ \cup \mathcal{S}_-$, whereas for a walk with mass one has $\mathcal{S} \coloneqq \mathcal{S}_+ \cup \mathcal{S}_- \cup \{\varepsilon\}$, ε being the identity element of the group G. We remark that a transition associated to the identity ε—namely, the walk does not move on the lattice—only affects the internal degree of freedom, for example by swapping the internal components, as for the Dirac walk. Accordingly, the off-diagonal matrix elements are independent of the momentum.

The iterated application of the update rule of Eq. (18) naturally leads to a representation of the evolution in terms of paths on the graph. In this way we are just employing a discrete version of Feynman's path-integral [66, 98] to express the evolution of a state $|\psi(0)\rangle \in \mathscr{H}$ driven by the walk W. In practice, as we will see, we need to compute the propagator of the walk heavily relying on the algebraic properties of the transition matrices.

Given, thus, an initial configuration of the walk $|\psi(0)\rangle \in \mathscr{H}$, we obtain the solution at time t by computing the sum of the contribution of each step for all the paths that join two given points on the graph. We denote by σ a path of length t with fixed endpoints x' and x, *i.e.* $\sigma = x' h_1 h_2 \cdots h_t x$, and we denote by $\Lambda_t(x', x)$ the set of all such paths. The collection of all the paths ending in a given point x is denoted as $\mathcal{C}_t(x) \coloneqq \{x' \in G \mid \Lambda_t(x', x) \neq \emptyset\}$, namely it is the slice at time t of the *past causal cone*

of x. In this way the solution at time t is obtained by summing over all the points x' in the past causal cone of x for which there exist a path σ of length t joining x' to x:

$$|\psi_x(t)\rangle = \sum_{x' \in \mathcal{C}_t(x)} \sum_{h_1,\dots,h_t \in S} \delta(x^{-1}x' h_1 \cdots h_t) \mathcal{A}(h_1,\dots,h_t) \, |\psi_{x'}(0)\rangle \,, \tag{19}$$

where the function

$$\mathcal{A}(h_1, h_2, \dots, h_t) = A_{h_t^{-1}} \cdots A_{h_2^{-1}} A_{h_1^{-1}}$$

gives the overall matrix associated to a sequence of steps $h_1, h_2, \dots, h_t$. The delta function is needed to determine if a sequence $h_1, h_2, \dots, h_t$ actually forms a path from x' to x, namely determines if a given word w is the empty string ε:

$$\delta(w) = \begin{cases} 1, & \text{if } w = \varepsilon, \\ 0, & \text{otherwise.} \end{cases}$$

From Eq. (19) we see that the task at hand to obtain the explicit solution amounts to the evaluation of the propagator of the walk which gives the overall transition amplitude to go from a site x to a site x' in t time-steps:

$$\mathcal{K}(x, x'; t) \coloneqq \langle x' | W^t | x \rangle = \sum_{h_1,\dots,h_t \in S} \delta(x'^{-1} x h_1 \cdots h_t) \mathcal{A}(h_1^{-1}, \dots, h_t^{-1}).$$

We will see in Chapters 4 to 6 how we can exploit the algebraic properties of the transition matrices and the binary encoding of paths to obtain an analytical expression of the propagator for the Dirac QW in dimension $d = 1$ and for the Weyl QW in dimension $d = 2$ and $d = 3$.

3 NUMERICAL EVALUATION OF THE DIRAC QUANTUM WALK

Particles that evolve according to the Dirac equation can show a typical quivering motion known as *Zitterbewegung* due to the interference of particle and antiparticle components [99]. This phenomenon was first discovered by Schrödinger [100] who noticed that for free relativistic electrons the velocity operator does not commute with the Dirac Hamiltonian. As a consequence, this leads to an extra term in the evolution of the position operator, besides the classical motion [101], which is responsible for the fast oscillatory behaviour. It can be shown that this quivering motion happens with frequency $\frac{2mc^2}{\hbar}$ and its amplitude is given by the Compton wavelength $\frac{\hbar}{mc}$, where m is the mass of the relativistic particle. Moreover, this jittering motion is shown to fade for a wave-packet particle state [102]. Although the *Zitterbewegung* effect has never been observed, there are however example of simulations of this phenomenon by means of trapped ion systems [103, 104] and Bose–Einstein condensates [105].

In this chapter we are going to study the position operator of the Dirac QW (see Section 2.4). We observe, both analytically and numerically, that *Zitterbewegung* arises also for the walk evolution of wave-packets containing both positive and negative frequency eigenstates of the walk, which thus correspond to particle and antiparticle states in the Dirac theory. We focus on the interference effect due to the superposition of positive and negative energy states, although this is not strictly necessary to exhibit the quivering behaviour [106]. We analyse the evolution of wave-packets particle states peaked around a given value of the momentum such that they satisfy a dispersive differential equation. The walk evolution approximates for these states the one given by the Dirac equation.

In addition, we are going to present here also the evolution of perfectly localized states, that—since they involve very large momenta—exhibit an evolution that is very far from the one given by the Dirac equation. Indeed, for perfectly localized states one can appreciate the the finiteness of the speed of information propagation.

The numerical simulations of the Dirac QW in dimension $d = 1$ and $d = 3$ were performed employing the direct space update rule to obtain the time evolution. Regarding the preparation of the initial state, we need to compute the components of the state in the eigenbasis of the walk, which means that we have to employ the Fourier representation. For the details on the numerical implementation of the Fourier Transform (FT) on $\mathbb{Z}^d$ and

on the BCC lattice, we refer the reader to Appendix C. In the following we are going to present the analysis of the Dirac walk dynamics in dimension $d = 1$ and $d = 3$, showing also the results of the numerical evaluation of the walk for perfectly localized states and Gaussian wave-packets.

3.1 SMOOTH STATES

We consider the general case of states peaked around a given momentum that are also localized in position space. In order to exhibit a particle-like behaviour the walk dynamics should also preserve the localization of such states, at least for a sufficient long time before the diffusion takes over.

So we conveniently consider states $|\psi\rangle$ in dimension $d \leqslant 3$ that are wave-packets given by a smooth function $g_{k'} \in \mathcal{C}_0^\infty[B]$ peaked around some wave vector $\mathbf{k}'$ such that

$$\int_{B'_\sigma} d\mathbf{k}\, |g_{k'}(\mathbf{k})|^2 > 1 - \varepsilon/2, \quad \varepsilon, \sigma > 0, \tag{20}$$

where B'_σ is defined as

$$B'_\sigma \coloneqq \left\{ \mathbf{k} \in B \;\middle|\; |k_i - k'_i| \leqslant \sigma \right\}.$$

In order to study the evolution of such states, we conveniently extend the FT to continuous $\mathbf{x}$ and t; therefore, introducing the interpolating Hamiltonian $H(\mathbf{k})$ we can write the state as

$$\begin{aligned} |\psi(t,\mathbf{x})\rangle &\coloneqq \frac{e^{i(\omega_{k'}t - \mathbf{k}'\cdot\mathbf{x})}}{(2\pi)^{d/2}} \int_B d\mathbf{k}\; g_{k'}(\mathbf{k}) e^{-i(H(\mathbf{k})t - \mathbf{k}\cdot\mathbf{x})} |u(\mathbf{k})\rangle \\ &= \frac{e^{i(\omega_{k'}t - \mathbf{k}'\cdot\mathbf{x})}}{(2\pi)^{d/2}} \int_B d\mathbf{k}\; g_{k'}(\mathbf{k}) e^{-i(\omega_k t - \mathbf{k}\cdot\mathbf{x})} |u(\mathbf{k})\rangle \end{aligned} \tag{21}$$

where $|u(\mathbf{k})\rangle$ denotes any eigenvector of the walk. Let us consider now the Taylor expansion of the dispersion relation ω_k associated to the eigenvector $|u(\mathbf{k})\rangle$ around some wave vector $\mathbf{k}'$:

$$\omega_k - \omega_{k'} = \sum_{|\alpha| \geqslant 1} \frac{\omega^{(\alpha)}_{k'}}{\alpha!} (\mathbf{k} - \mathbf{k}')^\alpha,$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ is a multi-index and $\omega^{(\alpha)}_{k'}$ is defined by

$$\omega^{(\alpha)}_{k'} \coloneqq \partial^\alpha_k \omega_k \big|_{k=k'}, \qquad \partial^\alpha_k \omega_k \coloneqq \frac{\partial^{|\alpha|} \omega_k}{\partial k_x^{\alpha_1} \partial k_y^{\alpha_2} \partial k_z^{\alpha_3}}.$$

Accordingly, from Eq. (21) on can derive the corresponding differential equation satisfied by $|\psi(t,\mathbf{x})\rangle$:

$$i\partial_t |\psi(t,\mathbf{x})\rangle = \sum_{|\alpha|\geqslant 1} \frac{(-i)^\alpha \omega_{\mathbf{k}'}^{(\alpha)}}{\alpha!} \partial_{\mathbf{x}}^\alpha |\psi(t,\mathbf{x})\rangle\,, \tag{22}$$

where, by the dominated derivative theorem, we exchanged the integral sign with the spatial derivatives.

Since the states we are considering here are smooth states peaked around $\mathbf{k}'$, we can consider the approximate differential equation by truncating up to order n the expression in Eq. (22). Denoting by $|\varphi^n(t,\mathbf{x})\rangle$ the approximate solution up to order n, we derive a bound for the overlap between the exact and approximate solution:

$$\begin{aligned}
|\langle\varphi^n(t)|\psi(t)\rangle| &= \left|\int_B d\mathbf{k}\; e^{-it\sum_{|\alpha|\geqslant n+1}\frac{\omega_{\mathbf{k}'}^{(\alpha)}}{\alpha!}(\mathbf{k}-\mathbf{k}')^\alpha}|g_{\mathbf{k}'}(\mathbf{k})|^2\right| \\
&\geqslant \left|\int_{B'_\sigma} d\mathbf{k}\; e^{-it\sum_{|\alpha|\geqslant n+1}\frac{\omega_{\mathbf{k}'}^{(\alpha)}}{\alpha!}(\mathbf{k}-\mathbf{k}')^\alpha}|g_{\mathbf{k}'}(\mathbf{k})|^2\right| \\
&\quad - \left|\int_{B\setminus B'_\sigma} d\mathbf{k}\; e^{-it\sum_{|\alpha|\geqslant n+1}\frac{\omega_{\mathbf{k}'}^{(\alpha)}}{\alpha!}(\mathbf{k}-\mathbf{k}')^\alpha}|g_{\mathbf{k}'}(\mathbf{k})|^2\right| \\
&> \left|\int_{B'_\sigma} d\mathbf{k}\; e^{-it\sum_{|\alpha|\geqslant n+1}\frac{\omega_{\mathbf{k}'}^{(\alpha)}}{\alpha!}(\mathbf{k}-\mathbf{k}')^\alpha}|g_{\mathbf{k}'}(\mathbf{k})|^2\right| - \frac{\varepsilon}{2} \\
&> 1-\varepsilon - \left|\int_{B'_\sigma} d\mathbf{k}\,(-it)\sum_{|\alpha|\geqslant n+1}\frac{\omega_{\mathbf{k}'}^{(\alpha)}}{\alpha!}(\mathbf{k}-\mathbf{k}')^\alpha|g_{\mathbf{k}'}(\mathbf{k})|^2\right| \\
&> 1-\varepsilon - \sum_{|\alpha|\geqslant n+1}\frac{t|\omega_{\mathbf{k}'}^{(\alpha)}|}{\alpha!}\left|\int_{B'_\sigma} d\mathbf{k}\,|g_{\mathbf{k}'}(\mathbf{k})|^2(\mathbf{k}-\mathbf{k}')^\alpha\right|.
\end{aligned}$$

Noticing that for $\mathbf{k}\in B'_\sigma$ one has $|(\mathbf{k}-\mathbf{k}')^\alpha|\leqslant\sigma^{|\alpha|}$, then we can write

$$|\langle\varphi^n(t)|\psi(t)\rangle| > 1-\varepsilon-\sum_{|\alpha|\geqslant n+1}\frac{t\sigma^{|\alpha|}|\omega_{\mathbf{k}'}^\alpha|}{\alpha!}\int_{B'_\sigma} d\mathbf{k}\,|g_{\mathbf{k}'}(\mathbf{k})|^2.$$

In particular, we are interested in the expression of the overlap at the second order in the power expansion and we can finally write the following expression for the bound:

$$|\langle\varphi^n(t)|\psi(t)\rangle| > 1-\varepsilon-\gamma\sigma^3 t - \mathcal{O}(\sigma^5)t,$$

where γ is defined as

$$\gamma \coloneqq \sum_{|\alpha|=3} \frac{|\omega^{(\alpha)}|}{\alpha!} \int_{B'_\sigma} d\mathbf{k}\, |g_{\mathbf{k}'}(\mathbf{k})|^2.$$

We remark that, if we want an error less than some $\delta > 0$, so that the overlap is sufficiently close to 1, namely

$$|\langle \varphi^n(t) | \psi(t) \rangle| > 1 - \delta,$$

this means that the approximate solution can deviate significantly from the walk evolution after a time $t > \frac{\delta-\varepsilon}{\gamma\sigma^3}$.

As a final remark of the present discussion, we can interpret the terms appearing in Eq. (22) truncating the sum at the second order. The resulting approximate equation for the state evolution can be written in the following form:

$$i\partial_t |\varphi(t,\mathbf{x})\rangle = \left[-i\boldsymbol{v}_{\mathbf{k}'} \cdot \nabla - \frac{1}{2}\nabla^T \cdot \mathbf{D}_{\mathbf{k}'} \cdot \nabla\right] |\varphi(t,\mathbf{x})\rangle\,. \tag{23}$$

The vector $\boldsymbol{v}_{\mathbf{k}} = \nabla_{\mathbf{k}}\omega_{\mathbf{k}}$ denotes the drift vector that determines the group velocity of the wave-packet. The spreading of its distribution in direct space is described by the diffusion tensor $\mathbf{D}_{\mathbf{k}} = \nabla_{\mathbf{k}}\nabla_{\mathbf{k}}\omega_{\mathbf{k}}$. The evolution of a Gaussian state in dimension $d = 3$, satisfying the condition of Eq. (20), is depicted in Fig. 6.

3.2 PERFECTLY LOCALIZED STATES

In a QW scenario, besides smooth wave-packets whose evolution can be approximated by the differential equation (23), one can also consider perfectly localized states. For such a class of states we can expect the QW evolution to be very different from the usual evolution of a Dirac particle. In this regard, we remark that the usual relativistic dynamics of the Dirac equation can be recovered in the limit of wave vectors that are much smaller with respect to a given reference scale [61, 64]. Nevertheless, the study of such states is essential for the analysis of the diffusion properties in an QW scenario [16–18, 107].

Let us consider perfectly localized states for the Dirac QW in dimension $d = 3$, having the form

$$|\psi\rangle = |\mathbf{x}\rangle\,|\zeta\rangle\,, \qquad |\zeta\rangle \in \mathbb{C}^4.$$

In Fig. 7, we show the time evolution of the state $|0\rangle\,|\zeta\rangle$ with $|\zeta\rangle = (1,0,0,0)$ with mass parameter $m = 0.03$. The probability distribution is represented for $t = 0, 8, 16$ from left to right. Furthermore, in Fig. 8, the probability

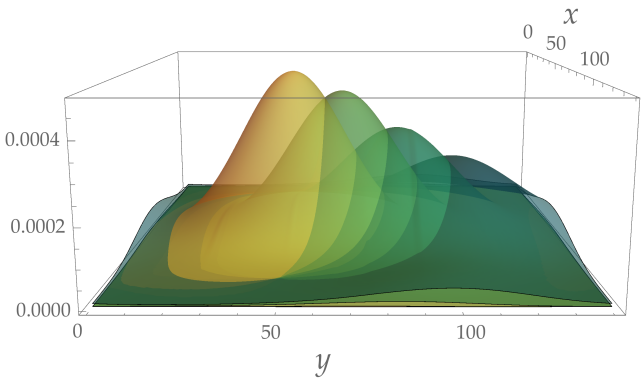


Figure 6.: Evolution of a wave-packet with only positive-frequency eigenstates for the Dirac QW in dimension $d = 3$. In the image it is represented the marginal distribution along the z-axis. The total number of time-steps is $t = 150$, whereas the probability distribution in position space is shown for $t = 0, 50, 100, 150$ with a colour gradient from light to dark (left to right). The initial state is a Gaussian wave-packet (see Eq. (20)) with mass $m = 0.02$, mean wave vector $\mathbf{k}' = (0, 0.01, 0)$ and width $\sigma = 32^{-1}$.

distribution is represented for the same state at time $t = 28$, showing also the projections on the three planes.

3.3 ZITTERBEWEGUNG OF THE DIRAC QUANTUM WALK

In this section we briefly discuss the phenomenon known as *Zitterbewegung* in the context of QWs. We consider smooth states similar to those described in Eqs. (20) and (21) containing both positive- and negative-energy components:

$$|\psi\rangle = \sum_{\mathbf{x}\in G} \sum_{r=1}^{s} g_r(\mathbf{x}) \, |\mathbf{x}\rangle \, |r\rangle \, ,$$

where we have introduced s smooth functions g_r (20) with $r = 1, \ldots, s$; and G denotes the vertex set of the lattice. In particular, for $d = 1$ we have $G = \mathbb{Z}$ and for $d = 3$ we can represent the BCC lattice with $G = 2\mathbb{Z}^3 \cup (2\mathbb{Z}^3 + \mathbf{t})$, $\mathbf{t} = (1, 1, 1)$.

We study the behaviour of the position operator

$$\mathbf{X} = \sum_{\mathbf{x}\in G} \mathbf{x} \, (|\mathbf{x}\rangle\langle\mathbf{x}| \otimes I)$$

on the aforementioned states that are superpositions of positive and negative frequencies components. In order to study the kinematics of the walk we need to define also the corresponding momentum operator. Although the definition of the momentum would require an interacting theory to be

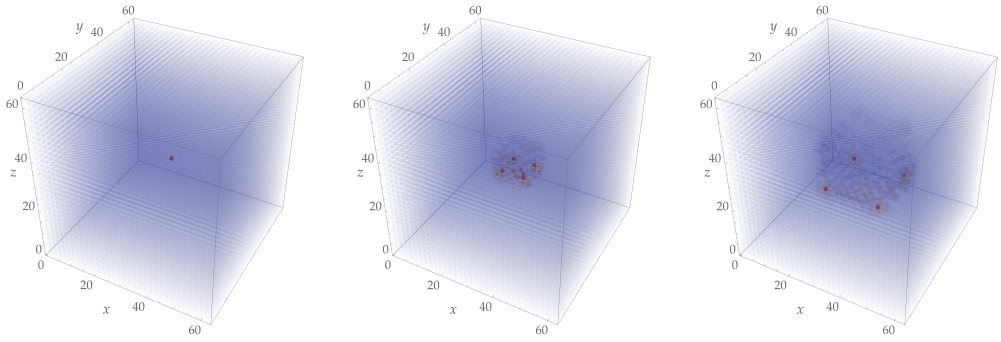


Figure 7.: Diffusion of a perfectly localized state in dimension $d = 3$ for the Dirac QW. The three different figures show the time evolution at three different steps, namely $t = 0, 8, 16$, from left to right. The value of the mass parameter is $m = 0.03$ and the internal state is $|\zeta\rangle = (1, 0, 0, 0)$.

defined, however, we can interpret the wave vector $\mathbf{k}$ *a posteriori* (see Section 2.4.2) as the momentum of the Dirac particle once we take limit for small wave vectors and masses. Therefore, we can take the operator

$$\mathbf{P} = \int_B d\mathbf{k}\, \mathbf{k}\, (|\mathbf{k}\rangle\langle\mathbf{k}| \otimes I)$$

as the momentum operator. The commutator between the position operator X_i and the momentum operator P_j, $i, j = 1, 2, 3$, reads

$$\langle\psi|\,[X_i, P_j]\,|\psi\rangle = i\delta_{ij}\left(1 - \frac{1}{2}\sum_r \left(|\hat{g}_r(\pi)|^2 + |\hat{g}_r(-\pi)|^2\right)\right), \tag{24}$$

where $\hat{g}(\mathbf{k})$ denotes the Discrete-Time Fourier Transform (DTFT) of $g(\mathbf{x})$, for any function g on the lattice. The extra term that appears in the commutator (24) is a boundary term that arises as a consequence of the discreteness of the lattice; moreover, for perfectly localized states the commutator vanishes. Nevertheless, in the following we will consider states for which the boundary term in Eq. (24) is negligible.

In order to appreciate the *Zitterbewegung* in the QW theory, we can study the behaviour of $\mathbf{X}(t) = U^{-t}\mathbf{X}U^t$. We report here the results of Ref. [108]. The operator $\mathbf{X}(t)$ can be analytically computed once we know the expression for the velocity and the acceleration operators:

$$\mathbf{V}(t) = i[H^D, \mathbf{X}(t)] = \int_B d\mathbf{k}\ |\mathbf{k}\rangle\langle\mathbf{k}| \otimes \mathbf{V}(\mathbf{k}),$$
$$\mathbf{A}(t) = i[H^D, \mathbf{V}(t)] = \int_B d\mathbf{k}\ |\mathbf{k}\rangle\langle\mathbf{k}| \otimes \mathbf{A}(\mathbf{k}),$$

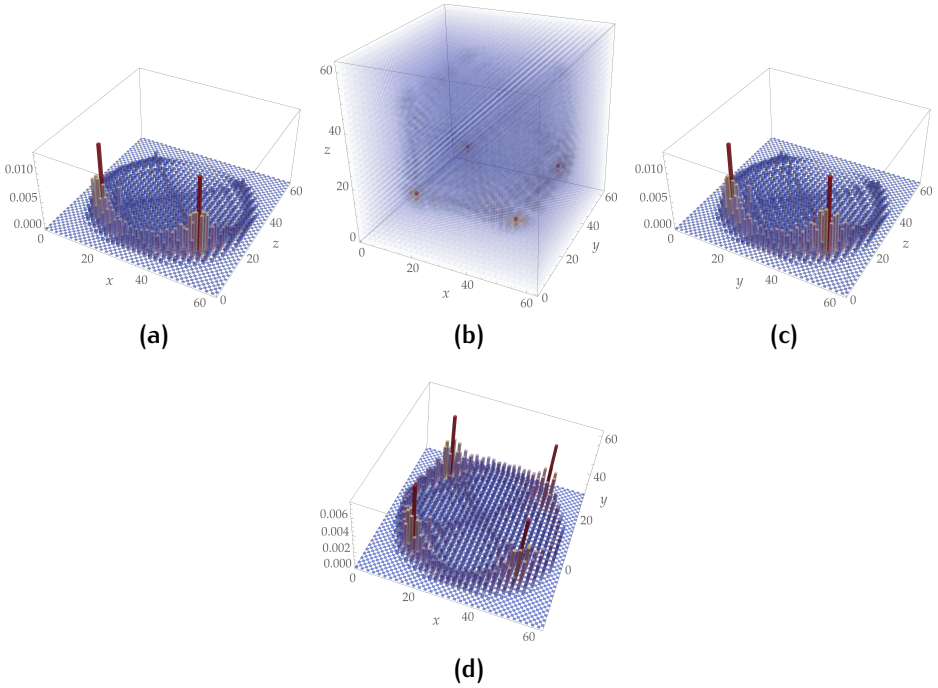


Figure 8.: Probability distribution for the same state as in Fig. 7 after $t = 28$ time-steps. Top-left: marginal distribution along the y-axis; top-right: marginal distribution along the x-axis; bottom: marginal distribution along the z-axis.

where H^D is the interpolating Hamiltonian of the Dirac walk given by Eq. (14):

$$H^D(\mathbf{k}) = \frac{\omega_{\mathbf{k}}}{\sin\omega_{\mathbf{k}}}(n\gamma_0\boldsymbol{\gamma}\cdot\mathbf{n}_{\mathbf{k}} - m\gamma_0).$$

By simple calculations, the velocity operator results to be

$$V_j(\mathbf{k}) = \frac{\sin\omega_{\mathbf{k}} - \omega_{\mathbf{k}}\cos\omega_{\mathbf{k}}}{\omega_{\mathbf{k}}\sin\omega_{\mathbf{k}}} H^D(\mathbf{k})(\boldsymbol{\nu}_{\mathbf{k}})_j + \frac{\omega_{\mathbf{k}}}{\sin\omega_{\mathbf{k}}} n\gamma_0\boldsymbol{\gamma}\cdot\partial_{k_j}\mathbf{n}_{\mathbf{k}},$$

and the acceleration operator reads

$$A_j(\mathbf{k}) = 2n\frac{\omega_{\mathbf{k}}^2}{\sin^2\omega_{\mathbf{k}}}\left(n\sum_{\mu<\nu}\gamma_\mu\gamma_\nu f^{(j)}_{\mu\nu} - m\boldsymbol{\gamma}\cdot\partial_{k_j}\mathbf{n}_{\mathbf{k}}\right),$$

where $f^{(j)}_{\mu\nu}$ is defined as

$$f^{(j)}_{\mu\nu} := \left((\mathbf{n}_{\mathbf{k}})_\nu\partial_{k_j}(\mathbf{n}_{\mathbf{k}})_\mu - (\mathbf{n}_{\mathbf{k}})_\mu\partial_{k_j}(\mathbf{n}_{\mathbf{k}})_\nu\right).$$

At this point we are able to compute the expression for $\mathbf{X}(t)$. First notice that the operator $\boldsymbol{A}(\mathbf{k},t) = e^{iH^D(\mathbf{k})t}\boldsymbol{A}(\mathbf{k})e^{-iH^D(\mathbf{k})t}$ actually evolves as

$$\boldsymbol{A}(\mathbf{k},t) = e^{2iH^D(\mathbf{k})t}\boldsymbol{A}(\mathbf{k}).$$

This is due to the fact that $\{H^D(\mathbf{k}), \boldsymbol{A}(\mathbf{k})\} = 0$ because of the relation $n_3 f_{12}^{(j)} - n_2 f_{13}^{(j)} + n_1 f_{23}^{(j)} = 0$. As such, by integrating the acceleration we have

$$\begin{aligned}
\mathbf{V}(\mathbf{k},t) &= \hat{\mathbf{V}}(\mathbf{k}) + \mathbf{Z}^V(\mathbf{k},t),\\
\hat{\mathbf{V}}(\mathbf{k}) &= \mathbf{V}(\mathbf{k}) - \mathbf{Z}^V(\mathbf{k},0),\\
\mathbf{Z}^V(\mathbf{k},t) &= \frac{1}{2i}H^{D,-1}(\mathbf{k})\boldsymbol{A}(\mathbf{k},t),
\end{aligned}$$

with $H^{D,-1}(\mathbf{k}) = \omega_{\mathbf{k}}^{-2}\, H^D(\mathbf{k})$. The integration of the velocity gives

$$\begin{aligned}
\mathbf{X}(t) &= \mathbf{X}(0) + \hat{\mathbf{V}}t + \mathbf{Z}^X(t) - \mathbf{Z}^X(0),\\
\mathbf{Z}^X(\mathbf{k},t) &= -\frac{1}{4}H^{D,-2}(\mathbf{k})\boldsymbol{A}(\mathbf{k},t),
\end{aligned} \tag{25}$$

where the operator $Z_j^X(\mathbf{k},t)$ is given by

$$Z_j^X(\mathbf{k},t) = -\frac{\omega_{\mathbf{k}}^3}{2\sin\omega_{\mathbf{k}}^3}e^{2iH^D(\mathbf{k})t}\Big(n^2\gamma^0\boldsymbol{\gamma}\cdot\boldsymbol{w}^{(j)} + nm\mathbf{n}\cdot\partial_{k_j}\mathbf{n} + m^2\gamma^0\boldsymbol{\gamma}\cdot\partial_{k_j}\mathbf{n}\Big),$$

with

$$\boldsymbol{w}^{(j)} \coloneqq \begin{pmatrix} n_3 f_{13}^{(j)} + n_2 f_{12}^{(j)} \\ -n_1 f_{12}^{(j)} + n_3 f_{23}^{(j)} \\ -n_1 f_{13}^{(j)} + n_2 f_{23}^{(j)} \end{pmatrix}.$$

From Eq. (25), we can see that the position operator presents an additional contribution besides the classical term given by $\hat{\mathbf{V}}t$, where $\hat{\mathbf{V}}$ denotes the classical component of the velocity which in the diagonal basis of the Hamiltonian is proportional to the group velocity: $\hat{\mathbf{V}}(\mathbf{k}) \propto (\sigma_z \otimes I)\boldsymbol{v}_{\mathbf{k}}$. This additional contribution consists in a time-dependent term denoted $\mathbf{Z}^X(t)$ and a constant shift denoted $\mathbf{Z}^X(0)$. Noticing that

$$\langle u_\mp(\mathbf{k})|\hat{V}_j(\mathbf{k})|u_\pm(\mathbf{k})\rangle = 0, \qquad \langle u_\pm(\mathbf{k})|Z_j^X(\mathbf{k})|u_\pm(\mathbf{k})\rangle = 0,$$

the expectation value of $\mathbf{X}(t)$ over a generic state $|\psi\rangle = |\psi_+\rangle + |\psi_-\rangle$ with both positive- and negative-frequency components can be expressed in the following form:

$$\langle\psi|\mathbf{X}(t)|\psi\rangle = \mathbf{x}_\psi^+(t) + \mathbf{x}_\psi^-(t) + \mathbf{x}_\psi^{\text{int}}(t),$$

where $x_\psi^\pm(t)$ is defined as

$$x_\psi^\pm(t) := \langle\psi_\pm|\mathbf{X}(0) + \hat{\mathbf{V}}t|\psi_\pm\rangle\,,$$

and $x_\psi^{\text{int}}(t)$ is given by

$$x_\psi^{\text{int}}(t) := 2\,\text{Re}\Big[\langle\psi_+|\mathbf{X}(0) - \mathbf{Z}^X(0) + \mathbf{Z}^X(t)|\psi_-\rangle\Big]. \tag{26}$$

The two contributions given by $x_\psi^\pm(t)$ represent the classical evolution of the particle and antiparticle components according to the classical velocity $\hat{\mathbf{V}}$, while the term $x_\psi^{\text{int}}(t)$ in Eq. (26) is responsible for the oscillatory behaviour of the state evolution which, hence, can be considered the analogue in the QW framework of the *Zitterbewegung* present in the Dirac theory. The oscillatory behaviour is clearly not present if the state has only positive or negative components. However, this oscillatory behaviour can be shown to vanish as $t \to \infty$ for smooth wave-packets generalizing Eq. (20) to superpositions of positive- and negative-frequency components:

$$|\psi\rangle = c_+\,|\psi_+\rangle + c_-\,|\psi_-\rangle\,, \qquad |c_+|^2 + |c_-|^2 = 1,$$

where $|\psi_\pm\rangle$ is defined by

$$|\psi_\pm\rangle = \int_B d\mathbf{k}\; g_{\mathbf{k}'}(\mathbf{k})\,|\mathbf{k}\rangle\,|u_{\pm,r}(\mathbf{k})\rangle$$

with $|u_{\pm,r}(\mathbf{k})\rangle$ denoting the walk eigenvectors of Eq. (17). The dumping of the oscillation is due to the fact that the wave-packets related to the positive and negative components separate in position space after many time-steps, suppressing in this way the interference between them. One can show that this dumping effect goes to 0 as $1/\sqrt{t}$ for $t \to \infty$ and that the amplitude of oscillations is bounded by the Compton wavelength $\hbar/(mc)$ in usual dimensional units (a proof in one spatial dimension is provided in Ref. [35]).

For the Dirac walk in one space dimension we show here also the numerical evaluation of a Gaussian state peaked around some value k' of the wave vector. In the specific case we chose $k' = 0.01\pi$ and the mass parameter $m = 0.15$. The width of the Gaussian wave-packet in momentum space is $\sigma = 40^{-1}$. The state is chosen with an equal superposition of particle and antiparticle eigenstates, namely $c_+ = c_- = 1/\sqrt{2}$. In Fig. 9 we show the evolution of this state for $t = 150$ time-steps, where one can appreciate the oscillating behaviour.

For the Dirac walk in dimension $d = 3$ we show the in Fig. 10 the evolution of the mean position for a Gaussian wave-packet peaked around $\mathbf{k}' = (0, 0.01\pi, 0)$ with width $\sigma = 32^{-1}$. The mass parameter of the walk is $m = 0.3$.

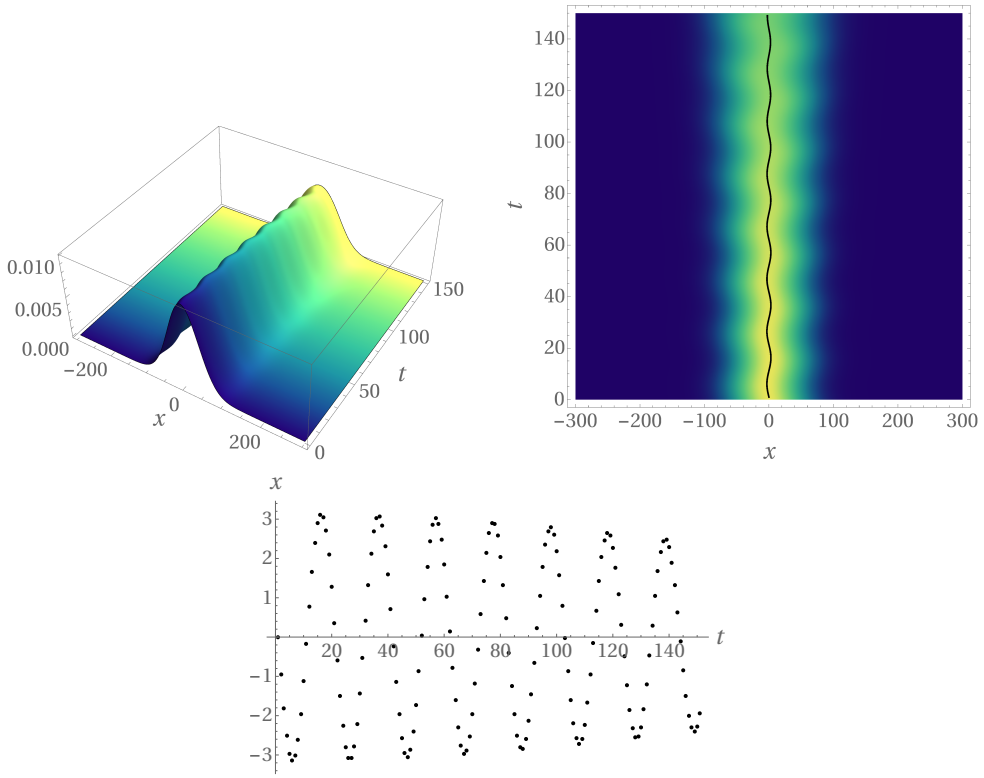


Figure 9.: The plots shows the evolution according to the Dirac QW in dimension $d = 1$ for $t = 150$ time-steps of a Gaussian state with both particle and an antiparticle eigenstates. The parameters are as follows: mass $m = 0.15$, width $\sigma = 40^{-1}$, mean wave vector $k' = 0.01\pi$, $c_+ = c_- = 1/\sqrt{2}$. Top: probability distribution of the position. Bottom: behaviour of the mean position.

We have seen that the position operator $\mathbf{X}$ mixes the positive- and negative-frequency components, as in QFT. However one can define, as in QFT, the operator $\mathbf{X}_{\mathrm{NW}}$, called Newton–Wigner position operator, that does not mix the particle and antiparticle components. We can see this by introducing the Foldy–Wouthuysen operator W_{FW} that provides the representation of the walk in which $H^D(\mathbf{k})$ is diagonal:

$$W_{\mathrm{FW}} = \int_B d\mathbf{k}\ |\mathbf{k}\rangle\langle\mathbf{k}| \otimes W_{\mathrm{FW}}(\mathbf{k}),$$
$$W_{\mathrm{FW}}^{-1}(\mathbf{k}) H^D(\mathbf{k}) W_{\mathrm{FW}}(\mathbf{k}) = \mathrm{diag}(\omega_{\mathbf{k}}, \omega_{\mathbf{k}}, -\omega_{\mathbf{k}}, -\omega_{\mathbf{k}}).$$

Accordingly, we can define the Newton–Wigner position operator, defined as

$$\mathbf{X}_{\mathrm{NW}} \coloneqq W_{\mathrm{FW}}^{-1} \mathbf{X} W_{\mathrm{FW}}.$$

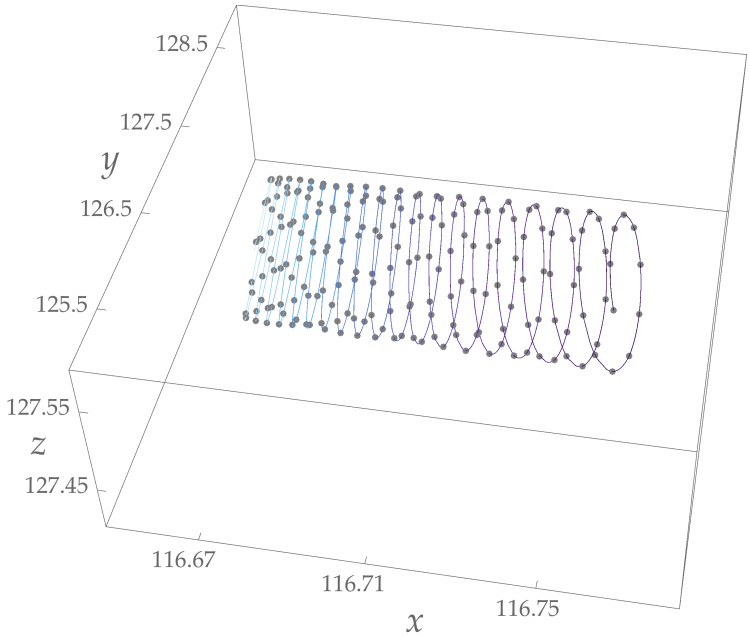


Figure 10.: The plot shows the mean-position evolution for the Dirac QW in dimension $d = 3$ for $t = 200$ time-steps. The state has both particle and antiparticle eigen. Here the states are Gaussian with parameters: mass $m = 0.3$, mean wave vector $\mathbf{k}' = (0, 0.01\pi, 0)$, width $\sigma = 32^{-1}$; the internal state is a superposition of $|u_{+,+}(k)\rangle$ and $|u_{-,+}(k)\rangle$, where these vectors are defined in Eq. (17). The time evolution is from left to right.

We can easily verify that the Newton–Wigner position operator does not present *Zitterbewegung*, as in the usual QFT; indeed, the velocity operator corresponds to the classical velocity operator:

$$\mathbf{V}_{NW}(t) = i[H^D, \mathbf{X}_{NW}(t)], \qquad \mathbf{V}_{NW}(k) = \hat{\mathbf{V}}(\mathbf{k}).$$

Consequently, since the acceleration vanish in this case, the evolution of $\mathbf{X}_{NW}$ is given by

$$\mathbf{X}_{NW}(t) = \mathbf{X}_{NW}(0) + \hat{\mathbf{V}}t,$$

showing in this way that the quivering behaviour disappears in the Foldy–Wouthuysen representation.

We have seen in this chapter the numerical evolution of gaussian states which show a particle-like behaviour satisfying a dispersive differential equation. For states which are superposition of particle and antiparticle components we provided the analysis of the behaviour of the position operator which exhibits the oscillating behaviour typical of the *Zitterbewegung* effect present in the Dirac theory. We also presented the evolution of a perfectly localized state in three spatial dimension showing the shape of the causal cone of the Dirac walk.

4 DIRAC QW IN ONE SPATIAL DIMENSION

We introduced the concept of QCA and the related one of QW in Chapter 2, showing how these structures emerge from simple assumptions. We review here the solution of the Dirac QW in $1+1$ dimensions, for the Cayley graph $\Gamma(\mathbb{Z}, \mathcal{S})$, $\mathcal{S} = \{\pm 1, 0\}$. The general discussion about the Dirac QW has been given in Section 2.4. We provide the solution in position space via a path-sum, exploiting the algebraic properties of the walk transition matrices.

The Dirac QW of Refs. [40, 42] describes the one-step evolution of a two-component quantum field on the line

$$|\psi_x(t)\rangle = \begin{pmatrix} \psi_x^L(t) \\ \psi_x^R(t) \end{pmatrix}, \quad x, t \in \mathbb{Z},$$

ψ_x^L and ψ_x^R denoting the *left* and the *right* mode of the field, respectively. The Hilbert space of the walk is $\mathscr{H} = \mathbb{C}^2 \otimes \ell^2(\mathbb{Z})$ and we will employ the factorized basis $|a\rangle\,|x\rangle$, with $a = L, R$. The evolution of the walk is provided by the unitary operator W of the form

$$W = \sum_{h \in \mathcal{S}} A_h \otimes T_h = A_L \otimes S + A_R \otimes S^\dagger + A_F \otimes I,$$

where the transition matrices are given by

$$A_L = \begin{pmatrix} n & 0 \\ 0 & 0 \end{pmatrix}, \; A_R = \begin{pmatrix} 0 & 0 \\ 0 & n \end{pmatrix}, \; A_F = \begin{pmatrix} 0 & -im \\ -im & 0 \end{pmatrix}, \tag{27}$$

with $n^2 + m^2 = 1$, $n, m > 0$, and the shift operator S defined by

$$S = \sum_{x \in \mathbb{Z}} |x-1\rangle\langle x|\,.$$

Here we conveniently identify $R \equiv -1$, $L \equiv 1$ and $F \equiv 0$. The operator T_h denotes the right-regular representation of $\mathbb{Z}$ on $\ell^2(\mathbb{Z})$, namely $T_h\,|x\rangle = |x-h\rangle$. The matrices in Eq. (27) have been derived in Refs. [40, 42] from the assumptions of unitarity, locality, homogeneity and isotropy. The resulting walk is not a *coined* QW as discussed in Section 2.3.2, since it can not be factorized as $W = TC$, where T is the translation operator and C is the coin-flip operator.

4.1 PATH-SUM SOLUTION

In this section we provide a brief review of the solution obtained in Ref. [72]. Given an initial configuration $|\psi(0)\rangle \in \mathscr{H}$, the evolution of the state is given by the repeated application of the walk unitary: $|\psi(t)\rangle = W^t |\psi(0)\rangle$. In terms of the transition matrices the update rule is given by

$$|\psi_x(t+1)\rangle = \sum_{h\in\mathcal{S}} A_h |\psi_{x+h}(t)\rangle , \tag{28}$$

where $|\psi_x(t)\rangle \in \mathbb{C}^2$ denotes the state at site $x \in \mathbb{Z}$, namely

$$|\psi(t)\rangle = \sum_{x\in\mathbb{Z}} |x\rangle |\psi_x(t)\rangle .$$

By iterating Eq. (28), as shown in Section 2.5, we can express the state at time t in terms of the sum over the paths that join the sites in the past causal cone $\mathcal{C}_t(x)$ of a given site x:

$$|\psi_x(t)\rangle = \sum_{y\in\mathcal{C}_t(x)} \sum_{\sigma\in\Lambda_t(y,x)} \mathcal{A}(\sigma) |\psi_y(0)\rangle ,$$

where σ is a path on $\mathbb{Z}$ joining a site y to the site x in t time-steps. Representing the path σ with the sequence of successive steps $h_1 h_2 \dots h_t$, where each h_i is a transition in $\mathcal{S}$, the function $\mathcal{A}(\sigma)$ is given by the product of the transition matrices corresponding to the steps h_i:

$$\mathcal{A}(h_1, h_2, \dots, h_t) \coloneqq A_{-h_t} \cdots A_{-h_2} A_{-h_1} .$$

We remark that, following our convention, the matrix A_h is associated to the step $-h$.

Our aim is now to evaluate the sum over σ in order to compute the propagator defined by

$$\begin{aligned} \mathcal{K}(x, y; t) &\coloneqq \langle y|W^t|x\rangle \\ &= \sum_{\sigma\in\Lambda(x,y)} \mathcal{A}(\sigma) \end{aligned} \tag{29}$$

and representing the probability amplitude to go from x to y in t time-steps.

Each path σ is formed by arranging successive R, L, F steps. We denote by $\hat{r}(\sigma)$, $\hat{l}(\sigma)$, $\hat{f}(\sigma)$ their respective occurrence number, which satisfy the conditions

$$\begin{cases} \hat{r}(\sigma) + \hat{l}(\sigma) + \hat{f}(\sigma) = t, \\ \hat{r}(\sigma) - \hat{l}(\sigma) = x - y; \end{cases}$$

then, we can express $\hat{r}$ and $\hat{l}$ in terms of the coordinates on the lattice and the parameter $\hat{f}$ as

$$\hat{r}(\sigma) = \frac{t - \hat{f}(\sigma) + x - y}{2}, \quad \hat{l}(\sigma) = \frac{t - \hat{f}(\sigma) - x + y}{2}.$$

We now evaluate the sum over σ in Eq. (29) as a function of the variables x, y, t. By direct inspection, one can recognize that the products of the transition matrices are easily expressed by adopting a suitable binary encoding:

$$A_R = nA_{11}, \quad A_L = nA_{00}, \quad A_F = -im(A_{01} + A_{10}), \tag{30}$$
$$A_{00} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad A_{11} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$
$$A_{01} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad A_{10} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

With this convention, the matrices satisfy the following composition rule:

$$A_{ab}A_{cd} = \frac{1 + (-1)^{b \oplus c}}{2} A_{ad}, \tag{31}$$

the symbol $\oplus$ denoting the sum modulo 2. The mass term A_F plays a special role in the computation of the path-sum, since it determines which paths connecting two given points are admissible. From Eq. (31) we see that the resulting matrix $\mathcal{A}(\sigma)$ depends only on the first and the last bit of the path. As a consequence we can parameterize the sum over $\sigma \in \Lambda_t(y, x)$ by considering the paths with $\hat{f}(\sigma) = f$ and with resulting matrix A_{ab} denoted as $\mathfrak{F}_{t,ab}(f)$. Thus, the sum over paths becomes:

$$|\psi_x(t)\rangle = \sum_{y \in \mathcal{C}_t(x)} \sum_{a,b \in \{0,1\}} \sum_{f=0}^{t-|x-y|} \alpha(f) c_{ab}(f) A_{ab} |\psi_y(0)\rangle, \tag{32}$$

where $\alpha(f) \coloneqq (-im)^f n^{t-f}$ and $c_{ab}(f) \coloneqq |\mathfrak{F}_{t,ab}(f)|$ counts how many paths σ with $\hat{f}(\sigma) = f$ contribute to give the matrix A_{ab}.

The problem is now to obtain an explicit expression for the coefficients c_{ab}. Again, the product rule of Eq. (31) gives us a hint on how to proceed: an R (L) transition can be followed only by other transitions of the same kind or an F transition. An F transition flips the components of the internal state and after it the walker can only proceed to the left (to the right) with an L transition (R transition). In other words, a generic path with $f < t$ transitions of the F kind has the general form

$$\tau_1 \, F \, \tau_2 \, F \, \tau_3 \, F \, \ldots \, F \, \tau_{f-1} \, F \, \tau_f \, F \, \tau_{f+1}.$$

The F transitions identify $f+1$ slots τ_i and, as we remarked, there are two classes of paths: the ones having any one of the odd slots τ_{2i+1} filled with R transitions and the ones having any one of the odd slots filled with L transitions. We denote the first class as $\Omega_R(f)$ and the second one as $\Omega_L(f)$, which are clearly disjoint if $f < t$. In order to compute the coefficients c_{ab}, it is convenient to separate the case of f even from then case of f odd. As one can readily check, we have that $c_{aa}(2f+1) = c_{01}(2f) = c_{10}(2f) = 0$. Moreover, only paths coming from $\Omega_R(2f)$ contribute to $c_{00}(2f)$, and, analogously, only paths in $\Omega_L(2f)$ contribute to $c_{11}(2f)$; the same goes in the odd case: $c_{01}(2f+1)$ counts paths in $\Omega_R(2f+1)$, while $c_{10}(2f+1)$ counts paths in $\Omega_L(2f+1)$. For $f = t$, the resulting matrix is $A_{00} + A_{11}$ when t is even and it is $A_{01} + A_{10}$ in the odd case.

At this point we are able to write the general expression for the coefficients $c_{ab}(f)$ (for any f):

$$c_{ab}(f) = \binom{\Delta_+ - \nu_{ab}}{\frac{f-1}{2} - \nu_{ab}} \binom{\Delta_- + \nu_{ab}}{\frac{f-1}{2} + \nu_{ab}}, \tag{33}$$

$$\Delta_\pm = \frac{t \pm (x-y) - 1}{2}, \quad \nu_{ab} = \frac{ab - \bar{a}\bar{b}}{2},$$

where $\bar{a} \coloneqq 1 - a$, and the binomials vanish for non integer arguments. Such an expression for the coefficients is justified by studying the combinatorial properties of the paths.

Let us start from the even case with $\hat{f}(\sigma) = 2f$, $r \coloneqq \hat{r}(\sigma)$ and $l \coloneqq \hat{l}(\sigma)$. If $\sigma \in \Omega_R(2f)$, we can extract two substrings of the form

$$\rho = R \ldots R\, F\, R \ldots R\, F\, R \ldots R,$$
$$\lambda = L \ldots L\, F\, L \ldots L,$$

with $\hat{r}(\rho) = r$, $\hat{f}(\rho) = f$, $\hat{l}(\lambda) = l$, and $\hat{f}(\lambda) = f - 1$. The coefficient $c_{00}(2f)$ is now easily computed since it is given by the product of the number of ρ and λ strings. The number of ρ strings can be computed with the method of *stars and bars* [109]: the number of strings is given by the number of permutations of $r + f$ and $l + f - 1$ symbols, respectively for ρ and λ strings. Analogously, we obtain the result for c_{11}, and therefore we have:

$$c_{00}(2f) = \binom{r+f}{f}\binom{l+f-1}{f-1} = \binom{\frac{t+x-y}{2}}{f}\binom{\frac{t-x+y}{2}-1}{f-1},$$
$$c_{11}(2f) = \binom{l+f}{f}\binom{r+f-1}{f-1} = \binom{\frac{t-x+y}{2}}{f}\binom{\frac{t+x-y}{2}-1}{f-1}.$$

The number of occurrences of the matrices A_{01} and A_{10} is counted in the same way. These matrices can only appear if $\hat{f}(\sigma) = 2f + 1$. In this case, the two substrings ρ and λ have the same number of F symbols given

by f. Considering separately the permutations of the symbols in the two substrings, we obtain the counting

$$c_{01}(2f+1) = c_{10}(2f+1) = \binom{r+f}{f}\binom{l+f}{f} = \binom{\frac{t+x-y-1}{2}}{f}\binom{\frac{t-x+y-1}{2}}{f}.$$

The analytical solution of the Dirac QW can be expressed in a compact form in terms of Jacobi polynomials $P_k^{(\zeta,\rho)}(z)$ computing the sum over f in Eq. (32):

$$|\psi_x(t)\rangle = \sum_{y\in\mathcal{C}_t(x)} \sum_{a,b\in\{0,1\}} \gamma_{ab} P_k^{(\overline{a\oplus b},-t)}\left(1+2\left(\frac{m}{n}\right)^2\right) A_{ab}\,|\psi_y(0)\rangle\,,$$

where $k \coloneqq \Delta_- - (ab+\bar{a}\bar{b})/2$, and

$$\gamma_{ab} \coloneqq -i^{a\oplus b} n^t \left(\frac{m}{n}\right)^{2-a\oplus b}\left(\frac{\Delta_+ + \frac{1}{2}}{\Delta_- + \frac{1}{2}}\right)^{1-ab},$$

assuming that $\gamma_{aa} = 0$ for $t+x-y$ odd and $\gamma_{01} = \gamma_{10} = 0$ for $t+x-y$ even.

We remark that for $x = t$ the only non-zero coefficient is c_{00} with $f = 0$. Substituting the expression of Eq. (33) we have $c_{00}(0) = 1$ and, choosing as initial state $|\psi_y(0)\rangle = \delta_{y,0}\,|\varphi\rangle$ with $|\varphi\rangle \in \mathbb{C}^2$, the state after t time-steps is given by

$$|\psi_t(t)\rangle = n^t \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} |\varphi\rangle\,.$$

Analogously, for $x = -t$ the only non-zero coefficient is c_{11} and thus we have

$$|\psi_{-t}(t)\rangle = n^t \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} |\varphi\rangle\,.$$

In this chapter we reviewed the solution of the Dirac QW in position space of Ref. [72]. The solution is obtained exploiting the path-sum method and the algebraic properties of the transition matrices, solving the combinatorial problem of counting the number of paths contributing with the same matrix. The result obtained here fits into the literature of solved QWs on the line: the coined QW [17] and the disordered coined QW [110]. We should also mention the solution of Kauffman and Noyes [69] to the Feynman checkerboard problem [66] obtaining a solution of the finite-difference Dirac equation for a fixed value of the mass. The approach of Kauffman

and Noyes simplifies previous attempts [67, 68]. We remark that the Feynman checkerboard problem is a different discretization approach from the one provided by the QW framework. Indeed, this is due to the fact that finite-difference equations—lacking, in general, strict unitary evolution—do not have a corresponding description in terms of QWs. As a future perspective, it would be interesting to study in position space the behaviour of the causal cone providing a better understanding of the dynamical properties of the walk.

5 WEYL QW IN TWO SPATIAL DIMENSIONS

We continue the discussion on the path-sum solution for quantum walks by presenting in this chapter a review of the solution for the Weyl QW in $2+1$ dimensions derived in Ref. [73].

The Weyl QW of Ref. [40] is the only unitary quantum walk satisfying the principles of locality, homogeneity and isotropy, with minimal computational complexity, that can be embedded in the two-dimensional Euclidean space [40, 65, 94]. The Weyl QW is defined on the Cayley graph of the group $\mathbb{Z}^2$, considered as the free Abelian group with two generators, say $R \equiv h_1 \coloneqq (1,0)$ and $U \equiv h_2 \coloneqq (0,1)$. The unitary operator W governing its dynamics acts on the Hilbert space $\mathscr{H} = \ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^2$ and the generic state of the walk is denoted as $|\psi\rangle = \sum_{x\in\mathbb{Z}^2} |x\rangle\,|\psi_x\rangle$, with $|\psi_x\rangle \in \mathbb{C}^2$ being the state at the site $x \in \mathbb{Z}^2$.

The walk unitary can be expressed in terms of the transition matrices as

$$W = \frac{1}{2}\sum_{h\in\mathcal{S}} T_h \otimes A_h, \tag{34}$$

where $\mathcal{S} = \{R, L, U, D\}$, with $L = -R$ and $D = -U$, and the transition matrices are given by

$$\begin{aligned} A_R &= \begin{pmatrix} 1 & 0 \\ -\nu & 0 \end{pmatrix}, \qquad A_U = \begin{pmatrix} 1 & 0 \\ \nu & 0 \end{pmatrix}, \\ A_L &= \begin{pmatrix} 0 & \nu^* \\ 0 & 1 \end{pmatrix}, \qquad A_D = \begin{pmatrix} 0 & -\nu^* \\ 0 & 1 \end{pmatrix}, \end{aligned} \tag{35}$$

with $|\nu| = 1$. Without loss of generality we assume $\nu = 1$. As before, T_h denotes the right-regular representation of $\mathbb{Z}^2$ on $\ell^2(\mathbb{Z}^2)$.

5.1 PATH-SUM SOLUTION

As for the one dimensional case of Chapter 4 we seek now an expression for the propagator $\mathcal{K}(\mathbf{x}', \mathbf{x}; t)$ of the Weyl QW in $d = 2$, which determines the probability amplitude to go from a site $\mathbf{x}'$ to a site $\mathbf{x}$ in t time-steps. The state is expressed in terms of the propagator by the following equation:

$$|\psi_{\mathbf{x}}(t)\rangle = \sum_{\mathbf{x}'\in\mathcal{C}_t(\mathbf{x})} \mathcal{K}(\mathbf{x}', \mathbf{x}; t)\,|\psi_{\mathbf{x}'}(0)\rangle\,,$$

where $|\psi(0)\rangle$ is the initial state. In terms of the transition matrices the propagator can be written as a path-sum:

$$\begin{aligned}\mathcal{K}(\mathbf{x}',\mathbf{x};t) &\coloneqq \langle \mathbf{x}|W^t|\mathbf{x}'\rangle \\ &= \frac{1}{2^t}\sum_{\sigma\in\Lambda_t(\mathbf{x}',\mathbf{x})}\mathcal{A}(\sigma),\end{aligned} \tag{36}$$

with $\mathcal{A}(\sigma)$ the generic product of the transition matrices associated to the path σ:

$$\mathcal{A}(\mathbf{h}_1,\mathbf{h}_2,\ldots,\mathbf{h}_t) \coloneqq A_{-\mathbf{h}_t}\cdots A_{-\mathbf{h}_2}A_{-\mathbf{h}_1}.$$

As in Section 2.5, the set $\Lambda_t(\mathbf{x}',\mathbf{x})$ is the set of paths of length t starting from the site $\mathbf{x}' \in \mathbb{Z}^2$ and ending in the site $\mathbf{x} \in \mathbb{Z}^2$.

In order to solve the path-sum of Eq. (36), we need to exploit the algebraic properties of the transition matrices, as we did in dimension $d = 1$ (see Section 4.1). The composition rule of the matrices can be expressed in a very simple way by introducing a 2-bit encoding: $R \to 00$, $L \to 11$, $U \to 10$, and $D \to 01$. In this way, the product of the matrices is given by

$$A_{ab}A_{cd} = (-1)^{(c\oplus a)(d\oplus b)}A_{cb}, \tag{37}$$

where the symbol $\oplus$ denotes the sum modulo 2. Throughout the manuscript, all the bit operations are also extended element-wise to binary strings. We remark that the composition rule of Eq. (37) entails that the set of transition matrices generate a semigroup. The binary encoding of the single steps induces a binary representation of the paths: a path σ of length t is encoded in a pair $(w^{(1)},w^{(2)})$ of binary strings, $w^{(j)}$ being the string made of the j-th bits of the encoding. We denote the set of all the binary strings of length t as $\mathfrak{B}_t \coloneqq \{0,1\}^t$ and the set of the strings with a fixed number of 1-bits as

$$\mathfrak{S}_t(K) \coloneqq \{\, w \in \mathfrak{B}_t \mid \iota(w) = K \,\}, \tag{38}$$

where, denoting with $|w|$ the length of the string w, $\iota(w) \coloneqq \sum_{k=1}^{|w|} w_k$ represents the Hamming weight of the string w and w_k denotes the k-th bit of w. In terms of $\mathfrak{S}_T(K)$, n-tuples of binary strings are defined by

$$\mathfrak{S}_t^n(K_1,\ldots,K_n) \coloneqq \mathfrak{S}_t(K_1)\times\cdots\times\mathfrak{S}_t(K_n). \tag{39}$$

From Eq. (37) it is easy to extend the composition rule to the product of an arbitrary number of matrices. For a path $\sigma = (w^{(1)},w^{(2)})$ the resulting matrix is given by

$$\mathcal{A}\left(w^{(1)},w^{(2)}\right) = (-1)^{(\overline{w}^{(1)}\oplus S\overline{w}^{(1)})\overline{w}^{(2)}}A_{\overline{w}_1^{(1)}\overline{w}_t^{(2)}}, \tag{40}$$

where $z^w := z^{\iota(w)}$ and we introduced the left circular shift S defined by $(Sw)_i = w_{(i \bmod t)+1}$, for all $i \in \{1, \dots, t\}$. Notice that in Eq. (40) the strings are negated since the matrix associated to the step $\mathbf{h}$ is exactly $A_{-\mathbf{h}}$, and, in terms of strings, this corresponds to negate the bits of the binary encoding.

Denoting as $\hat{r}(\sigma)$, $\hat{l}(\sigma)$, $\hat{u}(\sigma)$, $\hat{d}(\sigma)$ the number of occurrences of R, L, U, D steps in the path $\sigma \in \Lambda_t((x_1', x_2'), (x_1, x_2))$, it is straightforward to prove that the following conditions are satisfied (for $t - |x_1 - x_1'| - |x_2 - x_2'|$ even)

$$\begin{cases} \hat{r}(\sigma) - \hat{l}(\sigma) = x_1 - x_1', \\ \hat{u}(\sigma) - \hat{d}(\sigma) = x_2 - x_2', \\ \hat{r}(\sigma) + \hat{l}(\sigma) + \hat{u}(\sigma) + \hat{d}(\sigma) = t. \end{cases} \tag{41}$$

Furthermore, the Hamming weight of the path σ is related to the parameters r, l, u and d via the equations

$$\begin{cases} \iota(w^{(1)}) = \hat{l}(\sigma) + \hat{u}(\sigma), \\ \iota(w^{(2)}) = \hat{l}(\sigma) + \hat{d}(\sigma). \end{cases}$$

By using the relations of Eq. (41), we see that

$$\begin{aligned} \iota(w^{(1)}) - \iota(w^{(2)}) &= \hat{u}(\sigma) - \hat{d}(\sigma) = x_2 - x_2', \\ \iota(w^{(1)}) + \iota(w^{(2)}) &= t - (\hat{r}(\sigma) - \hat{l}(\sigma)) = t - (x_1 - x_1'), \end{aligned}$$

which finally gives

$$\begin{cases} \iota(w^{(1)}) = \frac{1}{2}(t - (x_1 - x_1') + (x_2 - x_2')), \\ \iota(w^{(2)}) = \frac{1}{2}(t - (x_1 - x_1') - (x_2 - x_2')). \end{cases} \tag{42}$$

As a consequence of this result, the admissible paths σ connecting $\mathbf{x}' = (x_1', x_2')$ to $\mathbf{x} = (x_1, x_2)$ are precisely those having a fixed number of 1-bits, according to Eq. (42), and are obtained by independent permutations of the bits of the encoding-strings $w^{(1)}$ and $w^{(2)}$.

In terms of the binary strings, the propagator $\mathcal{K}$ can be rewritten as

$$\begin{aligned} \mathcal{K}(\mathbf{x}', \mathbf{x}; t) &= \frac{1}{2^t} \sum_{\sigma \in \Lambda_t(\mathbf{x}', \mathbf{x})} \mathcal{A}(\sigma) \\ &= \frac{1}{2^t} \sum_{\boldsymbol{w} \in \mathfrak{S}_t^2(K_1, K_2)} (-1)^{(\overline{w}^{(1)} \oplus S\overline{w}^{(1)})\overline{w}^{(2)}} A_{\overline{w}_1^{(1)} \overline{w}_t^{(2)}} \\ &= \frac{1}{2^t} \sum_{\boldsymbol{w} \in \mathfrak{S}_t^2(t-K_1, t-K_2)} (-1)^{(w^{(1)} \oplus Sw^{(1)})w^{(2)}} A_{w_1^{(1)} w_t^{(2)}}, \end{aligned} \tag{43}$$

where $\boldsymbol{w} = (w^{(1)}, w^{(2)})$, $K_1 = (t - (x_1 - x_1') + (x_2 - x_2'))/2$, and $K_2 = (t - (x_1 - x_1') - (x_2 - x_2'))/2$. Therefore, since the resulting matrix depends only

on the first bit of $w^{(1)}$ and the last bit of $w^{(2)}$, we can collect together all the paths giving the same matrix:

$$\mathcal{K}(\mathbf{x}', \mathbf{x}; t) = \frac{1}{2^t} \sum_{a,b\in\{0,1\}} c_{ab}(t - K_1, t - K_2) A_{ab},$$

where the coefficients c_{ab} are defined by

$$c_{ab}(K_1, K_2) \coloneqq \sum_{w\in\mathfrak{S}^2_{t,ab}(K_1,K_2)} (-1)^{(w^{(1)}\oplus Sw^{(1)})w^{(2)}}, \tag{44}$$

and $\mathfrak{S}^2_{t,ab}(K_1, K_2) \subset \mathfrak{S}^2_t(K_1, K_2)$ is the subset of pairs $(w^{(1)}, w^{(2)})$ with $w^{(1)}_1 = a$ and $w^{(2)}_t = b$.

The computation of the coefficients c_{ab} can be done by exploiting the combinatorial properties of the binary strings. To this end, it is convenient to define a canonical form for strings.

Definition 5.1.1. We say that a binary string w is in *canonical form* if the following condition holds:

$$w_i \geqslant w_{i+1} \quad \forall i \in \{1, 2, \ldots, |w| - 1\}.$$

The main result of this chapter relies on a number of general results which we present in the following. The complete proofs of the results of this chapter are given in Appendix A. We denote with $v \frown w$ the concatenation of binary strings, which is extended naturally for A and B subsets of $\mathfrak{B}_t$:

$$A \frown B \coloneqq \{\, v \frown w \in \mathfrak{B}_t \mid v \in A,\ w \in B \,\}.$$

Lemma 5.1.1. *Take* $t, K, H \in \mathbb{N}$, *with* $K, H \leqslant t$, *and let* $v \in \mathfrak{S}_t(K)$ *be in canonical form. Then the string* v *induces a partition on* $\mathfrak{S}_t(H)$*:*

$$v \oplus \mathfrak{S}_t(H) = \bigcup_{n\in I} \mathfrak{W}(K, H, n),$$

$$\mathfrak{W}(K, H, n) \coloneqq \begin{cases} \mathfrak{S}_K(K - H + n) \frown \mathfrak{S}_{t-K}(n), & \text{if } K \geqslant H, \\ \mathfrak{S}_K(n) \frown \mathfrak{S}_{t-K}(H - K + n), & \text{otherwise,} \end{cases}$$

with $I = \{0, 1, \ldots, \min\{K, H, t - K, t - H\}\}$. *Defining* $r = \vartheta(K - H)$ *and* $\bar{r} = 1 - r$, *the size of each subset is given by*

$$|\mathfrak{W}(K, H, n)| = D(t, \bar{r}t + (-1)^{\bar{r}}H, rt + (-1)^{r}K, n),$$

$$D(t, p, m, n) \coloneqq \begin{cases} \binom{m}{n}\binom{t-m}{p-n}, & \text{if } 0 \leqslant n \leqslant m \leqslant t \text{ and } n \leqslant p, \\ 0, & \text{otherwise,} \end{cases}$$

and for all $w \in \mathfrak{W}(K, H, n)$ *the Hamming weight is given by* $\iota(w) = |K - H| + 2n$.

Corollary 5.1.1. *Given* K, H *as in Lemma 5.1.1, for all* $v \in \mathfrak{S}_t(K)$ *and for any* π_v *bitwise permutation of* $\mathfrak{B}_t$ *such that* $\pi_v(v)$ *is in canonical form, the following decomposition holds:*

$$v \oplus \mathfrak{S}_t(H) = \bigcup_{n \in I} \pi_v^{-1}(\mathfrak{W}(K, H, n))$$

with $I = \{0, 1, \ldots, \min\{K, H, t-K, t-H\}\}$ *and moreover*

$$|\pi_v^{-1}(\mathfrak{W}(K, H, n))| = |\mathfrak{W}(K, H, n)|,$$
$$\iota(\pi_v^{-1}(\mathfrak{W}(K, H, n))) = \iota(\mathfrak{W}(K, H, n)).$$

From Eq. (44) it is apparent that we need to find a classification of binary strings v and w according to the sign $(-1)^{(v \oplus Sv)w}$, which depends only on the parity of the Hamming weight of $(v \oplus Sv)w$. In order to aid the discussion, it is convenient to consider separately the classification induced by the functions $v \oplus Sv$ and $v'w$. So, let us start from the function $v \oplus Sv$. The following Lemma specialize the result of Corollary 5.1.1 to this case.

Lemma 5.1.2. *Let* $v \in \mathfrak{S}_t(K)$. *Then* $v \oplus Sv \in \pi_v^{-1}(\mathfrak{S}_K(n) \frown \mathfrak{S}_{t-K}(n))$, *for some* $n \in \{0, 1, \ldots, \min\{K, t-K\}\}$.

The result of Lemma 5.1.2 is not accurate to encompass the complete classification of the function $v \oplus Sv$ since in the summation of Eq. (44) the strings $w^{(1)}$ and $w^{(2)}$ must have, respectively, the first and the last bit fixed. Therefore, let us consider strings $v \in \mathfrak{S}_t(K)$ such that $v \oplus Sv \in \pi_v^{-1}(\mathfrak{S}_K(n) \frown \mathfrak{S}_{t-K}(n))$ with both the first and the last bit fixed, say $v_1 = a$ and $v_t = a'$. The set of all such strings is denoted as $\mathfrak{T}_{aa'}(t, K, n)$. The refined counting of Lemma 5.1.2 is then given by the following result (whose proof is given in Appendix A).

Lemma 5.1.3. *Taking* n *such that*

$$n_{\min}(K) \leqslant n \leqslant n_{\max}(K),$$

with $n_{\min}(K) \coloneqq \min\{1, K, t-K\}$ *and*

$$n_{\max}(K) \coloneqq \begin{cases} \min\{K - aa', t - K - 1 + aa'\}, & \text{if } 1 < K < t-1, \\ 1, & \text{if } K = 1 \text{ or } K = t-1, \\ 0, & \text{otherwise,} \end{cases}$$

the number $u_{aa'}(n)$ *of binary strings* $v \in \mathfrak{T}_{aa'}(t, K, n)$ *is given by*

$$u_{aa'}(n) = C_{K, n+aa'} C_{t-K, n+\bar{a}\bar{a}'},$$

where $C_{K,n}$ *is defined as*

$$C_{K,n} \coloneqq \begin{cases} \binom{K-1}{n-1}, & \text{if } K \geqslant n > 0, \\ 1, & \text{if } K = n = 0, \\ 0, & \text{otherwise.} \end{cases}$$

So far we have considered only the sum modulo 2 in $(v \oplus Sv)w$; the final counting is then obtained by considering that the Hamming weight of $(v \oplus Sv)w$ is given by the 1-bits of $v \oplus Sv$ selected via the string w. Since $v \in \mathfrak{T}_{aa'}(t, K_1, n)$ has fixed endpoints, we write formally $v = a\widetilde{v}a'$. Notice that we can write in a formal way $S(a\widetilde{v}a') = \widetilde{v}a'a$ and $|\widetilde{v}| = t-2$. Analogously, $w = \widetilde{w}b$, with $|\widetilde{w}| = t-1$ and $\iota(\widetilde{w}) = \iota(w) - b$. In this way we obtain

$$\begin{aligned} \iota[(v \oplus Sv)w] &= \iota[(a\widetilde{v}a' \oplus \widetilde{v}a'a)(\widetilde{w}b)] \\ &= \iota[(a\widetilde{v} \oplus \widetilde{v}a')\widetilde{w}] + (a \oplus a')b, \end{aligned}$$

and hence the expression for the coefficients c_{ab} is given by

$$c_{ab}(K_1, K_2) = \sum_{a'=0,1} \sum_{n=n_{\min}(K_1)}^{n_{\max}(K_1)} \sum_{\widetilde{v},\widetilde{w}} (-1)^{(a\oplus a')b} (-1)^{(a\widetilde{v}\oplus\widetilde{v}a')\widetilde{w}}. \tag{45}$$

The sign in the above expression is independent of permutation of the binary strings. Indeed, consider a bitwise permutation π_n of $\mathfrak{B}_{t-1}$ such that $\pi_n(a\widetilde{v} \oplus \widetilde{v}a') = c_n \in \mathfrak{S}_{t-1}(2n)$ with c_n canonical. Then we can write

$$(-1)^{\pi_n^{-1}(c_n)\widetilde{w}} = (-1)^{\pi_n^{-1}(c_n \pi_n(\widetilde{w}))} = (-1)^{c_n \pi_n(\widetilde{w})}$$

and therefore the sum over $\widetilde{v}$ in Eq. (45) gives precisely

$$u_{aa'}(n) = |\mathfrak{T}_{aa'}(t, K_1, n)|,$$

so that we obtain

$$c_{ab}(K_1, K_2) = \sum_{a' \in \{0,1\}} \sum_{n=n_{\min}(K_1)}^{n_{\max}(K_1)} (-1)^{(a\oplus a')b} u_{aa'}(n) \sum_{\widetilde{w}} (-1)^{c_n \widetilde{w}}. \tag{46}$$

The last sum can be performed by considering in how many ways one can select k bits, $0 \leqslant k \leqslant \mu$, $\mu \coloneqq 2n - a \oplus a'$, from the string c_n, for fixed n. This is tantamount to consider the following partition of the set $\mathfrak{S}_{t-1}(K_2 - b)$

$$\mathfrak{S}_{t-1}(K_2 - b) = \bigcup_{k=0}^{\mu} \mathfrak{S}_{\mu}(k) \mathfrak{S}_{t-\mu-1}(K_2 - k - b),$$

and the size of each subset is denoted as $w_{aa'b}(n,k)$:

$$\begin{aligned} w_{aa'b}(n,k) &\coloneqq |\mathfrak{S}_\mu(k)| \cdot |\mathfrak{S}_{t-\mu-1}(K_2-k-b)| \\ &= \binom{\mu}{k}\binom{t-\mu-1}{K_2-k-b}. \end{aligned}$$

The expression for the coefficients c_{ab} finally becomes:

$$c_{ab}(K_1,K_2) = \sum_{a'\in\{0,1\}} \sum_{n=n_{\min}(K_1)}^{n_{\max}(K_1)} \sum_{k=0}^{\mu} (-1)^{k+(a\oplus a')b} u_{aa'}(n) w_{aa'b}(n,k). \quad (47)$$

As a final remark on this result, the sum over k in Eq. (47) can be evaluated in terms of the hypergeometric function ${}_2F_1(a,b,c,z)$ as follows:

$$\sum_{k=0}^{\infty} (-1)^k w_{aa'b}(n,k) = \binom{t-\mu-1}{K_2-b} {}_2F_1(-K_2+b,-\mu,t-K_2-\mu+b,-1).$$

So, letting

$$F_{aa'b}(n) \coloneqq {}_2F_1(-K_2+b,-\mu,t-K_2-\mu+b,-1),$$

the coefficients c_{ab} can be written in the equivalent form:

$$c_{ab}(K_1,K_2) = \sum_{a'\in\{0,1\}} \sum_{n=n_{\min}(K_1)}^{n_{\max}(K_1)} (-1)^{(a\oplus a')b} \binom{t-\mu-1}{K_2-b} u_{aa'}(n) F_{aa'b}(n).$$

This concludes the computation of the propagator $\mathcal{K}(x',x;t)$ of the Weyl QW in $2+1$ dimensions. The analytical solution that we have obtained provides the first example of path-sum solution of a QW in two spatial dimensions, opening also the possibility of studying other walk in $2+1$ dimensions. Furthermore, a deeper analysis of the results is necessary, such as the scaling behaviour and the study of the causal cone evolution, and will be matter of future work.

In this chapter we have seen how the solution of the Weyl QW in dimension $d = 2$ can be obtained in position space. The solution relies on the semigroup property of the transition matrices and the topological properties of the lattice paths that can be encoded in binary strings. This approach allowed us to simplify the combinatorial problem of counting the number of paths contributing with the same transition matrix.

As a future perspective, it would be interesting to study also the massive case. The matrices for the Dirac walk in two spatial dimensions generate a closed algebra as well, meaning that it is likely that the path-sum can be successfully solved. The added complexity in this case is due to the presence of the mass term which makes the classification of the paths

contributing with the same matrix more involved. Nevertheless, one can expect that the results for the massless case prove to be relevant also in the massive case, simplifying in this way the computation of the propagator.

6 WEYL QW IN THREE SPATIAL DIMENSIONS

We reviewed in Chapters 4 and 5 the path-sum solutions of Refs. [72, 73] for the Dirac QW in $1+1$ dimensions and for the Weyl QW in $2+1$ dimensions. Now we present the continuation of these previous works by providing an analytical solution in position space of the Weyl QW in $3+1$ dimensions [74]. The solution deeply relies on the results of Chapter 5 since the structure of the transition matrices is similar; in fact, the product rule is modified by a phase factor that depends only on the Hamming weight of the binary strings involved.

The Weyl QW of Ref. [40] in $3+1$ dimensions is the only unitary quantum walk satisfying the principles of locality, homogeneity and isotropy, with minimal computational complexity, that can be embedded in the two-dimensional Euclidean space [40, 65, 94]. The walk is defined on a Cayley graph of the group $\mathbb{Z}^3$; in particular, the solution exists only for the BCC lattice $\Gamma(G, \mathcal{S}_+)$, where a convenient choice for the vertex set is $G = 2\mathbb{Z}^3 \cup (2\mathbb{Z}^3 + \mathbf{t})$, $\mathbf{t} = (1,1,1)$; moreover, the generating set is $\mathcal{S}_+ \coloneqq \{\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \mathbf{h}_4\}$ with

$$\mathbf{h}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{h}_2 = \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix}, \quad \mathbf{h}_3 = \begin{pmatrix} -1 \\ 1 \\ -1 \end{pmatrix}, \quad \mathbf{h}_4 = \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}.$$

The evolution is provided by the unitary operator $W = \sum_{\mathbf{h}\in\mathcal{S}} T_{\mathbf{h}} \otimes A_{\mathbf{h}}$ ($\mathcal{S} \coloneqq \mathcal{S}_+ \cup \mathcal{S}_-$ and $\mathcal{S}_- \coloneqq \mathcal{S}_+^{-1}$), acting on $\mathscr{H} = \ell^2(G) \otimes \mathbb{C}^2$, and the transition matrices are

$$\begin{aligned}
A_{\mathbf{h}_1} &= \zeta^* \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, & A_{\mathbf{h}_{-1}} &= \zeta \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}, \\
A_{\mathbf{h}_2} &= \zeta^* \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, & A_{\mathbf{h}_{-2}} &= \zeta \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \\
A_{\mathbf{h}_3} &= \zeta^* \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}, & A_{\mathbf{h}_{-3}} &= \zeta \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \\
A_{\mathbf{h}_4} &= \zeta^* \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, & A_{\mathbf{h}_{-4}} &= \zeta \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix},
\end{aligned}$$

with $\zeta = \frac{1\pm i}{4}$ and $\mathbf{h}_{-l} = -\mathbf{h}_l$. The two possible choices for the coefficient ζ correspond to the two inequivalent QW solutions existing on the BCC

lattice [40]. The state of the walk is written as $|\psi\rangle = \sum_{x\in G} |x\rangle\,|\psi_x\rangle$, where we denote with $|\psi_x\rangle \in \mathbb{C}^2$ the state at site $x \in G$.

6.1 COMPOSITION RULE OF THE TRANSITION MATRICES

The path-sum in the case of the Weyl QW in $d = 3$ can be studied in a very similar way as we did for the Weyl QW in $d = 2$. This is due to the algebraic properties of the transition matrices which are essentially the same. We employ also in this case a binary encoding for the generators $h \in \mathcal{S}$ so as the composition rule of the matrices takes a very simple form. Being the $|\mathcal{S}| = 8$, it is sufficient to find a three-bit encoding $b_1b_2b_3$: the binary functions involved in the evaluation of the path-sum take a convenient form with the identifications

$$\begin{aligned} &h_1 \to 011, \quad h_2 \to 110, \quad h_3 \to 101, \quad h_4 \to 000, \\ &h_{-1} \to 100, \quad h_{-2} \to 001, \quad h_{-3} \to 010, \quad h_{-4} \to 111. \end{aligned} \tag{48}$$

Accordingly, the transition matrices are encoded as

$$\widetilde{A}_{b_1b_2b_3} = (\pm i)^{b_1\oplus b_2\oplus b_3} B_{b_1b_2}, \qquad \widetilde{A}_{b_1b_2b_3} \coloneqq (\zeta^*)^{-1} A_{b_1b_2b_3},$$

where the matrices $B_{b_1b_2}$ are precisely the matrices of Chapter 5, with also the same encoding:

$$B_{00} = \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \qquad B_{10} = \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix},$$
$$B_{01} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \qquad B_{11} = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}.$$

Hence, the product rule for $B_{b_1b_2}$ is (as in Chapter 5):

$$B_{ab}B_{cd} = (-1)^{(c\oplus a)(d\oplus b)} B_{cb}.$$

Consequently, the transition matrices of the Weyl QW in $d = 3$ generate, up to phases, a finite semigroup, allowing for an effective solution of the path-sum. A path σ of length t on $\Gamma(G, \mathcal{S}_+)$ is represented by a triad of binary strings $(w^{(1)}, w^{(2)}, w^{(3)})$, with $w^{(j)} \in \mathfrak{B}_t$ the string made of the j-th

bits of the encoding (48). The product of the transition matrices associated to each step of a path $\sigma = (w^{(1)}, w^{(2)}, w^{(3)})$ can be written as

$$\begin{aligned}\widetilde{\mathcal{A}}\left(w^{(1)}, w^{(2)}, w^{(3)}\right) &\coloneqq \widetilde{A}_{\overline{w}_t^{(1)}\overline{w}_t^{(2)}\overline{w}_t^{(3)}} \cdots \widetilde{A}_{\overline{w}_1^{(1)}\overline{w}_1^{(2)}\overline{w}_1^{(3)}} \\ &= (-1)^{(\overline{w}^{(1)} \oplus S\overline{w}^{(1)})\cdot\overline{w}^{(2)}} (\pm i)^{\overline{w}^{(1)}\oplus\overline{w}^{(2)}\oplus\overline{w}^{(3)}} B_{\overline{w}_1^{(1)}\overline{w}_t^{(2)}}, \quad (49)\end{aligned}$$

where it is understood that $z^w \equiv z^{\iota(w)}$ and $\iota(w)$ is the Hamming weight of w defined as $\iota(w) \coloneqq \sum_{k=1}^{|w|} w_k$, w_k being the k-th bit of the string w. Recall that S denotes the left circular shift

$$(Sw)_k \coloneqq w_{(k \bmod |w|)+1}, \quad \forall k \in \{1, 2, \ldots, |w|\}.$$

6.2 PATH-SUM SOLUTION

In this section we present the derivation of the solution in position representation of the walk. Our aim is to obtain an expression for the evolution of a given initial configuration $|\psi(0)\rangle$—that is, we seek an expression for the propagator $\mathcal{K}(\mathbf{x}', \mathbf{x}; t)$ representing the probability amplitude to go from $\mathbf{x}'$ to $\mathbf{x}$ in t time-steps—exploiting the geometric and algebraic properties of the underlying graph as well as the semigroup property of the transition matrices. The state at time t can be written in terms of the propagator as

$$|\psi_{\mathbf{x}}(t)\rangle = \sum_{\mathbf{x}' \in \mathcal{C}_t(\mathbf{x})} \mathcal{K}(\mathbf{x}', \mathbf{x}; t)\, |\psi'_{\mathbf{x}}(0)\rangle\,,$$

$\mathcal{K}$ being the propagator of the Weyl QW for $d = 3$, defined as

$$\begin{aligned}\mathcal{K}(\mathbf{x}', \mathbf{x}; t) &\coloneqq \langle \mathbf{x}| W^t |\mathbf{x}'\rangle \\ &= \sum_{\sigma \in \Lambda_t(\mathbf{x}', \mathbf{x})} \mathcal{A}(\sigma), \quad (50)\end{aligned}$$

where $\mathcal{A}(\sigma)$ represents the product of the transition matrices associated to the steps of the path σ:

$$\mathcal{A}(\mathbf{h}_1, \mathbf{h}_2, \ldots, \mathbf{h}_t) \coloneqq A_{\mathbf{h}_t^{-1}} \cdots A_{\mathbf{h}_2^{-1}} A_{\mathbf{h}_1^{-1}}.$$

Again, following our convention, the matrix associated to a step $\mathbf{h}$ is $A_{\mathbf{h}^{-1}}$.

6.2.1 Characterization of the past causal cone

First of all we need to give a characterization of the points lying in the past causal cone $\mathcal{C}_t(\mathbf{x})$ of $\mathbf{x}$. To this end, we need to introduce the concept of

distance on the graph $\Gamma(G, \mathcal{S}_+)$, counting the minimum number of steps required to go from $\mathbf{x}'$ to $\mathbf{x}$. More formally this is given by

$$d(\mathbf{x}', \mathbf{x}) \coloneqq \inf_{\lambda \in \Lambda(\mathbf{x}', \mathbf{x})} l(\lambda),$$

where the infimum is taken over the set $\Lambda(\mathbf{x}', \mathbf{x})$ of paths starting at $\mathbf{x}'$ and ending in $\mathbf{x}$, and $l(\lambda)$ is the length of the path. The computation of the propagator (50), however, requires to consider paths of a given length t. A necessary condition, then, for a point $\mathbf{x}' \in G$ to lie in the past causal cone of $\mathbf{x} \in G$ is

$$\Delta_t(\mathbf{x}', \mathbf{x}) \coloneqq t - d(\mathbf{x}', \mathbf{x}) \geqslant 0.$$

Since G is Abelian, we can freely permute the steps of a path $\lambda = \mathbf{h}_1 \mathbf{h}_2 \dots \mathbf{h}_t$ without changing its endpoints. This meas that λ is characterized by a quadruple $(n_{\pm 1}, n_{\pm 2}, n_{\pm 3}, n_{\pm 4})$, $n_{\pm l}$ counting the number of steps in direction $\mathbf{h}_{\pm l}$, such that

$$\begin{cases} \sum_l (n_l - n_{-l}) h_{l,i} = x_i - x_i', \\ \sum_l (n_l + n_{-l}) = t. \end{cases} \tag{51}$$

Furthermore, introducing the number of steps in the positive- and negative-coordinate direction

$$\begin{aligned} x_i^+ &\coloneqq \sum_l [\vartheta(h_{l,i}) n_l + \vartheta(h_{-l,i}) n_{-l}], \\ x_i^- &\coloneqq \sum_l [\vartheta(-h_{l,i}) n_l + \vartheta(-h_{-l,i}) n_{-l}], \end{aligned}$$

ϑ being the Heaviside step function, for each $i = 1, 2, 3$ it holds that

$$\begin{cases} x_i^+ + x_i^- = t, \\ x_i^+ - x_i^- = x_i - x_i'. \end{cases} \tag{52}$$

Consequently, from Eq. (52), any closed path (*i.e.* a *cycle*), for which $\mathbf{x} = \mathbf{x}'$, should have an even number of steps. Suppose now that the distance of $\mathbf{x}$ from the origin is d and consider a permuted path

$$\lambda' = \mathbf{h}_1' \dots \mathbf{h}_d' \mathbf{h}_{d+1}' \dots \mathbf{h}_t'$$

such that the first d steps realize the distance. Hence, the other $t - d$ steps constitute a cycle joining $\mathbf{x}$ to itself, and the quantity $t - d$ must be even. Since this holds in general, we have that $\mathbf{x}' \in \mathcal{C}_t(\mathbf{x})$ if and only if $\Delta_t(\mathbf{x}', \mathbf{x})$ is even and non-negative.

For the BCC lattice the distance is given by

$$d(\mathbf{x}, \mathbf{x}') = \max_i |x_i - x_i'|. \tag{53}$$

Let us see why this is the case. Without loss of generality, let us compute the distance $d(0, \mathbf{x})$, for some $\mathbf{x} \in G$. Notice that for each path $\lambda \in \Lambda(0, \mathbf{x})$ it holds true that for each $i = 1, 2, 3$

$$|x_i| \leqslant \left| \sum_l (n_l - n_{-l}) \right| \leqslant \sum_l (n_l + n_{-l}) = l(\lambda),$$

namely every path satisfies $l(\lambda) \geqslant \max_i |x_i|$, making $\max_i |x_i|$ a good candidate to be the distance. Now, it only remains to prove that there exists a path with precisely that number of steps. From Eq. (51) it is apparent that if λ satisfies the system (51) with $(n_{\pm 1}, n_{\pm 2}, n_{\pm 3}, n_{\pm 4})$, then the path $\lambda' \in \Lambda(0, \mathbf{x})$ such that $n'_l = n_l - n_{-l}$ satisfies:

$$\sum_l n'_l h_{l,i} = x_i, \quad l(\lambda') = \sum_l |n'_l| \leqslant l(\lambda). \tag{54}$$

Therefore we can restrict ourselves to look for paths λ' having only steps either in the positive or in the negative direction for each $l = 1, \ldots, 4$. From Eq. (54) we obtain the following expressions for n'_2, n'_3 and n'_4:

$$\begin{cases} n'_2 = n'_1 - \frac{x_2 + x_3}{2}, \\ n'_3 = n'_1 - \frac{x_1 + x_3}{2}, \\ n'_4 = n'_1 - \frac{x_1 + x_2}{2}. \end{cases} \tag{55}$$

Suppose now that x_1 is maximal and non-negative. If we choose $n'_1 = a_1$, $n'_2 = a_2$, $n'_3 = -a_3$, $n'_4 = -a_4$, with $a_i \geqslant 0$, then $l(\lambda') = a_1 + a_2 + a_3 + a_4 = x_1$. Imposing the conditions of positivity of the a_i according to Eq. (55), we see that, for instance, a_1 has to satisfy the conditions

$$\begin{cases} a_1 \geqslant \frac{x_2 + x_3}{2}, \\ a_1 \leqslant \frac{x_1 + x_3}{2}, \\ a_1 \leqslant \frac{x_1 + x_2}{2}. \end{cases}$$

The last two inequalities entail that $a_1 \leqslant \frac{x_1 + \min\{x_2, x_3\}}{2}$ and since a_1 is arbitrary we can choose it to fulfil the bound, namely $a_1 = \frac{x_1 + \min\{x_2, x_3\}}{2}$. For the other cases we can follow a similar reasoning, proving in this way the result.

6.2.2 Binary string solution

So far we have studied the past causal cone $\mathcal{C}_t(\mathbf{x})$, yet we still do not know which paths, specifically, are in $\Lambda_t(\mathbf{x}', \mathbf{x})$. The characterization we seek is best studied by considering the binary description of paths. The binary en-

coding and the quadruple $(n_{\pm 1}, n_{\pm 2}, n_{\pm 3}, n_{\pm 4})$ are related by the following equations:

$$\begin{cases} \iota(w^{(1)}) = n_{-1} + n_2 + n_3 + n_{-4}, \\ \iota(w^{(2)}) = n_1 + n_2 + n_{-3} + n_{-4}, \\ \iota(w^{(3)}) = n_1 + n_3 + n_{-2} + n_{-4}. \end{cases}$$

Remarkably, the expressions for the Hamming weights of $w^{(1)}$, $w^{(2)}$ and $w^{(3)}$ are given precisely by the expressions defining the number of steps in the positive- and negative-coordinate direction:

$$\begin{cases} \iota(w^{(1)}) = x_3^- = \frac{t-(x_3-x_3')}{2}, \\ \iota(w^{(2)}) = x_1^+ = \frac{t+(x_1-x_1')}{2}, \\ \iota(w^{(3)}) = x_2^+ = \frac{t+(x_2-x_2')}{2}. \end{cases} \tag{56}$$

Hence, as for the case $d = 2$, the number of 1-bits in each encoding string is fixed by the coordinates. It is then convenient to introduce the set of string tuples

$$\mathfrak{S}_t^n(K_1, \ldots, K_n) \coloneqq \mathfrak{S}_t(K_1) \times \cdots \times \mathfrak{S}_t(K_n), \tag{57}$$

where

$$\mathfrak{S}_t(K) \coloneqq \{\, w \in \mathfrak{B}_t \mid \iota(w) = K \,\}$$

is the set of strings with fixed Hamming weight K.

Therefore, in terms of binary strings, the path-sum of Eq. (50) can be rewritten as

$$\begin{aligned} \mathcal{K}(\boldsymbol{x}', \boldsymbol{x}; t) &= (\zeta^*)^t \sum_{\boldsymbol{w} \in \mathfrak{S}_t^3(K_1, K_2, K_3)} \widetilde{\mathcal{A}}(\boldsymbol{w}) \\ &= (\zeta^*)^t \sum_{\boldsymbol{w} \in \mathfrak{S}_t^3(t-K_1, t-K_2, t-K_3)} \alpha^{(12)} \beta^{(123)} B_{w_1^{(1)} w_t^{(2)}}, \end{aligned} \tag{58}$$

where the parameters K_1, K_2 and K_3 are given by

$$K_1 = \frac{t-(x_3-x_3')}{2}, \qquad K_2 = \frac{t+(x_1-x_1')}{2}, \qquad K_3 = \frac{t+(x_2-x_2')}{2}.$$

Moreover, the symbols $\alpha^{(12)}$ and $\beta^{(123)}$ denote the phase factors:

$$\alpha^{(12)} \coloneqq (-1)^{(w^{(1)} \oplus S w^{(1)}) \cdot w^{(2)}}, \tag{59}$$

$$\beta^{(123)} \coloneqq (\pm i)^{w^{(1)} \oplus w^{(2)} \oplus w^{(3)}}. \tag{60}$$

Since the resulting matrix depends only on the first bit of $w^{(1)}$ and the last bit of $w^{(2)}$, we can define some coefficients c_{ab} representing the contribution to the probability amplitude associated to the matrix B_{ab}:

$$c_{ab}(K_1, K_2, K_3) \coloneqq \sum_{w \in \mathfrak{S}^3_{t,ab}(K_1,K_2,K_3)} \alpha^{(12)}\beta^{(123)}, \tag{61}$$

where we defined $\mathfrak{S}^3_{t,ab}(K_1, K_2, K_3) \subset \mathfrak{S}^3_t(K_1, K_2, K_3)$ as the subset of string triads $(w^{(1)}, w^{(2)}, w^{(3)})$ with $w^{(1)}_1 = a$ and $w^{(2)}_t = b$. In this way the propagator can be computed as

$$\mathcal{K}(x', x; t) = (\zeta^*)^t \sum_{a,b\in\{0,1\}} c_{ab}(t - K_1, t - K_2, t - K_3)\, B_{ab}. \tag{62}$$

We have now to evaluate the sums in Eq. (61). Since $\alpha^{(12)}$ does not depend on $w^{(3)}$, we can first compute the sum

$$\sum_w (\pm i)^{v\oplus w}$$

alone with $\iota(w) = H$ for a given H and for some fixed $v \in \mathfrak{S}_t(K)$. Let us recall that $\sum_w z^{v\oplus w}$, $z \in \mathbb{C}$, is independent of bitwise permutations of the string v; indeed, suppose $c = \pi_v(v)$ is canonical (see Definition 5.1.1), then

$$\begin{aligned}\sum_w z^{\pi_v^{-1}(c)\oplus w} &= \sum_w z^{\pi_v^{-1}(c\oplus\pi_v(w))} \\ &= \sum_w z^{c\oplus\pi_v(w)} \\ &= \sum_w z^{c\oplus w}.\end{aligned}$$

Therefore, we only need to classify the strings w according to the Hamming weight of $c \oplus w$. All the results regarding this classification are already given in Chapter 5. In particular, from Lemma 5.1.1, taking $K \geqslant H$, the partition

$$\mathfrak{S}_t(H) = \bigcup_n \mathfrak{S}_K(H - n) \frown \mathfrak{S}_{t-K}(n)$$

gives the correct counting for $c \in \mathfrak{S}_t(K)$ since the size of each subset is preserved:

$$c \oplus \mathfrak{S}_t(H) = \mathfrak{W}(K, H, n) \coloneqq \bigcup_n \mathfrak{S}_K(K - H + n) \frown \mathfrak{S}_{t-K}(n),$$

with

$$|\mathfrak{W}(K, H, n)| = \binom{K}{H-n}\binom{t-K}{n}.$$

Moreover, all the elements of $\mathfrak{W}(K, H, n)$ share the same Hamming weight:

$$\iota(w) = |K - H| + 2n, \quad \forall w \in \mathfrak{W}(K, H, n).$$

Therefore, summing $z^{c\oplus w}$ over w, we have

$$\begin{aligned}\sum_{w\in\mathfrak{S}_t(H)} z^{c\oplus w} &= \sum_n \sum_{w\in\mathfrak{W}(K,H,n)} z^w \\ &= \sum_n \sum_{w\in\mathfrak{W}(K,H,n)} z^{|K-H|+2n} \\ &= z^{|K-H|} \sum_n \binom{K}{H-n}\binom{t-K}{n} z^{2n}.\end{aligned}$$

The general result is summarized in the following proposition, whose proof in given in Appendix B.

Proposition 6.2.1. *Given* $t, K, H \in \mathbb{N}$, *with* $K, H \leqslant t$, *and* $z \in \mathbb{C}$, *for all* $v \in \mathfrak{S}_t(K)$ *we have that*

$$\sum_{w\in\mathfrak{S}_t(H)} z^{v\oplus w} = \xi(K, H; z), \tag{63}$$

where

$$\xi(K, H; z) := z^{|K-H|} \sum_{n\in I} D(t, \bar{r}t + (-1)^{\bar{r}}H, rt + (-1)^r K, n)\, z^{2n},$$

with $I = \{0, 1, \ldots, \min\{K, H, t-K, t-H\}\}$.

So far we have obtained the expression for the sum of $\beta^{(123)}$ (60) over $w^{(3)}$:

$$\sum_{w^{(3)}\in\mathfrak{S}_t(K_3)} (\pm i)^{w^{(1)}\oplus w^{(2)}\oplus w^{(3)}} = \xi\Big(\iota\Big(w^{(1)} \oplus w^{(2)}\Big), K_3; \pm i\Big).$$

We still have to evaluate the sum of $\alpha^{(12)}$ (59) over $w^{(1)}$ and $w^{(2)}$, together with $\xi(\iota(w^{(1)} \oplus w^{(2)}), K_3; \pm i)$, in order to obtain the final expression for the coefficients c_{ab}:

$$c_{ab}(K_1, K_2, K_3) = \sum_{w\in\mathfrak{S}^2_{t,ab}(K_1,K_2)} \alpha^{(12)} \xi\Big(\iota\Big(w^{(1)} \oplus w^{(2)}\Big), K_3; \pm i\Big). \tag{64}$$

The classification of strings according to the values of

$$\alpha^{(12)} = (-1)^{(w^{(1)}\oplus Sw^{(1)})w^{(2)}}$$

has already been given in Chapter 5. We recall that $w^{(1)}$ and $w^{(2)}$ have fixed endpoints, say $w^{(1)}_1 = a$, $w^{(1)}_t = a'$ and $w^{(2)}_t = b$. The classification for

the function $w^{(1)} \oplus Sw^{(1)}$ is provided by Lemma 5.1.3, where the number of strings $w^{(1)}$ such that

$$\iota(w^{(1)} \oplus Sw^{(1)}) = 2n,$$

for some n and with $w^{(1)}_i = a$ and $w^{(1)}_t = a'$, is given by

$$u_{aa'}(n) = C_{K_1,n+aa'} C_{t-K_1,n+\bar{a}\bar{a}'},$$

$C_{K,n}$ being the number of n-compositions of K:

$$C_{K,n} \coloneqq \begin{cases} \binom{K-1}{n-1} & \text{if } K \geqslant n > 0, \\ 1, & \text{if } K = n = 0, \\ 0, & \text{otherwise.} \end{cases}$$

The last step of our discussion is the analysis of the classification of the strings $w^{(2)}$ according to the values of both $\iota((w^{(1)} \oplus Sw^{(1)})w^{(2)})$ and $\iota(w^{(1)} \oplus w^{(2)})$. Suppose for definiteness that $K_1 \geqslant K_2$ and $a = a' = 0$. The other cases are treated with a similar discussion. To emphasize the fact that the strings have fixed endopoints, we write $0v_n0$ to denote a string belonging to $\mathfrak{T}_{00}(t, K_1, n)$. Notice that the action of the circular shift S can be viewed as $S(0v_n0) = v_n00$. Similarly, wb denotes a string in $\mathfrak{S}_t(K_2)$ such that $w \in \mathfrak{S}_{t-1}(K_2 - b)$. On the one hand, as we know from Corollary 5.1.1, we can parametrize the sum modulo 2 of $0v_n0$ and wb as

$$\iota(0v_n0 \oplus wb) = |K_1 - K_2| + 2J,$$

for some parameter J. On the other hand, we also need to find all the strings w for which

$$\iota((0v_n \oplus v_n0)w)$$

has the same value varying w, for each fixed v_n. In order to have a better understanding of what is going on, we introduce a particular notation for labeled strings. A labeled string is a string made of pairs of bits (p, q) and we will identify the pairs of kind $(p, 1)$ as $\bar{p}$ and the pairs of kind $(p, 0)$ as $\dot{p}$. In particular, for a given binary string $v \in \mathfrak{T}_{aa'}(t, K_1, n)$, we consider the labeled string $\bar{v}$ such that $\bar{v}_i = (v_i, (v \oplus Sv)_i) = (v_i, v_i \oplus v_{(i \bmod t)+1})$. Let us see a concrete example: take $0v0 = 001100110010$ and $wb = 11000010010b$, then we have

$$\dot{0}\bar{v}\dot{0} = \dot{0}\bar{0}\dot{1}\bar{1}\dot{0}\bar{0}\dot{1}\bar{1}\dot{0}\bar{0}\bar{1}\dot{0}$$

and

$$\begin{array}{cccc|c||ccc|ccc} \bar{v} & \dot{0} & \dot{0} & & \bar{1} & \bar{1} & \bar{1} & \dot{1} & \dot{1} & \bar{0} & \bar{0} & \bar{0} & \dot{0} & \dot{0} & \dot{0} & \dot{0} \\ wb & 1 & 1 & 0 & 0 & & & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & b \end{array}$$

where we have arranged the bits of $\bar{v}$ by writing first the barred 1-bits and the dotted ones, then the barred and dotted 0-bits, *i.e.* we used a modified

canonical arrangement. In the general case, we can view the structure of the binary strings as follows:

$$\begin{array}{c|c|c||c|c|c}
 & n & K_1-n & n & t-K_1-n-1 & \\
\bar{v}\dot{0}\dot{0} & \bar{1}\dots\bar{1} & \dot{1}\dots\dot{1} & \bar{0}\dots\bar{0} & \dot{0}\dots\dot{0} & \dot{0} \\
wb & k & K_2-J-k & k' & J-k'-b & b \\
(0v0)\oplus wb & n-k & K_1-K_2+J-n+k & k' & J-k'-b & b
\end{array}$$

where the first row shows the length of each section and for wb we have indicated the number of 1-bits present in each section, *i.e.* the bits used to select the bars of the labeled string $\dot{0}\bar{v}\dot{0}$. The last row contains the number of 1-bits in each part for the string $(0v0)\oplus wb$. This structure suggets to choose a partition of the set $\mathfrak{S}_{t-1}(K_2-b)$ as follows:

$$\begin{aligned}
\mathfrak{S}_{t-1}(K_2-b) &= \bigcup_{J=b}^{\min\{K_2,t-K_1-1\}} \bigcup_{k=0}^{n} \bigcup_{k'=0}^{n} \mathfrak{Z}_b^{(1)}(J,k)\mathfrak{Z}_b^{(0)}(J,k'), \\
\mathfrak{Z}_b^{(1)}(J,k) &= \mathfrak{S}_n(k)\mathfrak{S}_{K_1-n}(K_2-J-k), \\
\mathfrak{Z}_b^{(0)}(J,k') &= \mathfrak{S}_n(k')\mathfrak{S}_{t-K_1-n-1}(J-k'-b).
\end{aligned}$$

For strings w in each subset of the partition we get

$$\alpha^{(12)} = (-1)^{[(0v0)\oplus(v00)](wb)} = (-1)^{k+k'},$$

and also that

$$\iota[(0v0)\oplus(wb)] = K_1-K_2+2J.$$

Therefore, the coefficients c_{ab} can be written as

$$c_{ab}(K_1,K_2,K_3) = \sum_{a'}\sum_{n,J} u_{aa'}(n)\varphi_{aa'b}(n,J;-1)\xi(\tau_J,K_3;\pm i),$$

where $\tau_J = K_1-K_2+2J$ and

$$\varphi_{aa'b}(n,J;z) = \sum_{k,k'} z^{k+k'+(a\oplus a')b}\left|\mathfrak{Z}_b^{(1)}(J,k)\right|\left|\mathfrak{Z}_b^{(0)}(J,k')\right|.$$

This concludes the discussion for the derivation of the solution in position space of the Weyl QW in $d=3$. The general result is summarized by the following proposition, whose proof is given in Appendix B.

Proposition 6.2.2. *For $t \geqslant 2$ the coefficients of Eq. (64) take the form*

$$c_{ab}(K_1, K_2, K_3) = \sum_{a'=0,1} \sum_{n=n_{\min}(K_1)}^{n_{\max}(K_1)} \sum_{J=b}^{K_2} u_{aa'}(n)\varphi_{aa'b}(n, J; -1)\xi(\tau_J, K_3; \pm i), \tag{65}$$

where, letting $r \coloneqq \vartheta(K_1 - K_2)$, we have that $\tau_J \coloneqq |K_1 - K_2| + 2J$, and

$$\begin{aligned}
&\varphi_{aa'b}(n, J; z) \coloneqq w^{(1)}_{aa'b}(n, J; z) w^{(0)}_{aa'b}(n, J; z), \\
&w^{(s)}_{aa'b}(n, J; z) \coloneqq \sum_{k=0}^{n-\gamma^{(s)}_{aa'}} z^{k+\gamma^{(s)}_{aa'},b} D(\eta^{(s)}_{a'}, \kappa^{(s)}_{a'b}(J), n - \gamma^{(s)}_{aa'}, k), \\
&\kappa^{(s)}_{a'b}(J) \coloneqq (r \oplus \bar{s})K_2 + (-1)^{\bar{s}}(\bar{r}K_1 - J) - (\bar{s} \oplus a')b, \\
&\eta^{(s)}_{a'} \coloneqq \bar{s}(t-1) + (-1)^{\bar{s}}(K_1 - a'), \quad \gamma^{(s)}_{aa'} \coloneqq (s \oplus a)(\bar{s} \oplus a').
\end{aligned} \tag{66}$$

We have seen in this chapter a technique suitable to solve the walk evolution in position space employing the algebraic properties of the transition matrices and the combinatorics of the binary strings. We suggest the possible use of the same technique also in other cases, even for Cayley graphs of non-Abelian groups. The main obstacle in the non-Abelian case is represented by the solution of the word problem of the group (see [111, 112]) which, in general, is not an easy task.

7 THE THIRRING QCA

In the previous chapters we presented models of discrete dynamics suitable for the description of physical systems in a discrete scenario. The usual dynamics is recovered at a scale where the discreteness can not be probed. So, for example, if we take the Planck scale as the fundamental scale—at which the QCA operates—the usual relativistic dynamics described by the Dirac equation is recovered in the limit of small wave-vectors and small masses. Therefore, the wave-vector in the automaton theory can be interpreted, a *posteriori*, as the momentum of the particle, and the mass parameter as its mass. The system described, however, can be regarded as a gas of free particles. In the QCA framework one can accommodate, as well, interactions between particles introducing a non-linear step in the automaton evolution operator.

In this section we are going to study a particular interacting QCA having as free term (see Appendix D) the Dirac QCA. For the interaction we assume a local interaction resembling the Hubbard model of solid state physics (for a comprehensive treatment of the Hubbard in one spatial dimension see Ref. [113]). The Hubbard model has been solved in $d = 1$ by Lieb and Wu using the Bethe Ansatz.

We review in this chapter the results regarding the Thirring QCA in dimension $d = 1$ presented in Ref. [75] and we show a brief sketch of the basic construction of the perturbation theory for this automaton.

7.1 REVIEW OF THE DIRAC QW IN ONE SPATIAL DIMENSION

In Chapter 4 we introduced the Dirac QW in dimension $d = 1$. We want to give here an equivalent formulation employing relativistic notation. The Dirac QW describes the linear local evolution of a two-component quantum field

$$\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix},$$

where ψ_L and ψ_R denote the left- and right-mode of the field respectively. We assume the statistics to be Fermionic, with the field operators satisfying the canonical anticommutation relations:

$$\{\psi_A(x), \psi_B(x')\} = 0,$$
$$\{\psi_A(x), \psi_B^\dagger(x')\} = \delta_{A,B}\delta_{x,x'}.$$

In position space, the walk operator, seen as a unitary operator over $\mathscr{H} = \mathbb{C}^2 \otimes \ell^2(\mathbb{Z})$, can be written as:

$$W = \begin{pmatrix} nS & -im \\ -im & nS^\dagger \end{pmatrix}, \qquad n^2 + m^2 = 1, \tag{67}$$

where S denotes the left shift $S|x\rangle = |x-1\rangle$. From this expression of the walk, we can derive a finite difference equation governing the evolution of $|\psi(t)\rangle \in \mathscr{H}$ written compactly as:

$$(i\not{D} - m)|\psi(t)\rangle = 0, \tag{68}$$

where $\not{D} = \gamma^\mu D_\mu$ with metric signature $(1,-1)$ and $D = (D^0, D^1)$ is defined as

$$D^0 \coloneqq W - n\frac{S+S^\dagger}{2},$$
$$D^1 \coloneqq -n\frac{S-S^\dagger}{2},$$

with the trivial identification of S and $I_2 \otimes S$, where I_2 represents the identity matrix on $\mathbb{C}^2$. We will also identify a matrix M on $\mathbb{C}^2$ with its extension $M \otimes I$ to $\mathscr{H}$, I being the identity operator on $\ell^2(\mathbb{Z})$. The gamma matrices are taken in the chiral representation, *i.e.*

$$\gamma^0 \coloneqq \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \gamma^1 \coloneqq i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

As usual, the chiral projections are obtained in terms of the γ^5 matrix

$$\gamma^5 \coloneqq \gamma^0\gamma^1 = -\sigma_z = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

via the equations

$$|\psi_L\rangle = \frac{1-\gamma^5}{2}|\psi\rangle, \qquad |\psi_R\rangle = \frac{1+\gamma^5}{2}|\psi\rangle.$$

7.1.1 Solutions of the Dirac QW in one space dimension

The solutions of the walk are obtained in the Fourier representation as follows. By taking $|k\rangle = \sum_{x\in\mathbb{Z}} e^{ikx}|x\rangle$, with $k \in B := [-\pi, \pi]$, the shift operator is diagonal in this basis: $S|k\rangle = e^{ik}|k\rangle$. The operator W can thus be written as

$$W = \int_B dk\, W_k \otimes |k\rangle\langle k|, \qquad W_k = \begin{pmatrix} ne^{ik} & -im \\ -im & ne^{-ik} \end{pmatrix}.$$

We can solve now the eigenvalue problem for W_k:

$$W_k|s,k\rangle = e^{-is\omega_k}|s,k\rangle, \quad s = \pm. \tag{69}$$

The spectrum of the walk is then given by $\{e^{-i\omega_k}, e^{i\omega_k}\}$, where

$$\omega_k := \arccos(n\cos k) \tag{70}$$

is its dispersion relation. The eigenvenctors $|s,k\rangle$ can be written as

$$|s,k\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1-sv_k} \\ s\sqrt{1+sv_k} \end{pmatrix},$$

v_k being the group velocity, namely

$$v_k := \frac{d\omega_k}{dk} = \frac{n\sin k}{E_k}, \qquad E_k := \sin\omega_k = \sqrt{n^2\sin^2 k + m^2}.$$

If we define the map

$$(\omega, k) \mapsto p(\kappa) := (\sin\omega, n\sin k)$$

the eigenvalue equation (69) can be stated in the following equivalent form:

$$(\not{p} - sm)u_s(k) = 0, \qquad p_\mu p^\mu = m^2. \tag{71}$$

The solutions u_s are chosen so that

$$u_s(k)\bar{u}_s(k) = \not{p} + sm,$$

where, as usual, $\bar{u}$ is defined as

$$\bar{u} := u^\dagger\gamma^0.$$

Notice, however, that our choice for u_- implies that it is an eigenvector for $-k$. Moreover, we can readily compute the orthogonality relations as follows. Firstly, we need to compute the quantity $(\not{p} + sm)\gamma^0(\not{p} + sm)$:

$$\begin{aligned}(\not{p} + sm)\gamma^0(\not{p} + sm) &= \not{p}\gamma^0\not{p} + sm(\gamma^0\not{p} + \not{p}\gamma^0) + m^2\gamma^0 \\ &= \not{p}(2p^0 - \not{p}\gamma^0) + 2smp^0 + m^2\gamma^0 \\ &= 2p^0\not{p} - p_\mu p^\mu\gamma^0 + 2smp^0 + m^2\gamma^0 \\ &= 2E_k(\not{p} + sm).\end{aligned}$$

Knowing this relation, we can compute $\|u_s(k)\|$. To this end we compute the quantity $u_s u_s^\dagger u_s u_s^\dagger \gamma^0$:

$$u_s u_s^\dagger u_s u_s^\dagger \gamma^0 = \|u_s\|^2(\not{p} + sm).$$

Explicitly we have that

$$\begin{aligned}u_s u_s^\dagger u_s u_s^\dagger \gamma^0 &= u_s\bar{u}_s\gamma^0 u_s\bar{u}_s \\ &= (\not{p} + sm)\gamma^0(\not{p} + sm) \\ &= 2E_k(\not{p} + sm),\end{aligned}$$

which therefore entails that $\|u_s\|^2 = 2E_k$. As for the orthogonality relation we can compute the following expression:

$$\begin{aligned}u_+(k)u_+^\dagger(k)u_-(-k)u_-^\dagger(-k) &= u_+(k)\bar{u}_+(k)\gamma^0 u_-(-k)\bar{u}_-(-k)\gamma^0 \\ &= u_+(k)\bar{u}_+(k)u_-(k)\bar{u}_-(k) \\ &= (\not{p} + m)(\not{p} - m) \\ &= p_\mu p^\mu - m^2 = 0.\end{aligned}$$

In this calculation, we made use of the conjugation relation

$$\gamma^0 u_s(k)\bar{u}_s(k)\gamma^0 = u_s(-k)\bar{u}_s(-k),$$

which can be straightforwardly verified:

$$\begin{aligned}\gamma^0 u_s(k)\bar{u}_s(k)\gamma^0 &= \gamma^0(\not{p} + sm)\gamma^0 \\ &= (p^0\gamma^0 - p^1\gamma^0\gamma^1\gamma^0 + sm) \\ &= (p^0\gamma^0 + p^1\gamma^1 + sm) \\ &= (E_k\gamma^0 - n\sin(-k)\gamma^1 + sm) \\ &= u_s(-k)\bar{u}_s(-k).\end{aligned}$$

The evolution governed by the Dirac QW approximates in a suitable regime that of the Dirac equation. Indeed, this fact can be checked by

considering the eigenvalue equation of Eq. (71) for $m \ll 1$ and $k \ll 1$. Considering for simplicity the equation for u_+, let us write it as

$$H(k)u_+(k) = E_k u_+(k),$$

where the operator $H(k)$ is given by

$$H(k) \coloneqq n \sin k \gamma^0 \gamma^1 + m\gamma^0.$$

At first order in the power expansion $n = 1 + \mathcal{O}(m^2)$, so that in the end we get

$$H(k) = k\gamma^0\gamma^1 + m\gamma^0 + \mathcal{O}(m^2) + \mathcal{O}(k^2),$$

which, interpreting m as the mass of the particle and k as its momentum, gives at first order precisely the Dirac Hamiltonian in the momentum representation.

7.1.2 Fermion doubling and deformed Lorentz transformations

The dynamics of the QW is governed by a dispersion relation which is not the usual relativistic one and so we may certainly expect that it is not invariant under Lorentz transformations. For $d = 1$ the Lorentz group consists only in the boost transformations, which in the energy-momentum sector are represented by the linear map

$$L_\beta \colon (\omega, k) \mapsto (\omega', k') = \Gamma(\omega - \beta k, k - \beta\omega),$$

with $\Gamma \coloneqq (1-\beta^2)^{-1/2}$. In our case the quantity that should be left invariant by a change of reference QW is

$$p_\mu p^\mu = \sin^2 \omega - n^2 \sin^2 k = m^2, \tag{72}$$

for a generic $p = (\sin\omega, n \sin k)$, which is clearly not invariant under Lorentz transformations, when applied to (ω, k). This means that if we insist on the QW evolution we need to find another transformation representing a change of reference. This is done by considering a non-linear representation of the Lorentz group [64] (see [61] for the discussion in $d = 3$), *i.e.* instead of L_β we consider the map

$$L_\beta^{\mathcal{D}} \coloneqq \mathcal{D}^{-1} \circ L_\beta \circ \mathcal{D},$$

where $\mathcal{D} \colon \mathbb{R}^2 \to \mathbb{R}^2$ is the non-linear map

$$\mathcal{D} \colon (\omega, k) \longmapsto \mathcal{D}(\omega, k) \coloneqq \left(\frac{\sin\omega}{\cos k}, \tan k \right).$$

The deformed Lorentz transformations obtained in this way are then given by

$$\begin{cases} \sin\omega' = \Gamma\left(\dfrac{\sin\omega}{\cos k} - \beta\tan k\right)\cos\arctan\left(\Gamma\left(\tan k - \beta\dfrac{\sin\omega}{\cos k}\right)\right), \\ \tan k' = \Gamma\left(\tan k - \beta\dfrac{\sin\omega}{\cos k}\right). \end{cases}$$

By direct inspection, one can check that these transformation preserve the invariant for the Dirac QW (72).

As the authors show in Ref. [64] the map $\mathcal{D}$ has two invariant momenta $k = \pm\pi/2$ corresponding to the invariant "energy" $\omega_{inv} = \pi/2$. These fixed points induce a splitting of the Brillouin zone $B = [-\pi, \pi]$ into two separate regions B_1, B_2, $B = B_1 \cup B_2$, with $B_1 := [-\pi/2, \pi/2]$ and $B_2 = [-\pi, -\pi/2] \cup [\pi/2, \pi]$, invariant under any boost. Since the two invariant regions exhibit the same kinematics, they can be considered as two distinct Fermion species, as opposed to the single Fermion in the standard relativistic scenario. This is due essentially to the discreteness characterizing the QW description, for which this doubling of the particles is expected [114]. Therefore we introduce two quantum fields $\psi_0(t, x)$ and $\psi_1(t, x)$ representing the two Fermion species described by the Dirac QW. We can expand in modes the two fields as follows:

$$\psi_j(t, x) = \int_{B_{½}} \frac{dk}{2\pi} \sum_{s=\pm} \frac{u_{j,s}(k)}{\sqrt{2E_k}} a_{j,s}(k) e^{-si(\omega_k t - kx)}, \tag{73}$$

where $B_{½} := B_1 = [-\pi/2, \pi/2]$ and $a_{j,s}$ are fermionic operators satisfying the canonical anticommutation relations:

$$\begin{aligned} &\{a_{j,s}(k), a_{j',s'}(k')\} = 0, \\ &\{a_{j,s}(k), a^\dagger_{j',s'}(k')\} = 2\pi\delta_{s,s'}\delta_{j,j'}\delta_{2\pi}(k - k'). \end{aligned}$$

The vacuum state of the walk $|0\rangle$ is defined by $a_{j,s}(k)|0\rangle = 0$, for all $k \in B_{½}$ and $j = 0, 1$; this means we adopt here a local vacuum instead of the usual definition in QFT. The spinors $u_{j,s}$ are related to the solutions u_s by

$$u_{j,s}(k) = u_{(1-2j)s}(k),$$

giving the completeness relation

$$u_{j,s}\bar{u}_{j,s} = \not{p} + (-1)^j s m.$$

The total field, obtained by combining the two fields ψ_0 and ψ_1 is finally given by

$$\psi(t, x) = \psi_0(t, x) + (-1)^{t+x}\psi_1(t, x).$$

7.2 THE THIRRING QCA

In this section we present the Thirring QCA and review the solutions in the two particle sector derived in Ref. [75]. We then provide the results of the numerical evaluation of the case of two particles to demonstrate the properties of the model [115]. In order to have an interacting automaton we need to add a position-dependent extra step to the free evolution. In the general case, one could have a unitary operator of the form $U = U_f V$, where U_f is a translation invariant unitary describing the free evolution and V is position-dependent coin operator. We consider here an interaction term that acts non-identically only when the particles occupy the same lattice cell and in this case it acts via a fixed operator Γ. In the simplest case V simply multiplies the state with extra phase factor, namely $\Gamma = e^{i\chi} I$ for some real coupling constant χ.

We consider here an interaction commuting with the total particle number operator $\sum_x (n_R(x) + n_L(x))$ and thus preserving the number of particles. As a consequence, we can restrict our analysis to a fixed number of particles. The sector of N particles of the automaton can be described equivalently as a QW of N (interacting) particles. Accordingly we take a walk unitary of the form:

$$U_N = W_N V, \qquad W_N = W^{\otimes N},$$

where W denotes the unitary operator describing the Dirac QW of Eq. (67). In particular, we consider the interaction term

$$\begin{aligned} V &= e^{i\chi \sum_{x\in\mathbb{Z}} n_L(x) n_R(x)} \\ &= e^{i\chi \sum_{x\in\mathbb{Z}} \psi_L^\dagger(x)\psi_L(x)\psi_R^\dagger(x)\psi_R(x)}, \end{aligned} \tag{74}$$

where χ is a real coupling constant and $n_A(x)$ the number of particles at site x for the mode $A = R, L$. The Hilbert space of N particles is $\mathscr{H}_N = \mathscr{H}^{\otimes N}$, with $\mathscr{H}$ the single particle Hilbert space in one spatial dimension, namely $\mathscr{H} = \mathbb{C}^2 \otimes \ell^2(\mathbb{Z})$. As we said we can study separately the solutions for each fixed number of particles. We focus here on the case of two Fermions, which can be analytically solved by means of the Bethe Ansatz [75]. In this case we write

$$U_2 = W_2 V = (W \otimes W) V$$

where the interaction term can be written as

$$V = I - M + \Gamma M.$$

In the equation above, M denotes the projector on the collision subspace, namely

$$M = \sum_{x \in \mathbb{Z}} I \otimes |x\rangle\langle x| \otimes |x\rangle\langle x|,$$

and Γ is an operator that acts on the coin space by multiplying the state with a phase factor when the spins of the Fermions are different:

$$\Gamma = \begin{pmatrix} I & 0 & 0 & \\ 0 & e^{ix} I & 0 & 0 \\ 0 & 0 & e^{ix} I & 0 \\ 0 & 0 & 0 & I \end{pmatrix}.$$

The walk U_2 is conveniently expressed in the centre of mass basis

$$|A_1, A_2\rangle\, |y\rangle\, |w\rangle$$

for the two-particle Hilbert space $\mathscr{H}_2 = \mathbb{C}^4 \otimes \ell^2(\mathbb{Z})$, with $A_1, A_2 \in \{L, R\}$, $y = x_1 - x_2$ denoting the relative coordinate, and $w = x_1 + x_2$ the centre of mass coordinate. The free walk unitary W_2 can be expressed in momentum space denoting by $k = \frac{1}{2}(p_1 - p_2)$ the (half) relative momentum and by $p = \frac{1}{2}(p_1 + p_2)$ the (half) total momentum. In this way we have

$$W_2 = \int dk dp\; W_2(-p, -k) \otimes |k\rangle\langle k| \otimes |p\rangle\langle p|,$$

where $W_2(p, k) \coloneqq W(p + k) \otimes W(p - k)$. The eigenvectors of the free evolution are easily computed in terms of the eigenvectors of the single particle walk:

$$W_2(p, k) u^{sr}_{p,k} = e^{-i\omega_{sr}(p,k)} u^{sr}_{p,k}, \qquad u^{sr}_{p,k} \coloneqq v^s_{p+k} \otimes v^r_{p-k}, \tag{75}$$

where the dispersion relation $\omega_{sr}(p, k)$ is given by

$$\omega_{sr}(p, k) \coloneqq s\omega(p + k) + r\omega(p - k),$$

and $\omega(p) \coloneqq \operatorname{Arccos}(n \cos p)$ is the one-particle dispersion relation. In this section, we take the eigenvectors v^s_p in the form:

$$v^s_p = \frac{1}{|\alpha_s(p)|} \begin{pmatrix} -im \\ g_s(p) \end{pmatrix},$$
$$g_s(p) = -i(s \sin \omega(p) + n \sin p),$$

with $|\alpha_s(p)|^2 = |g_s(p)|^2 + m^2$. Since U_2 commutes with the translations in the centre of mass coordinate w the total momentum p is a conserved quantity and therefore we can study the walk solutions for fixed p. It

is convenient to represent the walk in the hybrid basis $|A_1, A_2\rangle |y\rangle |p\rangle$; for fixed value of p the walk reduces to a one-dimensional QW with a four dimensional coin:

$$U_2 = \int dp\, U_2(-p) \otimes |p\rangle\langle p|,$$

where $U_2(p) = W_2(p)V$ and

$$U_2(p) = mn \begin{pmatrix} \frac{n}{m} e^{i2p} & -ie^{ip} T_y & -ie^{ip} T_y^\dagger & -\frac{m}{n} \\ -ie^{ip} T_y & \frac{n}{m} T_y^2 & -\frac{m}{n} & -ie^{-ip} T_y \\ -ie^{ip} T_y^\dagger & -\frac{m}{n} & \frac{n}{m} T_y^{\dagger 2} & -ie^{-ip} T_y^\dagger \\ -\frac{m}{n} & -ie^{-ip} T_y & -ie^{-ip} T_y^\dagger & \frac{n}{m} e^{-i2p} \end{pmatrix},$$

where T_y represents the translation operator in the relative coordinate y. The interaction term now reads

$$V = I - M + \Gamma M,$$

where M is now defined only on the relative coordinate:

$$M = |0\rangle\langle 0| \otimes I,$$

which means that in the relative coordinate the interaction acts only at the origin $y = 0$.

From now on we omit the explicit dependence on the total momentum p. Since we are interested in Fermionic particles, we consider here only the antisymmetric solutions of the interacting walk, *i.e.* we seek only the eigenvectors of $U_2(p)$ in the antisymmetric subspace. Following Ref. [75] it is useful to define the following sets, allowing the relative momentum k to have non-vanishing imaginary part, *i.e.* $k = k_R + ik_I$:

$$\begin{aligned} \Gamma_f &:= \{ k \in S \mid k_I = 0 \}, \\ \Gamma_z &:= \left\{ k \in S \;\middle|\; k_R = z\frac{\pi}{2} \right\}, \end{aligned} \tag{76}$$

$$\begin{aligned} \Omega_f^{sr} &:= \left\{ e^{-i\omega_{sr}(p,k)} \;\middle|\; k \in \Gamma_f \right\}, \\ \Omega_z^{sr} &:= \left\{ e^{-i\omega_{sr}(p,k)} \;\middle|\; k \in \Gamma_z \right\}, \end{aligned} \tag{77}$$

where $z = 0, \pm 1, 2$ and the set S is defined as

$$S := \{ k \in \mathbb{C} \mid k_R \in (-\pi, \pi] \wedge k_I \in \mathbb{R} \}.$$

Let us now summarize the solutions to the equation

$$U_2(p) f = e^{i\omega} f, \quad f \colon \mathbb{Z} \to \mathbb{C}^4, \quad \omega \in \mathbb{C}. \tag{78}$$

We are interested in the antisymmetric solutions, namely f is antisymmetric under exchange of the two particles:

$$f(y) = -Ef(-y),$$

where E is the exchange matrix:

$$E = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

As proven in Ref. [75], the solutions can be written as

$$\begin{aligned} f_k^{\pm}(y) &= c_1 f_k^{\pm,f}(y) + c_2 f_k^{\pm,i}(y), \qquad (79)\\ f_k^{\pm,f}(y) &= [u_k^{+\pm} + (-1)^y u_{k-\pi}^{-\mp}]e^{-iyk} - [u_{-k}^{\pm+} + (-1)^y u_{\pi-k}^{\mp-}]e^{iyk}, \\ f_k^{\pm,i}(y) &= \begin{cases} e^{-i\delta_{y,0}\chi}\{[u_k^{+\pm} - (-1)^y u_{k-\pi}^{-\mp}]e^{-iyk} + \\ \quad -T_{\pm}[u_{-k}^{\pm+} - (-1)^y u_{\pi-k}^{\mp-}]e^{iyk}\} & y \geqslant 0, \\ \text{antisymmetrized} & y < 0, \end{cases} \\ T_{\pm} &:= \frac{g_+(p+k) + e^{-i\chi} g_{\pm}(p-k)}{g_{\pm}(p-k) + e^{-i\chi} g_+(p+k)}, \end{aligned}$$

where $c_1, c_2 \in \mathbb{C}$. We remark that the continuous spectrum of the interacting walk is the same of the free one[1]. From Eq. (79), one obtains the generalized eigenvector of $U_2(p)$ for $k \in \Gamma_f$ which correspond to the continuous spectrum given by $\Omega_f^{++} \cup \Omega_f^{--}$. The functions $f_k^{\pm,f}$ are solutions of the free walk that are also solutions in the interacting case; indeed we have that $f_k^{\pm,f}(0) = 0$ and thus these solutions are not affected by the interaction which is localized at the origin. The solutions $f_k^{\pm,i}$, instead, can be interpreted as scattering solutions and $T_{\pm}$ can be considered as the transmission coefficient of the plane waves.

Besides the scattering solutions, the Thirring QW exhibits also molecule states, *i.e.* bound states, for which the probability distribution decades exponentially with the relative coordinate y. As proven in Ref. [75], such solutions are obtained for $c_1 = 0$, $c_2 \neq 0$ and $k \notin \Gamma_f$ with $k_I = \mathrm{Im}(k) < 0$, so that $T_{\pm} = 0$. If $p \neq z\pi/2$ and if $e^{i\chi} \notin \{e^{\pm i2p}, 1, -1\}$, then the solution is unique, *i.e.* there exists a unique $k \in \Gamma_0 \cup \Gamma_{-1} \cup \Gamma_1 \cup \Gamma_2$ with $k_I < 0$ for which either $T_+ = 0$ or $T_- = 0$. In other words, for each value of the coupling constant χ and a given value of the momentum p the walk $U_2(p)$ has one eigenvector corresponding to an eigenvalue in the discrete spectrum. On the contrary, in the case of the Hadamard walk [117]—which also features molecule states—the spectrum of the bound states is discontinuous as a

1 As it is well known from scattering theory since the interaction term is a compact perturbation of the free evolution (see Theorem IV 5.35 of Ref. [116]).

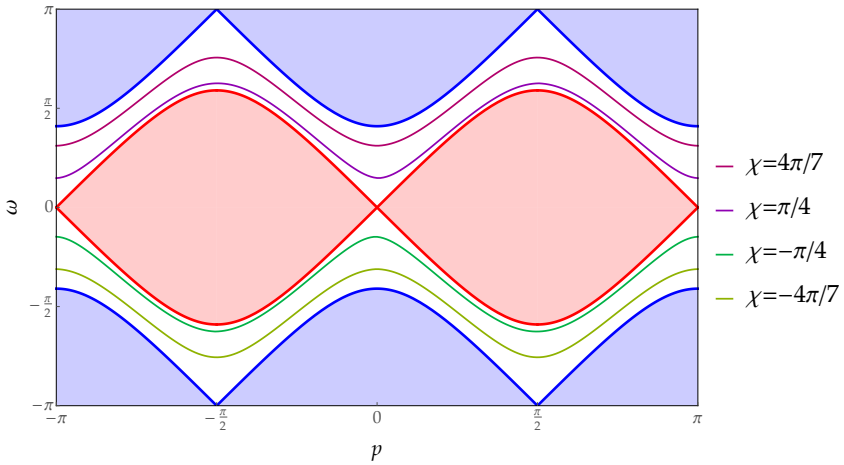


Figure 11.: Spectrum in the two-particle sector for the interacting walk as a function of the total momentum p. The mass parameter is $m = 0.6$. The blue and red regions constitute the continuous spectrum of the walk which is the same as the one of the free walk. The solid lines in the gaps represent the discrete spectrum for different values of the coupling constant: from top to bottom, $\chi = 4\pi/7$, $\pi/4$, $-\pi/4$, $-4\pi/7$.

function of p; furthermore, there are two bound states, if any, for fixed coupling constant and total momentum.

In Fig. 11 we show the spectrum of the interacting case for two particles with mass parameter $m = 0.6$ (provided in Ref. [115] which is in progress). The plot represent the spectrum for different values of the total momentum p. The continuous bands in blue and red represent the continuous spectrum which is the same as in the free case. The solid curves in the gaps between the continuous bands, instead, represent the discrete spectrum for different values of the coupling constant. The discrete spectrum has been computed for the values $\chi = -4\pi/7, -\pi/4, \pi/4, 4\pi/7$. Such discrete spectrum represents the bound states of the two particles.

In Fig. 12 we show for comparison the evolution in the free case and in the interacting case (the numerical analysis is provided in Ref. [115]). The plots show the joint probability distribution after $t = 32$ time-steps of evolution of the singlet state localized at the origin. In the left panel is depicted the probability distribution for the state evolved with the free walk. In the right panel the same state is evolved with the interacting walk for $\chi = \pi/2$, which is the same image as the image on the cover of this manuscript. One can see that in the latter case there is a concentration of probability along the diagonal, showing the appearance of the bound state component. The shape of this distribution shows the typical behaviour of a one-dimensional QW as for the Hadamard walk [117].

There also other solutions not encompassed by the previous analysis, namely solutions for which $e^{i\chi} = e^{\pm i2p}$ with eigenvalues $e^{\pm i2p}$. We remark that these eigenvalues belong to the discrete spectrum which is continuous

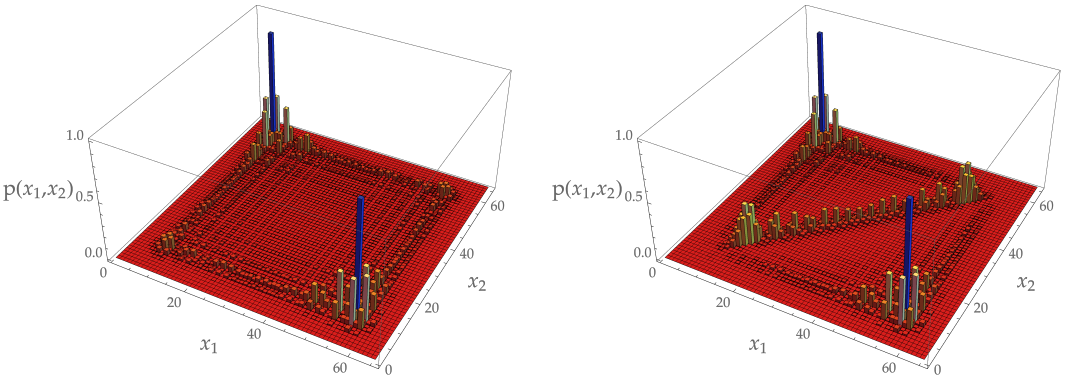


Figure 12.: Probability distribution in position space of two particles. The number of time steps is $t = 32$ and the mass parameter is $m = 0.6$. The initial state is a singlet located at the orgin. In the left panel is depicted the evolution in the free case ($\chi = 0$). In the right panel the same initial state is evolved according to the interacting walk for $\chi = \pi/2$. Besided the diffusive components that are present as in the free case, one can see also the appearance of a molecule component.

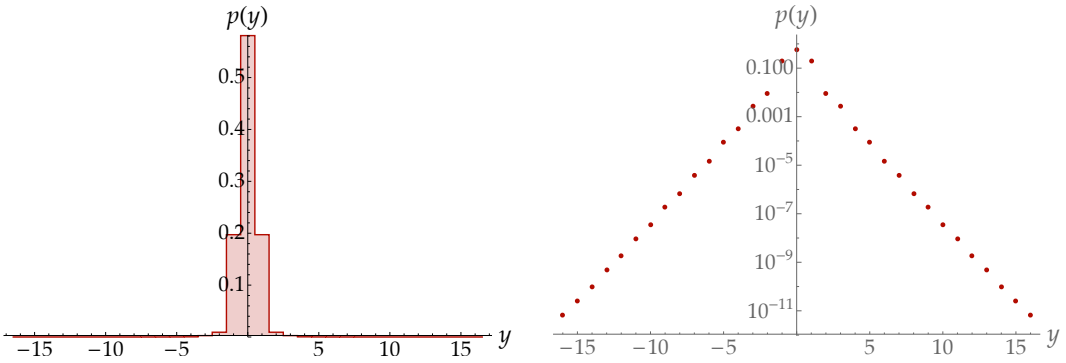


Figure 13.: Probability ditribution in position space for the eigenstate u_k^{+-} (see Eq. (75)) of the free walk of two Fermions with total momentum $p = 0$ and mass $m = 0.6$. On the left it shown the plot with linear scale, while on the right the same plot with logarithmic scale.

as a function of p. The corresponding eigenvectors are non-zero only on three sites and are given by

$$f_{\pm\infty}(y) = \begin{cases} ie^{\pm ip}\left(-\frac{1\pm1}{2}, 0, 0, -\frac{1\mp1}{2}\right)^T, & y = 1, \\ \left(0, \frac{m}{n}, -\frac{m}{n}, 0\right)^T, & y = 0, \\ ie^{\pm ip}\left(\frac{1\pm1}{2}, 0, 0, \frac{1\mp1}{2}\right)^T, & y = -1, \\ 0, & \text{otherwise.} \end{cases} \tag{80}$$

The final analysis of Ref. [75] regards the cases $p = z\frac{\pi}{2}$ that were missing in the previous results. Since the analysis for $z \neq 0$ is similar to the case $z = 0$, we consider only $p = 0$. In this case we have $\omega_{\pm\pm}(0, k) = 2\omega(k)$ and $\omega(k) \in \mathbb{R}$ if and only if $k \in \Gamma_f \cup \Gamma_0 \cup \Gamma_2$. We have instead $\omega_{\pm\mp}(0, k) =$

0 for all $k \in \mathbb{C}$. One can prove[2] that 1 belongs to the point spectrum of $U_2(0)$ and the corresponding eigenstates are stationary bound states. This feature is present also for $\chi = 0$, showing an essential difference with respect to similar Hamiltonian models. For instance, we show in Fig. 13 the probability distribution in position space for the (normalized) state (see Eq. (75))

$$|\psi\rangle = \int_{-\pi}^{\pi} dk \; |u_{-k}^{+-}\rangle \, |k\rangle \, ,$$

corresponding to the case $p = 0$ and $\chi = 0$. As expected all the states u_k^{+-} with $k \in (-\pi, \pi]$ correspond to the eigenvalue 1, meaning that they form a subspace on which the walk acts identically. This feature relies on the fact that the dispersion relation of the one-dimensional Dirac QW is an even function of k. The same is not true, for instance, in dimension $d = 3$ (see Eqs. (4) and (13)) where one should perform a different analysis of the spectral properties of the walk operator. The numerical analysis for the case $d = 1$ is provided in Ref. [115].

7.3 PERTURBATION THEORY FOR THE THIRRING QCA

We introduced in Section 7.2 the Thirring QCA and we discussed the analytical solutions derived in Ref. [75] for the two particle sector. In this section we introduce the basic concepts regarding the perturbation theory of the Thirring automaton.

Recall the expression for interaction term of the Thirring automaton (74):

$$\begin{aligned} V_{\text{int}} &= e^{i\chi \sum_{x\in\mathbb{Z}} n_L(x) n_R(x)} \\ &= e^{i\chi \sum_{x\in\mathbb{Z}} \psi_L^\dagger(x)\psi_L(x)\psi_R^\dagger(x)\psi_R(x)}, \end{aligned} \tag{81}$$

where χ is a real coupling constant and $n_{L,R}$ is the number operator of the left and right mode respectively. Since we are interested here in the case where the coupling constant is small, we can regard the interaction term as a perturbation of the free evolution of the Dirac walk. It is convenient to study the perturbation theory in the interaction picture (see Appendix D). In this representation the states evolve according to the interaction term, whereas the observables evolve according to the free term. From Eq. (81), we can write the interaction Hamiltonian:

$$H_I = \frac{1}{4}(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi) \tag{82}$$

$$= \psi_L^\dagger\psi_L\psi_R^\dagger\psi_R. \tag{83}$$

2 The technical details are presented in Ref. [75].

Usually one is interested in the computation of the scattering amplitude for some particular process. We assume that, before the particles interact, they are well describe by eigenstates of the free theory. Analogously, waiting enough time after the interaction has happened, the particles are assumed to be free and thus again we are allowed to describe them in terms of eigenstates of the free theory. Therefore, we consider the matrix elements of the S matrix (100) between free states of the theory. The goal is then to compute the amplitude representing a physical process to a given order in the perturbation expansion (we are considering here small values of the coupling constant χ). Explicitly, one computes the matrix elements of the S matrix at a given order in the power expansion in the coupling constant:

$$\langle f|S - I|i\rangle = \sum_{n=1}^{+\infty} \langle f|S_N^{(n)}|i\rangle\,,$$
$$S^{(n)} \coloneqq \frac{(-i\chi)^n}{n!} \sum_{t_1,x_1} \cdots \sum_{t_n,x_n} T \prod_{i=1}^{n} H_I(t_i, x_i),$$

for N-particle states $|i\rangle$ and $|f\rangle$. In the following analysis we consider the single-particle states with fixed momentum k given by

$$|k, j, s\rangle \coloneqq \sqrt{2E_k}\, a^\dagger_{j,s}(k)\,|0\rangle\,, \tag{84}$$

or equivalently

$$|k, s\rangle \coloneqq \sqrt{2E_k}\, a^\dagger_{s}(k)\,|0\rangle\,, \tag{85}$$

where in the latter one should choose k in B_1 or B_2 explicitly (recall Section 7.1.2 for the discussion about Fermion doubling).

7.3.1 Feynman rules for the Thirring QCA

We will give in this section the basic elements to compute scattering amplitudes from Feynman diagrams. We can represent a given process at order n in the perturbation expansion by a diagram with n vertices joined by lines representing the propagation of particles. The simplest process that we can consider in the present theory is the scattering of two particles. Let us focus on the following amplitude:

$$S_2^{(1)} \equiv \langle f|S^{(1)}|i\rangle = -\frac{i\chi}{4} \sum_{t,x} \langle 0|a'_1 a'_2 (\bar\psi\gamma^\mu\psi)(\bar\psi\gamma_\mu\psi) a^\dagger_1 a^\dagger_2|0\rangle\,, \tag{86}$$

where in short it is understood that $a_i \equiv a_{s_i}(k_i)$, $a'_i \equiv a_{s'_i}(k'_i)$. Since the interaction term commutes with the translations on the lattice, the total momentum is a conserved quantity, meaning that we can write $S_2^{(1)}$ as

$$S_2^{(1)} = -i\chi(2\pi)^2\delta^2_{2\pi}(\widetilde{k}'_1 + \widetilde{k}'_2 - \widetilde{k}_1 - \widetilde{k}_2)i\mathcal{M},$$

where $\widetilde{k}_i = s_i(\omega_i, k_i)$ and $i\mathcal{M}$ is the amplitude of the process given by the sum of all the possible contractions (by Wick's theorem [118]) in the expression

$$\langle 0|a'_1 a'_2 \psi^\dagger_L \psi_L \psi^\dagger_R \psi_R a^\dagger_1 a^\dagger_2|0\rangle\,. \tag{87}$$

The computation of $i\mathcal{M}$ involves the computation of the external leg contractions:

$$\begin{aligned}\langle 0|\psi(t,x)|k,s\rangle &= u_s(k)e^{-si(\omega_k t - kx)},\\ \langle k,s|\bar{\psi}(t,x)|0\rangle &= \bar{u}_s(k)e^{si(\omega_k t - kx)}.\end{aligned}$$

So for each external leg we write u_s for an incoming particle and $\bar{u}_s$ for an outgoing particle.

We also need to compute the propagator of the walk. By direct computation, since the field ψ contains only annihilation operators, we have

$$\begin{aligned}\langle 0|T[\psi_A(t,x)\bar{\psi}_B(t',x')]|0\rangle &= \vartheta(t-t')\,\langle 0|\psi_A(t,x)\bar{\psi}_B(t',x')|0\rangle\\ &= K_{AB}(t-t', x-x'),\end{aligned}$$

that is K vanish for $t < t'$. Explicitly, K is given by

$$\begin{aligned}K(t,x) &= \vartheta(t)\int_B \frac{dk}{2\pi}\,\frac{1}{2E_k}\left[(\not{p}+m)e^{-i[\omega_k t - kx]} + (\not{p}-m)e^{i[\omega_k t - kx]}\right]\\ &= \int_{\mathbb{B}} \frac{d\mu(\omega,k)}{(2\pi)^2}\,\widetilde{K}(\omega,k)e^{-i(\omega t - kx)},\end{aligned} \tag{88}$$

with $\mathbb{B} = \mathbb{R}\times B$ and $d\mu(\omega,k) = d\omega\cos\omega\,dk$. We introduced in Eq. (88) the propagator in momentum space:

$$\widetilde{K}(\omega,k) \coloneqq i\frac{\not{p}+m}{p^2-m^2}.$$

In order to obtain the retarded Green function the prescription to compute the integral is to translate the poles at $z = \pm E_k$ to $\pm E_k - i\varepsilon$, as depicted in Fig. 14; the contour, then, should be closed below the x-axis for $t > 0$ and above it for $t < 0$.

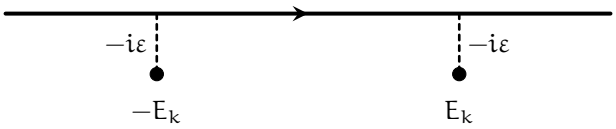


Figure 14.: Contour used to compute the propagator.

Contractions between internal fields in Eq. (87) give no contributions as one can readily verify. Such contractions correspond to evaluate the propagator for $t = x = 0$:

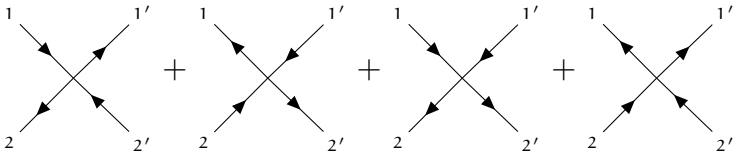
$$\begin{aligned} K(0) &= \int_B \frac{dk}{2\pi} \left(\gamma^0 - \frac{n \sin k}{E_k} \gamma^1 \right) \\ &= \gamma^0. \end{aligned}$$

Therefore, we have that

$$\begin{aligned} \gamma_\mu \langle 0|\psi\bar{\psi}|0\rangle \gamma^\mu &= \gamma_\mu K(0) \gamma^\mu \\ &= \gamma_\mu \gamma^0 \gamma^\mu \\ &= \gamma^0 \gamma^0 \gamma^0 - \gamma^1 \gamma^0 \gamma^1 \\ &= \gamma^0 - \gamma^0 = 0, \end{aligned}$$

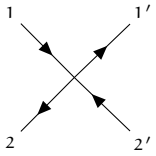
implying that at first order there are no loops in the Feynman diagrams.

By the considerations made so far, only four terms contribute to the amplitude of Eq. (87):

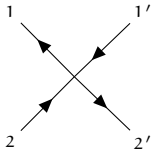
$i\mathcal{M} =$ 

The arrows on the legs of the diagrams correspond to the left and right modes of the field. In order to compute these diagrams, we have to follow

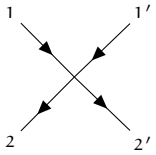
the arrows starting from the right and going backwards. The computation of the four possible diagrams contributing to the amplitude of Eq. (87) gives



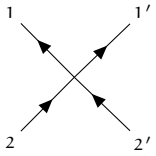
$$= (u^\dagger_{1'})_R(u_1)_R(u^\dagger_{2'})_L(u_2)_L = (u_1\bar{u}_{1'}\gamma^0)_{RR}(u_2\bar{u}_{2'}\gamma^0)_{LL},$$



$$= (u^\dagger_{1'})_L(u_1)_L(u^\dagger_{2'})_R(u_2)_R = (u_1\bar{u}_{1'}\gamma^0)_{LL}(u_2\bar{u}_{2'}\gamma^0)_{RR},$$



$$= (u^\dagger_{1'})_L(u_1)_R(u^\dagger_{2'})_R(u_2)_L = (u_1\bar{u}_{1'}\gamma^0)_{RL}(u_2\bar{u}_{2'}\gamma^0)_{LR},$$



$$= (u^\dagger_{1'})_R(u_1)_L(u^\dagger_{2'})_L(u_2)_R = (u_1\bar{u}_{1'}\gamma^0)_{LR}(u_2\bar{u}_{2'}\gamma^0)_{RL},$$

where in short $u_i \equiv u_{s_i}(k_i)$ and $u_{i'} \equiv u_{s'_i}(k'_i)$.

Let us consider the case where we have particles (positive energy) both in input and in output. As proved in Ref. [75], the conservation of two-momentum entails that the two particles either retain the same momenta as the initial ones, or exchange their momenta. Hence, in the first case we have that

$$\begin{aligned}(u_i\bar{u}_i\gamma^0)_{AA} &= \left[(\not{p}_i + m)\gamma^0\right]_{AA} \\ &= (p^0_i - p^1_i\gamma^1\gamma^0)_{AA} \\ &= p^0_i - p^1_i(\delta_{A,l} - \delta_{A,r})\end{aligned}$$

and for $A \neq B$

$$\begin{aligned}(u_i\bar{u}_i\gamma^0)_{AB} &= \left[(\not{p}_i + m)\gamma^0\right]_{AB} \\ &= m.\end{aligned}$$

Putting all together we obtain the total amplitude:

$$\begin{aligned}i\mathcal{M} &= (p^0_1 + p^1_1)(p^0_2 - p^1_2) + (p^0_1 - p^1_1)(p^0_2 + p^1_2) - 2m^2 \\ &= 2(p_1 \cdot p_2 - m^2).\end{aligned} \tag{89}$$

As a remark on this result, it is worth noticing that if the momenta of the two particles are equal, then the amplitude $i\mathcal{M}$ vanishes, as can be expected since the two particles occupy the same state.

On the other hand, the case where the two particles exchange their momenta amounts to swap $1 \leftrightarrow 2$ in Eq. (89) and therefore we get the same result. The same goes for the scattering of two antiparticles. However, when the scattering process happens between a particle and an antiparticle, the amplitude results to be

$$i\mathcal{M} = 2(p_1 \cdot p_2 + m^2).$$

In this case we see that the amplitude vanishes if the momenta are opposite, which agrees with the result of Eq. (89). Finally, since the two particles are identical, one can not in practice distinguish the case where the particles exchanged their momenta from the case where the momenta were not exchanged. So in the end one should add up the probability amplitude for the two situations. This concludes this brief introduction on the perturbation theory of the Thirring automaton.

In this chapter we presented an interacting QCA, the Thirring automaton. We reviewed the analytical solutions of the model in the sector of two particles. In the last section we presented a preliminary study on the perturbation theory of the Thirring automaton providing the computation of the tree-level diagrams for two particles.

8 CONCLUSIONS

The present dissertation focused on the derivation of the solutions in position space of the Dirac Quantum Walk in one spatial dimension and of the Weyl Quantum Walk in two and three spatial dimensions. Furthermore, we addressed the study of the basic aspects of the perturbation theory of the Thirring Quantum Cellular Automaton. The present thesis integrates in the recent line of research regarding the foundational aspects of Quantum Field Theory in a quantum-informational background. This line of research dates back to the informational paradigm advocated by Wheeler and synthesised in his dictum "it from bit". The problem undertaken by the informational paradigm connects various aspects regarding the foundational questions arising in the study of the basic features of Quantum Theory. In such regard, Quantum Information Theory plays a prominent role since it has been proven to lead to a deeper understanding of *entanglement* and *non-locality* which are distinctive features of Quantum Theory. Following the informational paradigm of Wheeler, we consider the possible fundamental mechanism underlying the physical world to be the processing of quantum information from which the usual dynamics of particles physics should emerge as an effective dynamics at large scales. One can show that the usual relativistic dynamics described by the Dirac equation can be recovered as a good approximation of a discrete evolution happening at the hypothetical Planck scale.

The next step in this scenario is, thus, the reconsideration in terms of the informational background also of the mechanical part of the physical world—particles or quantum fields, along with the dynamical equations governing their evolution in time—which lies under the framework of Quantum Field Theory, nowadays the best theory available to us describing the elementary constituents of our reality. So, the task at hand, is to give a formulation of Quantum Field Theory in terms of basic principles regarding the properties of the interaction network existing between the elementary objects constituting this "quantum computer" underlying our reality. Considering Quantum Theory the fundamental theory of systems, we assume that the basic objects constituting the primitive notions are quantum systems obeying the Fermi statistics. The idea that there can not be an infinite amount of information in any finite region of space [84–86] requires our fundamental description to involve a denumerable set of finite dimensional quantum systems. The theoretical framework in which we should develop such a description of natural phenomena is therefore that of Quantum Cellular Automata [5], since they represents precisely the

unitary evolution of countably-many quantum systems in local interaction. The premisses underlying our investigation of the Quantum Cellular Automaton theory consist in the principles of *unitarity*, *linearity*, *locality*, *homogeneity*, and *isotropy*. One can show that the emergent structure of the interaction network satisfying these assumptions indeed corresponds to a Quantum Cellular Automaton. The bridge between the automaton theory and the usual relativistic physics is given by a suitable approximation of the automaton theory that recovers the Dirac equation in the limit of small momenta with respect to a given reference scale [27, 28, 40, 42].

The program then regards, as we said, the idea of considering Quantum Cellular Automata as a fundamental description—in the sense that it operates at a scale much smaller than the scale of particle physics, as could be the Planck scale—underlying Quantum Field Theory, which should emerge in the end as an effective theory. Previous works have confirmed the present goal of the program which, at this stage, encompasses in the Quantum Cellular Automaton description systems of free particles, while an interacting theory has just recently began to be developed and the path towards a reconstruction of Electrodynamics is still missing, as well as the description in the setting of Quantum Cellular Automata of more general gauge theories.

Being a theory that is "quantum" *ab initio*, the Quantum Cellular Automaton theory can be also a fertile ground to explore the possible formulation of a quantum theory of gravity. In this respect, space-time itself is considered an emergent notion since the quantum systems constituting the causal network of the automaton are not "placed" in any background and time is just the "clock" that takes from one computational step to the other: this means that time is an inherent discrete notion and that the continuum of space-time is recovered as a large scale limit where the effects of the discreteness can not be detected. Information can play an even more fundamental role in theoretical physics as the relation with the *holographic principle* confirms [119–121]. The holographic principle, supposedly a feature of quantum gravity, has been proposed by 't Hooft [119, 121] and originates in the context of string theories. It states that the information needed to describe a volume of space can be encoded on a lower-dimensional boundary region and its most successful and rigorous realization of the principle comes from the AdS/CFT correspondence [122]. The interest in the holographic principle was inspired by black-hole thermodynamics [84, 85] and recently it was considered as a possible mechanism for the origin of gravity [123, 124].

The present dissertation started by exposing and presenting in Chapter 2 the theoretical framework at the core of the informational paradigm [4] that we considered in this work. We provided a brief review of the general construction of the notion of Quantum Cellular Automata on Cayley graphs following Refs. [40, 62, 63]. We then provided a review of the Dirac

Quantum Walk of Refs. [40, 42] obtained as the unique coupling of two Weyl walks satisfying the principles of unitarity, locality, homogeneity, and isotropy. We showed how in the relativistic limit of small momenta and masses the Dirac walk recovers the Dirac equation. Since this thesis is mainly devoted to the solution of these walks in position space by exploiting the path-sum formulation, we presented in the same chapter also the general formulation of the path-sum approach to calculate the propagator of a Quantum Walk on the Cayley graph of an arbitrary group.

In Chapter 3 we presented a numerical evaluation of the Dirac walk in one and three spatial dimensions exploiting the Fourier representation, which is suitable to implement fast algorithms, such as the Fast Fourier Transform of Ref. [125]. Furthermore, we show that the Dirac walk manifests *Zitterbewegung*, as the Dirac field, by analysing the evolution of the position operator on the lattice.

In Chapter 4 we showed the derivation of the analytical expression of the propagator for the Dirac walk in one spatial dimension given in Ref. [72]. The solution relies on the algebraic properties of the transition matrices of the walk. Remarkably, one can show that the matrix corresponding to an arbitrary sequence of steps depends only on the first and last bit of a suitable encoding of paths. This feature inspired and made possible the subsequent work in higher dimensions.

In Chapter 5 we presented a reformulation of the derivation of the position-space solution of Ref. [73] for the Weyl Quantum Walk in two spatial dimensions taking under consideration the results in dimension three of Ref. [74]. This reformulation is due to the similarity between the transition matrices of the Weyl walks in two and three spatial dimensions that allows us to exploit similar combinatorial properties of the binary encoding of paths.

In Chapter 6 we finally specialized the results of Chapter 5 to the case of the Weyl Quantum Walk in three spatial dimensions. The computation of the propagator relies then on similar features such as the dependence of the transition matrix associated to a path only on the first and last bits of the binary encoding of the path. As a consequence one can translate the algebraic properties of the transition matrices and geometric ones of the lattice paths to the algebraic properties of binary strings, which are easy to manipulate.

In Chapter 7 we discussed the Thirring Quantum Cellular Automaton on the line. This model is characterized by a local on-site interaction—namely, two particles interact only if they collide on the same lattice cell—and it has the Thirring model [126], representing the self-interactions of the Dirac field, as the relativistic limit of large scales. The Thirring automaton shares this type of interactions with the Hubbard model [113, 127], representing the simplest model in solid-state physics describing the on-site interaction of particles. As the Hubbard model, the Thirring automaton can be similarly solved exploiting the Bethe Ansatz [128]. We review in this chapter

the solution provided by Ref. [75] for the two-particle sector, in which case the automaton can be described by a Quantum Walk (Thirring walk). The Thirring walk shows distinctive features with respect to other interacting walks known in the literature such as the one based on the Hadamard Quantum Walk [117]. In particular, there exists a unique bound state for every choice of the coupling constant and of the total momentum. Furthermore, the Thirring walk is also characterized by stationary bound states even for vanishing coupling constant, due to the spectral properties of the free evolution operator. In the same chapter, we also provide a reformulation of the Thirring walk suitable for exploiting the perturbative approach. The full derivation of the Feynman rules and the Feynman diagrams for the Thirring automaton is still in an unpolished and unripe form, and it still needs a thorough investigation.

The thesis addressed different aspects of the automaton theory, in order to gain a deeper insight on the features of some instances of Quantum Cellular Automata. The Quantum Cellular Automaton framework poses a solid theoretical background for a reconstruction of Quantum Field Theory based on informational principles; however, we still need a consistent way to formulate a gauge theory, since we lack a formal way that selects the kind of interactions that can be defined on an automaton.

As a future perspective, an automaton theory could be also an effective way to explore the physics beyond the Standard Model. Another aspect that the informational paradigm could address is a formulation of a theory of gravity in a scenario that is quantum *ab initio* and the study of the connection with the holographic principle. Another possible continuation of the present work could be the application of the path-sum approach, exploiting the algebraic structure of the transition matrices, to the interacting case of the Thirring automaton. Furthermore, the path-sum approach could be applied also in more general situations to Quantum Walks defined on non-Abelian groups—for which the Fourier analysis can be difficult since their representations are generally unknown—providing an alternative strategy to study the diffusion properties of these walks. For instance, it could be interesting to study quantum walks defined on hyperbolic groups, such as Fuchsian groups. The main obstacle in this case is represented by the fact that the word problem [129] is not straightforwardly solvable and this affects the issue of finding a classification of the paths on the graph.

A PROOFS FOR THE WEYL QW IN TWO SPATIAL DIMENSIONS

Proof of Lemma 5.1.1. Suppose for definiteness that $K \geqslant H$ (the case $K < H$ is very similar). Take $v \in \mathfrak{S}_t(K)$ canonical and $w \in \mathfrak{S}_t(H)$. Then we can arrange the strings in the following way:

$$\begin{array}{cc|c} & K & t-K \\ v & 1\ldots1 & 0\ldots0 \\ w & H-n & n \end{array}$$

This corresponds to consider a splitting of w into two subtrings $L_K w = w_1 \ldots w_K$ and $R_K w = w_{K+1} \ldots w_t$, so that $\iota(R_K w) = n$ for some n and $\iota(L_K w) = H - n$. Since $\mathfrak{S}_K(n) \cap \mathfrak{S}_K(m) = \emptyset$ for $n \neq m$, we have then a partition of $\mathfrak{S}_t(H)$:

$$\mathfrak{S}_t(H) = \bigcup_{n \in I} \mathfrak{S}_K(H-n) \frown \mathfrak{S}_{t-K}(n), \tag{90}$$

with $n \in I = \{0, 1, \ldots, \min\{H, t-K\}\}$. The $\oplus$ operation preserves the size of the subsets and therefore one obtains

$$\begin{aligned} v \oplus \mathfrak{S}_t(H) &= \bigcup_{n \in I} v \oplus [\mathfrak{S}_K(H-n) \frown \mathfrak{S}_{t-K}(n)] \\ &= \bigcup_{n \in I} [L_K v \oplus \mathfrak{S}_K(H-n)] \frown [R_K v \oplus \mathfrak{S}_{t-K}(n)] \\ &= \bigcup_{n \in I} \mathfrak{S}_K(K-H+n) \frown \mathfrak{S}_{t-K}(n) \\ &= \bigcup_{n \in I} \mathfrak{W}(K, H, n). \end{aligned}$$

The Hamming weight of a string $w \in \mathfrak{W}(K, H, n)$ is given by

$$\iota(w) = \iota(L_K w) + \iota(R_K w) = K - H + 2n,$$

and, finally, the size of each factor $\mathfrak{W}(K, H, n)$ is given by

$$|\mathfrak{W}(K, H, n)| = \binom{K}{H-n}\binom{t-K}{n}. \qquad \square$$

Proof of Corollary 5.1.1. Let $v \in \mathfrak{S}_t(K)$ and let π_v be a bitwise permutation such that $\pi_v(v)$ is canonical, then we have that

$$\begin{aligned}\pi_v(v \oplus \mathfrak{S}_t(H)) &= \pi_v(v) \oplus \pi_v(\mathfrak{S}_t(H)) \\ &= \pi_v(v) \oplus \mathfrak{S}_t(H).\end{aligned}$$

Therefore, using the decomposition of Lemma 5.1.1, we can write

$$\begin{aligned}v \oplus \mathfrak{S}_t(H) &= \pi_v^{-1}\left(\bigcup_{n\in I} \mathfrak{W}(K, H, n)\right) \\ &= \bigcup_{n\in I} \pi_v^{-1}(\mathfrak{W}(K, H, n)).\end{aligned}$$

□

Proof of Lemma 5.1.2. Let $v \in \mathfrak{S}_t(K)$. From Lemma 5.1.1 and Corollary 5.1.1 we know that $\iota(v \oplus Sv) = 2n$, for some n. Then letting $c \coloneqq \pi_v(v)$, we have that

$$\begin{aligned}\iota(v \oplus Sv) &= \iota(\pi_v(v \oplus Sv)) \\ &= \iota(c \oplus \pi_v Sv) \\ &= \iota(L_K c \oplus L_K \pi_v Sv) + \iota(R_K \pi_v Sv) \\ &= \iota(\overline{L_K \pi_v Sv}) + \iota(R_K \pi_v Sv) \\ &= K - \iota(L_K \pi_v Sv) + \iota(R_K \pi_v Sv).\end{aligned}$$

On the other hand, it holds true that

$$\iota(L_K \pi_v Sv) + \iota(R_K \pi_v Sv) = \iota(\pi_v Sv) = \iota(Sv) = \iota(v) = K.$$

Therefore, the Hamming weight of $v \oplus Sv$ reads

$$\iota(v \oplus Sv) = 2K - 2\iota(L_K \pi_v Sv)$$

and we have the result:

$$\iota(\overline{L_K \pi_v Sv}) = \iota(R_K \pi_v Sv) = n.$$

□

Proof of Lemma 5.1.3. Consider a string $v \in \mathfrak{S}_t(K)$ such that $\iota(v \oplus Sv) = 2n$ and $v_1 = v_t = 0$, *i.e.* a string $v \in \mathfrak{S}_{00}(t)Kn$. This string can be viewed as follows:

$$\boxed{0\ldots0}\,|\,\boxed{1\ldots1}\,\cdots\,\boxed{0\ldots0}\,\cdots\,\boxed{1\ldots1}\,|\,\boxed{0\ldots0}$$

where there are exactly $2n$ interfaces $|$ separating 0-boxes from 1-boxes. The number of boxes is n for both 0-boxes $\boxed{0\ldots0}$ and 1-boxes $\boxed{1\ldots1}$ (in the general case one would have $n + \bar{a}\bar{a}'$ and $n + aa'$ respectively). We then need to count how many strings can be constructed for a fixed number of

interfaces. Let us start from the 1-boxes: we have K elements to distribute in n boxes, but we have to leave at least one bit in a box in order to identify it. So we have only $K-n$ bits that can be arranged freely. In order to count in how many ways we can do this, we can think to arrange the $K-n$ 1-bits represented by the symbol $\star$ together with some bars $|$ to denote the slots:

$$\star\star|\star|\star\star|\star\star\star$$

Given n slots, $n-1$ bars are sufficient to indentify the slots, hence we have to permute $K-n+n-1 = K-1$ objects of which $n-1$ are equal: this is given by the number of permutations with repetitions

$$\frac{(K-1)!}{(n-1)!(K-n)!} = \binom{K-1}{n-1}.$$

The problem can be interpreted in another way. An integer number K can be written in several ways as the sum of a sequence of other (strictly) positive integers. For instance, the number 5 has 16 compositions:

$$\begin{aligned}
&5,\\
&4+1,\\
&3+2,\\
&3+1+1,\\
&2+3,\\
&2+2+1,\\
&2+1+2,\\
&2+1+1+1,\\
&1+4,\\
&1+3+1,\\
&1+2+2,\\
&1+2+1+1,\\
&1+1+3,\\
&1+1+2+1,\\
&1+1+1+2,\\
&1+1+1+1,
\end{aligned}$$

of which we need only those with a fixed number of parts, say 3:

$$\begin{aligned}
&3+1+1,\\
&2+2+1,\\
&2+1+2,\\
&1+3+1,\\
&1+2+2,\\
&1+1+3.
\end{aligned}$$

Two sequences that differ in the order of their terms define different *compositions* of K, whereas if we disregard the order, the two sequences define the same *partition*. The case we are looking for is the first one, since sequences differing in the order of their terms generate different binary strings and thus different paths on the lattice. So we have to count the number of composition of K into n parts which is given precisely by $\binom{K-1}{n-1}$ [109].

We denote here as $C_{K,n}$ the number of n-compositions of an integer K:

$$C_{K,n} = \begin{cases} \binom{K-1}{n-1}, & \text{if } K \geqslant n > 0, \\ 1, & \text{if } K = n = 0, \\ 0, & \text{otherwise.} \end{cases}$$

For the 0-bits the same argument applies, so the counting results to be $C_{t-K,n+1}$, since there are $n+1$ boxes where one can arrange the $t-K$ 0-bits. So the total number of binary strings is given by

$$\begin{aligned}
u_{00}(n) &= \binom{K-1}{n-1}\binom{t-K-1}{n} \\
&= C_{K,n}C_{t-K,n+1}.
\end{aligned}$$

In the end, for generic a and a' the cardinality of $\mathfrak{T}_{aa'}(t,K,n)$ turns out to be

$$u_{aa'}(n) \coloneqq |\mathfrak{T}_{aa'}(t,K,n)| = C_{K,n+aa'}C_{t-K,n+\bar{a}\bar{a}'}. \qquad \square$$

B PROOFS FOR THE WEYL QW IN THREE SPATIAL DIMENSIONS

Proof of Proposition 6.2.1. Suppose that $K \geqslant H$ and let $v \in \mathfrak{S}_t(K)$, $w \in \mathfrak{S}_t(H)$. Naming c the canonical string in $\mathfrak{S}_t(K)$, we then have

$$\begin{aligned}\sum_{w\in\mathfrak{S}_t(H)} z^{v\oplus w} &= \sum_{w\in\mathfrak{S}_t(H)} z^{c\oplus w} \\ &= \sum_{n=0}^{\min\{H,t-K\}} \sum_{w\in\mathfrak{W}(K,H,n)} z^{w}.\end{aligned}$$

In the first step we used the bitwise-permutation independence: for any π bitwise permutation it holds that

$$\begin{aligned}\sum_{w} z^{v\oplus w} &= \sum_{w} z^{\pi(v\oplus w)} \\ &= \sum_{w} z^{\pi(v)\oplus\pi(w)} \\ &= \sum_{w} z^{\pi(v)\oplus w}.\end{aligned}$$

In the second step we employed the result of Lemma 5.1.1:

$$\begin{aligned}\mathfrak{S}_t(H) &= \bigcup_n \mathfrak{S}_K(H-n) \frown \mathfrak{S}_{t-K}(n) \\ &= \bigcup_n \mathfrak{W}(K,H,n).\end{aligned}$$

Moreover, one has

$$\iota(w) = K - H + 2n \quad \forall w \in \mathfrak{W}(K,H,n).$$

Therefore we can write

$$\begin{aligned}\sum_{w\in\mathfrak{W}(K,H,n)} z^{w} &= |\mathfrak{W}(K,H,n)|\, z^{K-H+2n} \\ &= \binom{K}{H-n}\binom{t-K}{n} z^{K-H+2n},\end{aligned}$$

so that

$$\sum_{w} z^{v\oplus w} = \xi(K,H;z)$$
$$= z^{|K-H|} \sum_{n=0}^{\min\{H,t-K\}} \binom{K}{H-n}\binom{t-K}{n} z^{2n}. \qquad \square$$

Proof of Proposition 6.2.2. Let us consider the case $K_1 \geqslant K_2$ as the other one is a simple variation of the following construction. First of all, let us implement the result of Lemma 5.1.3 in the expression for the coefficients (64):

$$c_{ab} = \sum_{v,w} (-1)^{(v\oplus Sv)w} \xi(\iota(v\oplus w), K_3; \pm i)$$
$$= \sum_{a'=0,1} (-1)^{(a\oplus a')b} \sum_{n} c'_{aa'b}(n),$$

where

$$c'_{aa'b}(n) := \sum_{v',w'} (-1)^{(av'\oplus v'a')w'} \xi(\iota(av'\oplus w') + a'\oplus b, K_3; \pm i),$$

and $av'a' \in \mathfrak{T}_{aa'}(t,K_1,n)$ and $w' \in \mathfrak{S}_{t-1}(K_2-b)$. Consider for now the case $a = a' = 0$ (the others are pretty much similar). We can define a particular "canonical" labeled string $\bar{v}' = (\lambda'_{(1)}, \lambda'_{(2)})$ such that $\lambda'_{(1)}$, $L_{K_1}(\lambda'_{(2)})$ and $R_{K_1}(\lambda'_{(2)})$ are all canonical; moreover we require $\lambda'_{(1)}$ and $\lambda'_{(2)}$ to have Hamming weight n. In this way we have:

$$c'_{00b}(n) = \sum_{v',w'} (-1)^{\lambda'_{(2)}w'} \xi\Big[\iota\Big(\lambda'_{(1)}\oplus w'\Big), K_3; \pm i\Big]$$
$$= u_{aa'}(n) \sum_{w'} (-1)^{\lambda'_{(2)}w'} \xi\Big[\iota\Big(\lambda'_{(1)}\oplus w'\Big), K_3; \pm i\Big].$$

Such form of the sum for $c_{00b}(n)$ suggests to split the set $\mathfrak{S}_{t-1}(K_2-b)$ as follows:

$$\mathfrak{S}_{t-1}(K_2-b) = \bigcup_{J=b}^{\min\{K_2,t-K_1-1\}} \bigcup_{k=0}^{n} \bigcup_{k'=0}^{n} \mathfrak{Z}_b^{(1)}(J,k)\mathfrak{Z}_b^{(0)}(J,k'),$$
$$\mathfrak{Z}_b^{(1)}(J,k) = \mathfrak{S}_n(k)\mathfrak{S}_{K_1-n}(K_2-J-k), \tag{91}$$
$$\mathfrak{Z}_b^{(0)}(J,k') = \mathfrak{S}_n(k')\mathfrak{S}_{t-K_1-n-1}(J-k'-b). \tag{92}$$

With this splitting, the coefficients c'_{00b} can then be written as

$$c'_{00b}(n) = u_{00}(n) \sum_{J,k,k'} \sum_{\widetilde{w}_{(1)},\widetilde{w}_{(0)}} (-1)^{k+k'} \xi(K_1-K_2+2J, K_3; \pm i),$$

where $\widetilde{w}_{(1)} \in \mathfrak{Z}_b^{(1)}(J,k)$ and $\widetilde{w}_{(0)} \in \mathfrak{Z}_b^{(2)}(J,k')$. So finally we have

$$\begin{aligned} c'_{00b}(n) &= u_{00}(n) \sum_{J,k,k'} (-1)^{k+k'} \xi(K_1 - K_2 + 2J, K_3; \pm i) \cdot \\ &\qquad \cdot \binom{n}{k} \binom{K_1 - n}{K_2 - J - k} \binom{n}{k'} \binom{t - K_1 - n - 1}{J - k' - b} \\ &= u_{00}(n) \sum_{J} \varphi_{00b}(n, J; -1)\, \xi(K_1 - K_2 + 2J, K_3; \pm i), \end{aligned}$$

where the function $\varphi_{00b}(n, J; z)$ is given by

$$\begin{aligned} \varphi_{00b}(n, J; z) &= \sum_{k,k'} z^{k+k'} \left| \mathfrak{Z}_b^{(1)}(J,k) \right| \left| \mathfrak{Z}_b^{(0)}(J,k') \right| \\ &= w^{(1)}_{00b}(n, J; z) w^{(0)}_{00b}(n, J; z). \end{aligned}$$

□

C DISCRETE FOURIER TRANSFORM

The simulations performed to generate the plots of Chapter 3 employed the Fourier representation to generate the initial configuration. We provide here a brief review of the Discrete Fourier Transform (DFT) employed to implement the QW algorithm in a computer program.

The evolution a QW can certainly be implemented exploiting the local update rule in position space (see Eq. (18)). Although this approach is generally straightforward to implement numerically, it requires, however, the repeated application of the one-step update rule at each time-step. For large lattices, especially in dimensions higher than one, or many-particle systems this can be a resource-intensive task. On the contrary, the evolution in the Fourier representation changes only a phase, since we are just employing the eigenbasis of the walk, and the complexity of the computation is hidden in the computation of the FT. Nevertheless, there exist efficient algorithms that implement the DFT, such as the Cooley–Tukey Fast Fourier Transform (FFT) algorithm [125].

In the general case, we consider the Abelian group $\mathbb{Z}^d$ and its Cayley graphs. Having the numerical implementation in mind, we consider the restriction of the infinite lattice to a finite number of sites, or, equivalently, we take all the functions on the lattice to be periodic also in the direct space. In particular, we are going to discuss the DFT on a rectangular lattice in dimension d and then we will specialize to the case of the DFT on the BCC lattice.

Our goal is the implementation of the update rule of a given QW. The Hilbert space associated to the QW is $\mathscr{H} \coloneqq \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^s$. The evolution of an initial state $|\psi(0)\rangle \in \mathscr{H}$ is given by the repeated application of the walk unitary W:

$$|\psi(t)\rangle = W^t |\psi(0)\rangle .$$

Expressing the initial state $|\psi(0)\rangle$ in the Fourier representation as

$$|\psi(0)\rangle = \int_B d\mathbf{k}\ |\mathbf{k}\rangle |\hat{\psi}(0,\mathbf{k})\rangle , \qquad |\hat{\psi}(0,\mathbf{k})\rangle \in \mathbb{C}^s,$$

and recalling the general expressions in Eqs. (2) and (3) providing the diagonal representation of the walk, the state at time t can be written as

$$|\psi(t,\mathbf{x})\rangle = \frac{1}{(2\pi)^{d/2}} \int_B d\mathbf{k}\ e^{-i\mathbf{k}\cdot\mathbf{x}} e^{-iH(\mathbf{k})t} |\hat{\psi}(0,\mathbf{k})\rangle ,$$

where

$$|\hat{\psi}(0,\mathbf{k})\rangle = \sum_{\mathbf{x}\in\mathbb{Z}^d} e^{i\mathbf{k}\cdot\mathbf{x}}\,|\psi(0,\mathbf{x})\rangle$$

is the FT of $|\psi(0,\mathbf{x})\rangle$.

From a practical point of view, we actually employ a finite data-set to represent the state of the walk. Suppose we have N_i samples in dimension i, for $i = 1,2,\ldots,d$. The dual space representation is given by a discrete sampling of the continuous FT at frequencies $\frac{2\pi}{N_i}k_i$, with $k_i \in \{-\lfloor N_i/2\rfloor,\ldots,\lceil N_i/2\rceil - 1\}$. This is equivalent to employ the periodic boundary conditions in position space on the infinite lattice.

C.1 RECTANGULAR DFT

For a given sequence $\varphi \in \ell^2(\mathbb{Z}^d)$ we consider a restriction $f\colon \mathbb{Z}^d \to \mathbb{C}$ on a finite region $\mathcal{N} = \{\mathbf{m}\in\mathbb{Z}^d \mid 0 \leqslant m_i < N_i,\, i = 1,\ldots,d\}$, where N_i is the number of samples in dimension $i = 1,\ldots,d$, such that $f|_{\mathcal{N}} = \varphi|_{\mathcal{N}}$. Assuming periodic boundary conditions, the function f is extended to the whole lattice with periodicity matrix $\mathbf{N} = \mathrm{diag}(N_1,\ldots,N_d)$:

$$f_{\mathbf{n}+\mathbf{N}\mathbf{r}} = f_{\mathbf{n}}, \quad \forall\,\mathbf{n},\mathbf{r}\in\mathbb{Z}^d.$$

The representation in the dual space of the function f corresponding to the dual representation of φ coincides with the DFT, namely we have

$$\hat{f}_{\mathbf{k}} = \mathcal{F}(f)(\mathbf{k}) \coloneqq \frac{1}{\sqrt{|\mathcal{N}|}}\sum_{\mathbf{n}\in\mathcal{N}} f_{\mathbf{n}} e^{-2\pi i \mathbf{p}^\intercal \mathbf{N}^{-1}\mathbf{n}} e^{2\pi i \mathbf{k}^\intercal \mathbf{N}^{-1}\mathbf{n}}, \quad \mathbf{k}\in\mathcal{N}, \tag{93}$$

where $N = |\mathcal{N}| = \det(\mathbf{N})$ and $p_i = \left\lfloor \frac{N_i}{2}\right\rfloor$. The reason of the extra phase factor is that the frequencies actually computed should lie in the range $[-\pi,\pi]$, while the indices of the sequence are conveniently chosen in the range $\{0,\ldots,N_i-1\}$ for each dimension. The inversion formula is given by the following expression:

$$f_{\mathbf{n}} = \mathcal{F}^{-1}(\hat{f})(\mathbf{n}) = e^{2\pi i \mathbf{p}^\intercal \mathbf{N}^{-1}\mathbf{n}} \frac{1}{\sqrt{|\mathcal{N}|}}\sum_{\mathbf{k}\in\mathcal{N}} \hat{f}_{\mathbf{k}} e^{-2\pi i \mathbf{k}^\intercal \mathbf{N}^{-1}\mathbf{n}}. \tag{94}$$

The two relations given in Eqs. (93) and (94) are all we need to implement numerically the walk evolution in the Fourier representation. At each time-step, though, we need to perform the inverse DFT to obtain the probability distribution in position space. The effectiveness and efficiency of algorithms based on the FFT are better exploited of we need only the state at some specific time t, rather than the case where we are interested in the complete time evolution of the state. In the latter case, it may be more con-

venient to employ directly the one-step update rule of the walk since it is usually straightforward to implement numerically.

In the following section, we specialize the discussion to the BCC lattice which is the lattice where the Dirac QW in dimension $d = 3$ is defined.

C.2 DFT ON THE BCC LATTICE

In dimension $d = 3$ the only lattice that admits a QW satisfying the assumptions of Section 2.3 is the BCC lattice [40]. In this case, the DFT is slightly different since the first Brillouin zone of the BCC lattice is not a cube, but instead is a *rhombic dodecahedron*, as depicted in Fig. 5. Nevertheless, the problem of computing the DFT on the BCC lattice can be reduced to the computation of two rectangular DFTs [130]. In this way, one can rely on fast algorithms to compute the FT such as the usual rectangular FFT algorithm [125].

In order to compute the DFT we have to choose a suitable finite region of the lattice; a convenient choice is obtained considering that the BCC lattice can be described by the vertex set $G = 2\mathbb{Z}^3 \cup (2\mathbb{Z}^3 + \mathbf{t})$, with $\mathbf{t} = (1, 1, 1)$. In this way, we can choose as fundamental region the set $\mathcal{B} \coloneqq 2\mathcal{N} \cup (2\mathcal{N} + \mathbf{t})$. A sequence $f_{\mathbf{n}}$ defined on the fundamental region $\mathcal{B}$ can be split into two subsequences $f^0_{\mathbf{n}}$ and $f^1_{\mathbf{n}}$ each one having as fundamental region the rectangular region $\mathcal{N}$. The two new sequences are defined, respectively, on the even and odd indices of the original sequence, namely

$$f^0_{\mathbf{n}} = f_{2\mathbf{n}}, \qquad f^1_{\mathbf{n}} = f_{2\mathbf{n}+\mathbf{t}}, \qquad \forall \mathbf{n} \in \mathcal{N},$$

and are periodic with periodicity matrix $\mathbf{N} = \operatorname{diag}(N_1, N_2, N_3)$:

$$f^j_{\mathbf{n}+\mathbf{N}\mathbf{r}} = f^j_{\mathbf{n}}, \quad \forall \mathbf{n}, \mathbf{r} \in \mathbb{Z}^3, \quad j = 0, 1.$$

In the Fourier representation the periodicity matrix is given by $2\mathbf{N}$, so that the total number of frequencies is $\det(2\mathbf{N}) = 8N_1N_2N_3 = 8|\mathcal{N}|$. Therefore, the correct definition for the FT of $f_{\mathbf{n}}$ is given by

$$\hat{f}_{\mathbf{k}} = \mathcal{F}(f)(\mathbf{k}) \coloneqq \frac{1}{2\sqrt{|\mathcal{B}|}} \sum_{\mathbf{n}\in\mathcal{B}} f_{\mathbf{n}} e^{2\pi i \mathbf{k}^\intercal (2\mathbf{N})^{-1}\mathbf{n}}, \qquad \forall \mathbf{k} \in \mathcal{K}, \tag{95}$$

$\mathcal{K}$ being the set of Fourier indices that can be chosen as

$$\mathcal{K} = \left\{ \mathbf{k} \in \mathbb{Z}^3 \;\middle|\; -N_i \leqslant k_i < N_i,\ i = 1, 2, 3 \right\}.$$

In order to compute the DFT in Eq. (95), we do not need to compute the function for the whole set $\mathcal{K}$ since, of the 8 replica of the fundamental region $\mathcal{N}$ that are included in $\mathcal{K}$, only two are inequivalent, say $\mathcal{N}$ and $\mathcal{N} -$

$\mathbf{t}$. As proved in details in [130], this means that, exploiting the geometry of the BCC lattice, we can restrict the sequence $\hat{f}_{\mathbf{k}}$, with $\mathbf{k} \in \mathcal{K}$, to two subsequences $\hat{f}^0_{\mathbf{k}}$ and $\hat{f}^1_{\mathbf{k}}$ with $\mathbf{k}$ in $\mathcal{N}$. In this way, we reduce the problem of the computation of the DFT on the BCC lattice in terms of two rectangular DFTs:

$$\hat{f}^0_{\mathbf{k}} = \frac{1}{\sqrt{2}}\Big[\mathcal{F}(f^0)(\mathbf{k}) - a_{\mathbf{k}}\mathcal{F}(f^1)(\mathbf{k})\Big],$$
$$\hat{f}^1_{\mathbf{k}} = \frac{1}{\sqrt{2}}\Big[\mathcal{F}(f^0)(\mathbf{k}) + a_{\mathbf{k}}\mathcal{F}(f^1)(\mathbf{k})\Big],$$

with $\mathbf{k} \in \mathcal{N}$ and $a_{\mathbf{k}} \coloneqq e^{i\pi \mathbf{k}^\intercal \mathbf{N}^{-1}\mathbf{t}}$. Finally, we can compute the inversion formulae to get back to the direct space representation:

$$f^0_{\mathbf{n}} = \frac{1}{\sqrt{2}}\mathcal{F}^{-1}(\hat{f}^0 + \hat{f}^1)(\mathbf{n}),$$
$$f^1_{\mathbf{n}} = \frac{1}{\sqrt{2}}\mathcal{F}^{-1}(a^*(\hat{f}^1 - \hat{f}^0))(\mathbf{n}).$$

D INTERACTION PICTURE

The interaction picture is an intermediate representation between the Schrödinger picture and the Heisenberg picture. It is a useful viewpoint in QM to describe the dynamics of a quantum system in presence of interactions that can be regarded as small perturbations to a well-understood dynamics, as a free QFT. If we are given a QCA described by a unitary operator A, the states and the operators evolve in the Schrödinger picture as

$$\begin{aligned} |\psi(t+1)\rangle_S &= A\,|\psi(t)\rangle_S\,, \\ O_S &\coloneqq O_S(t) = O_S(0). \end{aligned}$$

In the present case, for an interacting QCA, the unitary operator providing the time evolution consists actually in two steps. At each step of the automaton we are actually doing two distinct steps

$$A = A_{\text{int}} A_f,$$

where A_f denotes a *free* evolution, describing a linear nearest-neighbours QCA such as the free Dirac QW, and A_{int} represents an interaction term that is non-linear in the fields.

In order to obtain the interaction picture description, we consider A_{int} as a perturbation of the analytically solved free evolution given by A_f. In the interaction picture both states and operators are time-dependent; the evolution of the states is governed by interacting term, whereas the observables evolve via the free operator A_f:

$$\begin{aligned} |\psi(t)\rangle_I &\coloneqq (A_f^\dagger)^t\,|\psi(t)\rangle_S\,, \\ O_I(t) &\coloneqq (A_f^\dagger)^t O_S A_f^t. \end{aligned}$$

Consequently, letting

$$A_I(t) \coloneqq (A_f^\dagger)^t A_{\text{int}} A_f^t$$

to denote the time evolution operator in the interaction picture, we then obtain

$$\begin{aligned} |\psi(t+1)\rangle_I &= (A_f^\dagger)^{t+1}\,|\psi(t+1)\rangle_S \\ &= (A_f^\dagger)^{t+1} A_{\text{int}} A_f\,|\psi(t)\rangle_S \\ &= (A_f^\dagger)^{t+1} A_{\text{int}} A_f A_f^t\,|\psi(t)\rangle_I \\ &= A_I(t+1)\,|\psi(t)\rangle_I\,. \end{aligned} \tag{96}$$

The solution of Eq. (96) for an arbitrary time is easily obtained:

$$|\psi(t+n)\rangle_I = U(t+n,t)\,|\psi(t)\rangle_I\,, \tag{97}$$
$$U(t+n,t) \coloneqq \prod_{j=0}^{n-1} A_I(t+n-j).$$

We assume here that the interaction term has the following expression:

$$A_{int} = e^{-i\lambda H_{int}}$$

where H_{int} is the interaction Hamiltonian and λ is a real coupling constant. The operator $A_I(t)$ can thus be written as

$$\begin{aligned} A_I(t) &= (A_f^\dagger)^t e^{-i\lambda H_{int}} A_f^t \\ &= e^{-i\lambda H_I(t)} \\ &= \sum_n (-i\lambda)^n \frac{(H_I(t))^n}{n!}. \end{aligned} \tag{98}$$

By inserting the power expansion (98) into Eq. (97) we obtain the Dyson formula for the QCA:

$$U(t_+,t_-) = \mathsf{T}\left[\exp\left(-i\lambda \sum_{t=t_-+1}^{t_+} H_I(t)\right)\right]. \tag{99}$$

where T is the time ordering operator, *i.e.*

$$\mathsf{T}[A(t_1)B(t_2)] = \begin{cases} A(t_1)B(t_2), & \text{if } t_1 > t_2, \\ B(t_2)A(t_1), & \text{if } t_2 > t_1. \end{cases}$$

In a typical scenario we are interested in computing amplitudes and cross sections of scattering processes. This quantities are computed by means of the matrix elements of the so-called S-matrix, *i.e.*

$$\langle f|S|i\rangle \coloneqq \lim_{t_\pm \to \pm\infty} \langle f|U(t_+,t_-)|i\rangle\,, \tag{100}$$

where $|i\rangle$ and $|f\rangle$ are eigenstates of the free theory. The Dyson formula (99) allows us to compute the amplitudes of Eq. (100) as a power series in the coupling contant λ.

We now focus our analysis on local interactions, which are described by an Hamiltonian operator of the following kind:

$$H_{int} \coloneqq \sum_{x\in\mathbb{Z}} H_{int}(x). \tag{101}$$

By inserting Eq. (101) and Eq. (99) into Eq. (100) we obtain the power series

$$\langle f|S|i\rangle = \sum_{n=0}^{+\infty} \frac{(-i\lambda)^n}{n!} \sum_{X_1,\dots,X_n} \langle f|T[H_I(X_1)\cdots H_I(X_n)]|i\rangle\,, \tag{102}$$

where we introduced the notation

$$X_i \coloneqq (t_i, x_i), \qquad \sum_{X_i} O_I(X_i) \coloneqq \sum_{t_i=-\infty}^{+\infty} \sum_{x_i\in\mathbb{Z}} O_I(t_i, x_i).$$

Usually, $H_I(X_i)$ is a polynomial in the field operators $\psi_A(x)$, $\psi_A^\dagger(x)$. Therefore, from Eq. (102), we need to compute time order product of field operators that can be reduced to products of the contractions of all the possible pairs of field operators, according to Wick's theorem [118].

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