Towards quantum lattice-Boltzmann methods

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ABSTRACT

In these notes, formal models are proposed, mainly based on quantum walks, to simulate transport equations and beyond. Quantum walks are a composition of a scattering operator and a translation operator, formally equivalent to a quantum Boltzmann scheme. Assuming this correspondence, quantum walks are used to model a variety of physical situations, such as the dynamics of a quantum fluid in the relativistic and non-relativistic limit. In addition, the issue of transport simulation on arbitrary curved manifolds is addressed.

Contents

1.0 Introduction **2**

2.0 Quantum Walk **5**
2.1 Quantum Walks over square grids 5
2.2 Higher dimensional spaces 8

3.0 Discretization of transport equations **9**
3.1 Plastic Quantum Walk 10
3.1.1 The infinite line 10
3.2 Convergence 15
3.3 Discussion and open problems 15
3.4 QW over triangulations 16
3.4.1 The model 16

4.0 Quantum Lattice Boltzmann as Quantum Walk **20**
4.1 Operator splitting versus Quantum Walk for the Dirac equation 20
4.2 Quantum Lattice Boltzmann scheme from the Dirac equation to QWs 21
4.3 An example : Quantum Simulation of Hydrodynamics shocks 24

5.0 Introducing effective nonlinearities **27**

6.0 Hints for a QLB on curved surface **29**
6.1 Mimicking curved transport on the grid 29
6.2 A Quantum Walk over a generic 2D spatial triangulation 31
6.3 Discussion and perspectives 33

1.0 INTRODUCTION

Classical computation is based on the abstract model of the Turing Machine, defined in 1936 by the English mathematician Alan Turing and subsequently reworked by John von Neumann in the 1940s. Later, at the beginning of the 80s, when the quantum theory was sufficiently advanced, it became clear that to efficiently simulate a quantum system a classical computer was no longer sufficient. Just in those years Richard Feynman argued that no classical Turing Machine could simulate a quantum system without an exponential slowdown of its performance. This is due to the space complexity needed to describe a quantum state. In fact such a state is typically described by a number of parameters that grows as $O(\exp(N))$ with N size of the system and moreover, to simulate the temporal evolution of the system we also need a number of operations that grows exponentially with its size. Therefore, quantum theory lends itself to a combinatorial complexity of possible dynamic structures enormously large. It was Feynman himself in 1982 who proposed a solution to this problem. Quoting him: *"Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws." (Feynman, 1982)*...a quantum machine has the capacity to contain an exponential explosion of information avoiding the use of an exponentially large amount of physical resources. It is important to notice that, although N qubits can "carry" a larger amount of (classical) information (thanks to quantum superposition), the Holevo's theorem proved that the amount of classical information that can be retrieved, i.e. accessed, can be only up to N classical (non-quantum encoded) bits.

The idea that information can be stored in microscopic quantum states was an unprecedented challenge for scientists, since it opened the perspective of using quantum matter itself to make calculations. Unfortunately, the quantum coherence that would allow, e.g. quantum algorithms to work, is very fragile.

Before scientists could accept such a revolution, however, a few steps had to be taken in the world of atomic physics, of fundamental importance for the development of a quantum processor. The first steps in this direction was due to the physicist Hans Dehmelt (Nobel prize winner in 1989) who managed to isolate a single ion in a vacuum chamber and suspend it in the vacuum at a predetermined and controllable point. Then Zoller and Cirac realised that a single ion could act as a quantum gate, building the first quantum register with two distinct types of stored information depending on the physical characteristics of the ion. They had built the first qubit. The search for more stable and scalable quantum computer has never stopped. Today we can claim several technologies with up to 53 qubits, and capable of solving specific problems faster than classical computers.

Feynman's intuition led to the birth of a new theoretical computer science, that had repercussions in the theory of computability, complexity and logic. For the first time in history, the sacrosanct "hardware-independence" principle was shaken. The physical hardware became fundamental once more, as it would condition the entire logic of the algorithm. We need to be very careful to the choice of the physical system, to its initialization and to its measurement. Whilst classical Computer Science has soon managed to prescind from the physical machine, in quantum computation, this seems to be difficult or even impossible. A close collaboration between the two communities is necessary, as the new questions raised lie precisely at the frontier between computer science and physics. In fact, if with the advent of modern computers we have seen a progressive separation of computer scientists from physicists and mathematicians, quantum computer science raises new questions intimately at the frontier between physics and theoretical computer science.

It is in this increasingly vast and interdisciplinary boundary zone that as a student I took my first steps towards research and like me, hundreds of other young researchers. The increasing enthusiasm on these issues is not only related to the development of the first quantum computers, which in itself is attracting the interest of a large network of private and public actors. This enthusiasm has deeper roots: nowadays computing models conceived by computer scientists are becoming the new grammar for the study of natural processes. Information and its processing, after having conquered quantum mechanics and thermodynamics, have now become central in the study of gravity or biology. In this revolution, computer scientists and physicists will work together, to develop a common language, thirty years after Feynman's words.

One of the fields in which such a symbiosis seems strongest is quantum simulation. The idea of a quantum simulator has its origins in the early works of D. Deutsch and his Universal Quantum Turing Machine, which represents in quantum computability theory exactly what the Universal Turing Machine represents for classical computability. The idea of a universal quantum machine then led Lloyd in 1996 to prove that such a machine actually acts as a universal quantum simulator.

A quantum simulator requires by definition a discrete description of the phenomenon to be simulated, where discrete means a system made of disjointed components, e.g. qubits. The concept of discrete is different from the concept of discretized. In the latter we mean a system, at first continuous, resulting from a partition, seemingly arbitrary. If the phenomenon to be simulated is not discrete, the choice of finite element partitioning techniques is fundamental for the approximation to be sufficiently correct. Where "sufficiently" refers to the universal properties and symmetries of the original continuous system we are interested in. But these properties are generally not retained in the process of discretizing.

Let us take two symmetries very common to continuous systems, translation invariance and isotropy. Lattice models replace the translation invariance with the invariance under translation of step equal to an integer multiple of the step size of the lattice. Isotropy, which cannot be preserved in the discrete, is replaced by the invariance under the action of a finite group of rotations. Both these substitutions are well defined and in the limit in which the size of the lattice becomes various orders larger than the size of the elementary cell, they converge to the correct continuous symmetries. Evidently the debate on discretization procedures and the choice of the model cannot be limited to the symmetries and universal properties of the continuous system that is intended to be similar. Beyond computational techniques, there is also the choice of the scale of description and the nature of the phenomenon.

In these lectures we will focus our attention on a class of quantum phenomena, described by transport equations which are linear partial differential equations (PDE), which are essential to simulate natural transport phenomena. In the specific case of fluids, the equations are non-linear and present a challenge to those using quantum mechanics, which is linear. There are many proposals on this subject. In these lectures, we will try to provide formal tools rather than a solution to the specific problem. In particular, we will focus on how to simulate a transport equations on a discrete grid of qubits, by means of unitaires. We will first deal extensively with the linear case and then briefly discuss how to introduce non-linearities. Indeed, our approach is constructive. The need to simulate linear dynamics first comes from the algorithmic complexity in the multi-particle case, but also from the fact that reproducing such dynamics in extreme regimes (e.g. in the presence of a strong magnetic field), is often impossible in the laboratory. It is therefore fundamental to understand how to simulate such regimes by means of controllable and easily accessible physical systems.

There are essentially two methods to simulate a continuous quantum system on a lattice: one involves the series development of the continuous quantum operator, in terms of local units and its subsequent truncation to be implemented on a quantum computer, *aka* trotterization. This kind of scheme by trotterizing the global operator in local unitaries is usually in continuous time and we referred to it as Hamiltonian simulation. Moreover, truncating an infinite series induces an error in the simulation that can be estimated and controlled. An

alternative way is the construction of a network of local quantum gates, uniformly distributed across space and time. This solution is part of the vast class of quantum cellular automata (QCA) and can be historically presented in both continuous and discrete time. Both models have their advantages and disadvantages: the first one, due to the truncation, can introduce the breaking of some symmetries and therefore the non-preservation of quantities fundamental for the phenomenon we want to describe, but it has undoubtedly the advantage of building an ad hoc quantum circuit that could result, after all, in a good approximation. The QCA are a universal quantum computation system: defining sufficiently general unitaries on the grid allows us to choose appropriate parameters to converge in the limit to the correct continuous evolution. Recently such models have been used to describe the propagation of free particles, e.g. fermions, in the presence of fields of various nature [1–7], and also on arbitrary manifolds [5, 8–11] and lastly interacting systems [12, 13]. Such an idea is not new and goes back again to the brilliant Feynman, who first discretized the dynamics of fermions on a space-time checkboard [14].

The growing enthusiasm towards these discrete models is not only due to the ability to simulate quantum dynamical systems that are difficult to recreate in a laboratory, but to the fact that they themselves can be considered toy models of the way transport can be defined on a fundamentally discrete space-time structure. The issue of combining a discrete quantum phenomenon with the concept of continuous space-time has been the most fascinating enigma in the community of physicists for decades. Computer scientists can shed new light on this great challenge, by bringing concepts such as universality, classification and complexity to the ever richer frontier zone, enabling new perspectives to the quest for answers and ultimately to the scientific progress.

A further incentive to study such simulation models derives from a recent study, which for the first time has revealed how some natural mechanisms, such as the transport of a quantum particle, can naturally implement quantum algorithms, such as the Grover algorithm [15]. Simulating therefore a transport equation, might have as an additional result to suggest new ways in the short and medium term for the design of quantum algorithms.

The interlacement between quantum simulation, physics and algorithmics is the framework within which this course is inscribed. The humble contribution that we want to make is in particular the consideration of a discrete model of lattice simulation for a wide family of dynamics described by transport equations, known as Quantum Walks (QWs), which may be also seen as the one-particle sector of a QCA in discrete time. More importantly, It has been proven that a quantum walk formally coincides with a linear Boltzmann quantum scheme. This correspondence makes such models extremely interesting for computational fluid dynamics. Furthermore, the multi-body extension of a quantum walk, i.e. quantum cellular automata, are well understood and provided with a robust theoretical framework.

At first, we will give a gentle introduction of quantum walks, in the specific one-dimensional case, and briefly discuss extensions in higher dimensions. Next, we will demonstrate how in the continuous limit, in other words when the size of the discretization step tends to zero, the QWs equations converge to a very general class of transport equations. In this regard, we will also discuss ways in which a new family of QWs, referred to as *plastic*, might admit both a space and time limit, and a discrete space continuous time only limit, leaving the spatial grid to be discrete. This result is particularly important because it formally unifies for the very first time the Hamiltonian quantum simulators in continuous time we mentioned earlier, and those in discrete time, *i.e.* the QCAs.

Next, we will show, in the specific case of the Dirac equation, how isotropic discretization methods in fact coincide with the definition of Quantum Walk. And then we will prove that a quantum Boltzmann scheme, as introduced by Succi and collaborators [16] recently, formally coincides with a quantum walk and we will discuss an specific example : the simulation of a hydrodynamical shock by means of QW. In conclusion of this part, we will briefly discuss how nonlinear terms can be taken into account in such models.

At the end, we will try to approach a completely different problem. How can we simulate a fluid on a curved

surface? In line with what we explained so far, we will restraint ourself to the linear case. The methodology is abstract and formal but it can deliver a practical way to simulate multi-particles dynamics on an arbitrary manifold.

2.0 QUANTUM WALK

Quantum walks are the quantum counterpart of the Classical random walks (CRWs), which are employed to model phenomena as chemical reactions [17–19], genetic sequence location [20–22], optimal search strategies [23–25], diffusion and mobility in materials [26–28], exchange rate forecasts in economical sciences [29–31] and information spreading in complex networks [32–34]. Furthermore, they can successfully implement efficient algorithms, for example they can solve differential equations [35, 36], optimization [24, 37] and clustering problems [38, 39]. Random walks spread to every domain of science for more than a century and are still an important source for researchers nowadays. Even though in the second half of last century the interest in a quantum analogous to the classical stochastic process led to further investigation of quantum mechanics and quantum information, since the 1960s, numerous scientists [40–47] have extended the Brownian motion and stochastic calculus to particles which exhibited quantum effects. Schwinger was the first to demonstrate the importance of coherence effects in the evolution of a Brownian quantum particle. Just few years later, [48] proposed the first discrete model with the intention of recovering a quantum version of the CRW. This first example represented a quantum planar rotor on a lattice whose dynamics can be approximated by a random walk. Another important milestone was the work of Gudder [49], who studied systematically quantum Markov processes and established formally a connection with Feymann path integral formalism. Interestingly some years later, [50] and [51] had independently the same intuition of developing a quantum analogous to the CRW in discrete time and discrete space. Godoy and Fujita proposed a one-dimensional Markovian quantum walk displaying a diffusive behavior and [51] formalized the first model of unitary Quantum Walk (QW), whose dynamics was fully ballistic. Let us remark that, although the latter was defined as a QCA, this model is completely equivalent to the one proposed later by Aharonov [52]. Indeed, QWs may be seen as the one particle sector of a QCA, extensively reviewed in [53].

Thanks to its features, especially the unitarity, QWs were immediately considered a new and efficient tool for solving, in a wider range of applications, technical problems in a more convenient way than classical random walks.

2.1 Quantum Walks over square grids

In this section we will introduce the simplest quantum walk on a Cartesian grid, i.e. over a monohedral tessellation of a Euclidean space by congruent squares (or unit cubes in higher dimensions), where the vertices are point on the integer lattice. We will start by defining a QW on an infinite discrete line and treat its higher dimensional extension later. We need few ingredients to define a QW in discrete time: the walker, its internal state and an evolution unitary operator for both walker and coin.
The walker is represented by a quantum state $|\omega\rangle$ living in a Hilbert space $\mathcal{H}_{\mathbb{Z}}$ of infinite but countable dimension. The computational basis of this space is $|m\rangle \in \mathbb{Z}$, *i.e.*, the position sites of the walker. The walker $|\omega\rangle$ will be then denoted by any superposition of the form:

$$|\omega\rangle = \sum_{m\in\mathbb{Z}} \alpha_m |m\rangle \tag{1}$$

such that the normalisation condition $\sum_m |\alpha_m|^2 = 1$ holds.
The coin state $|\kappa\rangle$ is a quantum system, living in a $k-$dimensional Hilbert space $\mathcal{H}_\kappa$, spanned by the canonical basis $\{|0\rangle, |1\rangle, ..., |k-1\rangle\}$. Thus $|\kappa\rangle$ may be written as

$$|\kappa\rangle = \sum_s^{k-1} \beta_s |s\rangle \tag{2}$$

where $\sum_s |\beta_s|^2 = 1$. In the following we will consider the coin state as belonging to a $2-$dimensional Hilbert space $\mathcal{H}_2$, as the most natural extension of the notion of the classical bit. Thus the overall state, representing the QW, lies in both Hilbert spaces and it is spanned by the coin state and the position state basis.

Now, a QW over the one dimensional grid in discrete time is represented by the state Ψ, lying in the composite Hilbert space $\mathcal{H}_2 \otimes \mathcal{H}_\mathbb{Z}$. For the internal state we may choose some orthonormal basis $\{|0\rangle, |1\rangle\}$ and the overall state may be written

$$\Psi = \sum_m \psi_m^0 |0\rangle \otimes |m\rangle + \psi_m^1 |1\rangle \otimes |m\rangle, \tag{3}$$

where the complex probability amplitude ψ^0 and ψ^1 have to respect the following normalisation condition $\sum_m (|\psi_m^0|^2 + |\psi_m^1|^2) = 1$. The temporal evolution of a quantum walk is driven by the composite action of two unitary operators, one acting in combined position-coin space and the other in the coin space. Similar to the classical random walk, we need one operator to move the walker on the line and one operator to play the same role as the coin toss. The latter is crucial in the dynamical features of the QW. Unlike the classic case, where such an operator is represented by a stochastic matrix, in the case of the QW evolution there is no room for randomness before measurement and it is represented by an unitary matrix which acts as an internal rotation in the internal state space.

Quantum Coin The most general operator acting on a two-dimensional state is an arbitrary element of the unitary group $U(2)$, depending on four real parameters α, ξ, ζ, and θ in the following way:

$$\widehat{C}_{\theta,\alpha,\xi,\zeta} = e^{i\alpha} \begin{pmatrix} \cos\theta e^{i\xi} & \sin\theta e^{i\zeta} \\ -\sin\theta e^{-i\zeta} & \cos\theta e^{-i\xi} \end{pmatrix} \tag{4}$$

Taking advantage again of the analogy with a classical random walk, the shift operator, once the coin is flipped, moves the walker one step in a precise direction, depending on the state of the coin. While, in the classic case, the walker moves left or right, depending on whether the result is heads or tails, in the case of the unitary evolution of a QW, the walker will move in superposition of states:

Shift Operator A suitable conditioned shift operator for the QW has the form:

$$\widehat{S} = |0\rangle\langle 0| \otimes \sum_m |m+1\rangle\langle m| + |1\rangle\langle 1| \otimes \sum_m |m-1\rangle\langle m|. \tag{5}$$

At last we can introduce the unitary evolution operator acting on the Hilbert space $\mathcal{H}_2 \otimes \mathcal{H}_\mathbb{Z}$.

Evolution operator
Let us introduce $j \in \mathbb{N}$ to label instants and let the QW prepared for the initial time j' as a general product state 3 then

$$\Psi_{j'+1} = \widehat{W}\Psi_{j'} \tag{6}$$

where

$$\widehat{W} = \widehat{S}(\widehat{C}_{\theta,\alpha,\xi,\zeta} \otimes Id_{\mathbb{Z}}) \tag{7}$$

is the evolution unitary operator.

Notice that, due to the unitarity of W, the $\rho_{j'} \equiv |\Psi_{j'}|^2$ is a conserved real number all along the evolution and it is interpreted as the probability density of measuring the walker's being detected at any point of the space. It is usually normalised to one.

As an example, we will study the Hadamard Walk, the most common one-dimensional QW.

Hadamard Walk In the Hadamard Walk, the coin is the Hadamard operator, which coincides with $\widehat{H} = \widehat{C}_{\frac{\pi}{4},\frac{\pi}{2},\frac{-\pi}{2},\frac{-\pi}{2}}$:

$$\widehat{H} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{8}$$

One time step of the Hadamard Walk consists to apply to the initial state $\Psi_{j'}$ the Hadamard coin and then the shift operator, as introduced previously. Given the following generic initial state:

$$\Psi_{j'} = \sum_{s=0}^{1}\sum_{m=\infty}^{\infty} \psi^s_{m,j'}|s\rangle|m\rangle \tag{9}$$

the state at instant $j'+1$ reads:

$$\begin{aligned} \Psi_{j'+1} &= \sum_{m=\infty}^{\infty} \widehat{S}(\psi^0_{m,j'}\widehat{H}|0\rangle|m\rangle + \psi^1_{m,j'}\widehat{H}|1\rangle|m\rangle) = \\ &= \sum_{m=\infty}^{\infty}\left(\frac{\psi^0_{m,j'}+\psi^1_{m,j'}}{\sqrt{2}}|0\rangle|m+1\rangle + \frac{\psi^0_{m,j'}-\psi^1_{m,j'}}{\sqrt{2}}|1\rangle|m-1\rangle\right) \end{aligned} \tag{10}$$

From the above equation, once the final state is written as linear combination in the computational basis, we can extract the recursive relations for the coefficients, i.e., the walker probability amplitudes:

$$\begin{aligned} \psi^0_{m,j'+1} &= \frac{\psi^0_{m+1,j'}+\psi^1_{m+1,j'}}{\sqrt{2}} \\ \psi^1_{m,j'+1} &= \frac{\psi^0_{m-1,j'}-\psi^1_{m-1,j'}}{\sqrt{2}} \end{aligned} \tag{11}$$

For a given initial condition, the above equation can be solved numerically, generating the probability distribution and computing all the statistical property of the walker as the expected distance from the origin, i.e. the standard deviation, and other statistical momenta.

2.2 Higher dimensional spaces

The Eq. 6 may be extended to any d-dimensional regular grid, e.g. square in 2D and cubes in 3D. The simplest way to generalize the previous section is to introduce a Hilbert space for the position of the walker $\mathcal{H}_{\mathbb{Z}^d}$, where d is the connectivity of the vertices, and $\mathcal{H}_d$ for the coin state. The coin operator is then a d-dimensional matrix and the shift operator has to account a displacement towards the i^{th} neighbor among the d ones starting from a vertex. For instance, on a square lattice each vertex has four links and four neighbors, then the coin state encodes the probability amplitude to go towards each of the four possible directions. In a d-dimensional grid the most common one for the quantum coin is the Grover operator, introduced by Moore and Russell [54]:
Grover coin A d-dimensional Grover coin has elements $[C_d^G]_{i,j} = \frac{2}{d} - \delta_{i,j}$, i.e.:

$$C_d^G = \begin{pmatrix} 2/d-1 & 2/d & \cdot & 2/d \\ 2/d & 2/d-1 & \cdot & 2/d \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 2/d & 2/d & \cdot & 2/d-1 \end{pmatrix} \tag{12}$$

Notice that, except for $d = 4$, all Grover coins are biased since the diagonal entry is weighted differently from the off-diagonal ones. This particular coin has raised the interest of the community because it can be used to implement the two-dimensional Grover search algorithm [55].

As an example, let us consider the square grid: at each point of this infinite two-dimensional lattice, the walker has four possibilities to move ($d = 4$), which translates in four possible coin states. Such a QW lies in a composite Hilbert space $\mathcal{H}_{square} = \mathcal{H}_4 \otimes \mathcal{H}_{Z^2}$ where $\mathcal{H}_4$ is spanned by the orthonormal basis $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$. The shift operator is defined as follows:

$$\widehat{S} = \sum_{s=0}^{1} \sum_{m,n} (|s\rangle\langle s||m + (-1)^s, n\rangle\langle m, n|) + \sum_{s=2}^{3} \sum_{m,n} (|s\rangle\langle s||m, n + (-1)^s\rangle\langle m, n|) \tag{13}$$

and for the coin we can choose the Grover coin:

$$C_4^G = \frac{1}{2} \begin{pmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{pmatrix}. \tag{14}$$

Although the above walk completely describes the walker spread on the plane, and it seems to be the most natural and straightforward generalization of 6 in a spatial dimension higher then one, the use of a four dimensional state or two distinct qubits is really costly and nowdays very few feasible implementations have been proposed so far. To reduce the technological challenge, an alternative definition of 2D-dimensional QW has been introduced, which has been proven equivalent to the above one in the propagative regime [56]. This new family of QW, that we call alternate quantum walk (AQW) is a composition of two one-dimensional QW, each moving in the orthogonal u_x and u_y directions. The quantum coin is a single qubit, then is spanned by $\{|0\rangle, |1\rangle\}$ The time evolution of the QW will be then driven by the application of the coin operator, e.g., the Hadamard coin, and the shift operator along each basis vector of the grid u_i:

$$S_{u_x} = \sum_{m,n} (|m-1, n, 0\rangle\langle m, n, 0| + |m+1, n, 1\rangle\langle m, n, 1|) \tag{15}$$

and

$$S_{u_y} = \sum_{m,n} \left(|m, n-1, 0\rangle\langle m, n, 0| + |m, n+1, 1\rangle\langle m, n, 1| \right) \tag{16}$$

and in conclusion of this chapter, we give finally the following definition:

Alternate Quantum Walk The Alternate Quantum Walk is defined by the following unitary evolution

$$\Psi_{j'+1} = \widehat{W}\Psi_{j'} \tag{17}$$

and

$$\widehat{W} = \left(\widehat{S}_{u_x}(\widehat{H} \otimes Id_{\mathbb{Z}})\widehat{S}_{u_y}(\widehat{H} \otimes Id_{\mathbb{Z}}) \right) \tag{18}$$

Remark that using a single qubit system for the walker means that the *alternating* procedure can work only when d is even. For instance in the case of a hexagonal lattice, where $d = 3$, there not exist any splitting techniques for reducing a 3-dimensional system to a sequence of single qubit (2-dimensional) quantum walk.

3.0 DISCRETIZATION OF TRANSPORT EQUATIONS

The idea of simulating quantum systems with quantum computers was notably pointed out by Feynman [57], confronted with the insufficiency and intractability of classical computers' abilities to simulate quantum features. Several quantum simulation schemes have been sparked over the last few decades [58] and most of them can be divided into two different approaches: some of the methods being used for simulating quantum systems implemented over *discrete space* and *continuous time* lattices consist of constructing a Hamiltonian, which is historically the continuous time operator governing the time evolution of the system, which imitates a physical system, or trotterizing a constructed Hamiltonian to obtain unitaries [59, 60]. Problems with these approaches are discussed in Ref. [61] and include the breaking of Lorentz covariance as well as issues arising when recovering a bounded speed of light. The other approach concerns *discrete spacetime models*, which do not share the difficulties of their discrete space continuous time counterparts, such as the quantum circuit model and the quantum cellular automata or their one-particle sector, namely the discrete time quantum walk (DTQW). In particular this last quantum scheme have been proved a powerful tool to simulate a large spectra of quantum natural phenomena which are usually described by partial differential equations (PDE): indeed the continuous spacetime limit of various DTQWs defined on the regular lattice in arbitrary dimensions has been proved to be equivalent to a wide range of hyperbolic PDE (HPDE) describing in general quantum transport, eventually coupled with abelian [62–64] and non-abelian gauge field [3, 4, 65] on curved spacetime [11, 66–68].

The connection between continuous time and discrete space scheme with quantum walks has been investigated by [60, 69–71]. Although several techniques have been employed to study the connections between them, these two models have been apart for a long time. Recently a quantum simulation scheme known as a Plastic Quantum Walk (PQW) have been developed [61] which supports both a continuous spacetime limit and a continuous time-discrete space limit. Plasticity is the definitive element that makes the continuous limit process less rigid and therefore plastic. While remaining on the space-time grid, a PQW adapts anisotropically, modifying the speed at which space and discrete time converge to the continuous. This new quantum scheme not only encapsulates both historical approaches to simulate a quantum system, but unveils a previously inconsiderate property of the space-time grid.

For simplicity here we will explore plasticity in two space-time dimensions.

3.1 Plastic Quantum Walk

A large class of QW admits the continuous limit in space-time and there are few examples that admit the limit in time, leaving the space discrete. Here, we want to demonstrate that by introducing anistropic scaling on the space-time grid, we can find QWs that admit both limits. Such QWs will be called plastics. A **Plastic Quantum Walk (PQW)** is a QW which admits both a continuous limit in time and a continuous limit in spacetime depending on some parameters.

We will begin to study the simplest but not trivial case of Plastic QW, and in the results we will define and discern strong and weak forms of plasticity.

3.1.1 The infinite line

We consider a QW in one spatial dimension as defined in the previous section. To investigate the continuous limit, we first introduce a time discretization step Δ_t and a space discretization step Δ. We then introduce, for any discrete function ψ appearing in the QW evolution operator, a complex function $\bar{\psi} \in \mathbb{C}$ over the spacetime positions $\mathbb{R}^+ \times \mathbb{R}$, such that $\psi_{j,m} = \bar{\psi}(t_j, x_m)$, with $t_j = j\Delta_t$ and $x_m = m\Delta$. In other terms, we assume that the discrete function ψ samples exactly the continuous complex function $\bar{\psi}(t, x)$.

The Eq. 6 after a number of time steps τ reads:

$$\bar{\Psi}(t_j + \tau\Delta_t) = \widehat{W}^\tau \bar{\Psi}(t_j), \tag{19}$$

where

$$\widehat{W}^\tau = (\widehat{S}_{u_x}(\widehat{C}_{\theta,\alpha,\xi,\zeta} \otimes \mathrm{Id}_{\mathbb{Z}}))^\tau. \tag{20}$$

Now let us drop the bars to lighten the notation. We suppose that all functions are at least C^2, i.e. twice differentiable. The spacetime continuum limit, when it exists, coincides with the coupled differential equations obtained from Eq. 19 by letting both Δ_t and Δ go isotropically to zero, as for example in [62].

Now we will prove in the following that there is no room for plasticity in one spatial dimension if we compute the limit at each time iteration of the QW, for $\tau = 1$. Let us parametrize the time and space steps with a positive real number $\varepsilon \in \mathbb{R}^+$ and let consider the following jets:

$$\begin{aligned} \theta &= \theta^{(0)} + \varepsilon^b \theta^{(1)} \\ \alpha &= \alpha^{(0)} + \varepsilon^b \alpha^{(1)} \\ \xi &= \xi^{(0)} + \varepsilon^b \xi^{(1)} \\ \zeta &= \zeta^{(0)} + \varepsilon^b \zeta^{(1)} \end{aligned} \tag{21}$$

so that

$$\widehat{C}_{\alpha,\theta,\xi,\zeta} = \widehat{C}^{(0)} + \varepsilon^b \widehat{C}^{(1)} \tag{22}$$

where the exponent b is a real positive and smaller then 1. Let $\Delta_t = \varepsilon$ and $\Delta = \varepsilon^{1-a}$, where a is a real positive, such that $0 \leq a \leq 1$ and which traces the fact that both Δ_t and Δ may tend to zero anisotropically. If $\tau = 1$ and $\varepsilon \ll 1$ and $\Psi(t_j) \in C^2$, then Eq 6 admits only a continuous limit in space time and it coincides with the following couple of PDEs, namely the Dirac equation in (1+1) spacetime dimensions:

$$\partial_t \Psi = -\sigma_z \partial_x \Psi + \widehat{C}^{(1)} \Psi \tag{23}$$

if and only if $0 < b <= 1$ and

$$\begin{aligned} \theta^{(0)} &= 2q\pi \\ \alpha^{(0)} &= (q' + q")\pi \\ \xi^{(0)} &= (q' - q")\pi \end{aligned} \tag{24}$$

and $\forall\ \zeta^{(0)},\ \zeta^{(1)},\ \theta^{(1)}$ and where q, q' and $q" \in \mathbb{Z}$.

In order to prove the above statements, it is more suitable moving to Fourier space where the shift operator is diagonal. We can then write the Eq. 6 for $\tau = 1$ as follows:

$$\tilde{\Psi}(t + \Delta_t) = \widehat{W}_k \tilde{\Psi}(t). \tag{25}$$

where

$$\widehat{W}_k = e^{i\alpha} \begin{pmatrix} e^{i(\xi - k\Delta)} \cos\theta & e^{i(\zeta - k\Delta)} \sin\theta \\ -e^{-i(\zeta - k\Delta)} \sin\theta & e^{-i(\xi - k\Delta)} \cos\theta \end{pmatrix} \tag{26}$$

Notice that the vector $\tilde{\Psi}(t) \in C^2$ because its Fourier inverse is. Now we can Taylor expand the above equation around $\varepsilon = 0$ and up to the first order in $o(\varepsilon)$:

$$\tilde{\Psi}(t)(\mathrm{Id} - e^{-i\sigma_z k\varepsilon^{1-a}} \widehat{C}^{(0)}) = \varepsilon(\partial_t + e^{-i\sigma_z k\varepsilon^{1-a}} \varepsilon^{b-1} \widehat{C}^{(1)})\tilde{\Psi}(t) + o(\varepsilon^2) \tag{27}$$

We can now distinguish two cases: (i) if a is equal to 1 then $(\mathrm{Id} - e^{-i\sigma_z k} \widehat{C}^{(0)}) = 0$, implying that $\widehat{C}^{(0)} = e^{-i\sigma_z k}$ which is false because the coin does not depend on k. Thus, there not exist any continuous limit for $a = 1$. (ii) If $0 < a < 1$, then at the zeroth order, $\widehat{C}^{(0)}$ has to be the identity, which leads to Eqs. 24 after a simple and straightforward calculation. Thus, the leading order in $o(\varepsilon)$ reads:

$$(\partial_t - \varepsilon^{-a} \sigma_z ik + \varepsilon^{b-1} \widehat{C}^{(1)})\tilde{\Psi}(t) + o(\varepsilon) = 0 \tag{28}$$

where $\widehat{C}^{(1)}$ is solely a function of $(\theta^{(1)}, \alpha^{(1)}, \xi^{(1)})$ and ζ. Now, in order to avoid divergence $a = 0$ and b have to be greater than or equal to the unity. Finally taking the limit $\varepsilon \to 0$ and inverse Fourier transform, we converge to:

$$\begin{aligned} \partial_t \psi^0 &= e^{i\zeta} \theta^{(1)} \psi^1 - \partial_x \psi^0 + i(\alpha^{(1)} + \xi^{(1)})\psi^0, \\ \partial_t \psi^1 &= -e^{-i\zeta} \theta^{(1)} \psi^0 + \partial_x \psi^1 + i(\alpha^{(1)} - \xi^{(1)})\psi^1 \end{aligned} \tag{29}$$

which coincides with Eq. 23, where $\widehat{C}^{(1)} = i\mathrm{Id}\alpha^{(1)} + i\sigma_z \xi^{(1)} - i(\sigma_y \cos(\zeta) - \sigma_x \sin(\zeta))\theta^{(1)}$. and the $x-$, $y-$ and $z-$Pauli matrix read:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{30}$$

We have seen with the above Theorem that $a \neq 1$ precludes a continuous limit only in time (with discrete space) which means that there is no room for plasticity for $\tau = 1$. Actually, this result is true for every odd τ and the reader will find detailed evidence in the recent [72]. In the following, we will see that this problem can be encompassed considering $\tau = 2$ (or more in general an even number of time steps).

Starting from Eq. 19, we can derive the stroboscopic equation of period $\tau = 2$

$$\Psi(t_j + 2\Delta_t) = \widehat{W}^2 \Psi(t_j). \tag{31}$$

As in the previous case, we will work in the Fourier basis and we will use the same truncated Taylor expansion for the quantum coin's angles given in 22. Indeed, the zeroth order of the Taylor series of the stroboscopic equation 31, for any value $0 \leq a \leq 1$, cancels if and only if one of the following equations is satisfied:

1. $\forall a$, $\alpha^{(0)} = \frac{\pi}{2} + q\pi$ and $\theta^{(0)} = \frac{\pi}{2} + q'\pi$ $(C1)$
2. for $0 \leq a < 1$, $\alpha^{(0)} = \frac{\pi}{2} + q\pi$ and $\xi^{(0)} = \frac{\pi}{2} + q'\pi$ (C2)
3. for $0 \leq a < 1$, $\alpha^{(0)} = \frac{\pi}{2} q\pi$, $\xi^{(0)} = \frac{\pi}{2} q'\pi$ and $\theta^{(0)} = q"\pi$ (C3)

where q, q' and $q'' \in \mathbb{Z}$. Let us try to give you a glimps of the proof. Again we work in the Fourier basis. Then, let us Taylor expand 31 around $\varepsilon = 0$ and at order zero we get:

$$\tilde{\Psi}(t_j) + o(\varepsilon) = e^{-i\varepsilon^{1-a}\sigma_z k} \widehat{C}^{(0)} e^{-i\varepsilon^{1-a}\sigma_z k} \widehat{C}^{(0)} \tilde{\Psi}(t_j) \tag{32}$$

The above equation is satisfied if

$$e^{-i\varepsilon^{1-a}\sigma_z k} \widehat{C}^{(0)} e^{-i\varepsilon^{1-a}\sigma_z k} \widehat{C}^{(0)} = \mathrm{Id}, \tag{33}$$

which reduces to:

$$\cos^2(\varepsilon^{1-a}k)(\widehat{C}^{(0)})^2 - i\sin(\varepsilon^{1-a}k)\cos(\varepsilon^{1-a}k)\{\sigma_z, C^{(0)}\} - (\sigma_z C^{(0)})^2 \sin^2(\varepsilon^{1-a}k) = \mathrm{Id}. \tag{34}$$

Now we can distinguish two cases: (i) $a = 1$ and (ii) $0 \leq a < 1$. Case (i) implies:

$$\cos^2(k)(\widehat{C}^{(0)})^2 - i\sin(k)\cos(k)\{\sigma_z, C^{(0)}\} - (\sigma_z C^{(0)})^2 \sin^2(k) = \mathrm{Id}. \tag{35}$$

From the above equation it follows that:

$$\begin{aligned} (\widehat{C}^{(0)})^2 &= \mathrm{Id} \\ \{\sigma_z, C^{(0)}\} &= 0 \\ (\sigma_z C^{(0)})^2 &= -\mathrm{Id}. \end{aligned} \tag{36}$$

The first equation requires that $\widehat{C}^{(0)}$ be Hermitian, because $(\widehat{C}^{(0)})^2 = \mathrm{Id} = \widehat{C}^{(0)}(\widehat{C}^{(0)})^{-1}$ implies $(C^{(0)})^{-1} = C^{(0)}$. Notice that the last two conditions are equivalent. Both imply that $\widehat{C}^{(0)}$ be purely off diagonal, because the anti-commutation relations. Then, given $\widehat{C}^{(0)}$ the most general quantum coin introduced in the previous section, the only solution is that $\widehat{C}^{(0)} = -\sigma_y$, where the y-Pauli matrix

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{37}$$

for any value of ζ and ξ, which directly implies $\alpha^{(0)} = \frac{\pi}{2} + q\pi$ and $\theta^{(0)} = \frac{\pi}{2} + q'\pi$. Let us now prove the theorem for the conditions (ii). If $0 \leq a < 1$ is true then 33 reduces to:

$$\widehat{C}^{(0)} \widehat{C}^{(0)} = \mathrm{Id}, \tag{38}$$

which is satisfied in the following three cases (in the following we will denote them as C1, C2, C3):

1. $\alpha^{(0)} = \frac{\pi}{2} + q\pi$ and $\xi^{(0)} = \frac{\pi}{2} + q'\pi$
2. $\alpha^{(0)} = \frac{\pi}{2}q$, $\xi^{(0)} = \frac{\pi}{2}q'$ and $\theta^{(0)} = q"\pi$
3. $\alpha^{(0)} = \frac{\pi}{2} + q\pi$, and $\theta^{(0)} = \frac{\pi}{2} + q'\pi$

which proves the initial statement.

Notice that from the above result it follows that for $a = 1$ the continuous time limit in discrete space, for $\tau = 2$,exists only if

$$\begin{aligned} \alpha^{(0)} &= \frac{\pi}{2} + q\pi \\ \theta^{(0)} &= \frac{\pi}{2} + q'\pi \end{aligned} \tag{39}$$

where q and $q' \in \mathbb{Z}$.

Now using the above results we are now able to prove the following Theorem:

Continuous Limits for $\tau = 2$
Let the necessary conditions proved above be verified, consequently the continuous limit of the QW in one spatial dimension, for a stroboscopic period $\tau = 2$, exists and reads:

$$\begin{aligned} &\boldsymbol{a = 1:} \\ &\quad \partial_t \Psi = i\theta^{(1)} \sigma_y e^{-i\sigma_z(\zeta^{(0)}+\xi^{(0)})} \left(\widehat{S}^2 + e^{-2i\sigma_z \xi^{(0)}}\right) \Psi \\ &\boldsymbol{0 \leq a < 1:} \\ &\quad \partial_t \Psi = P\partial_x \Psi + Q\ \Psi, \end{aligned} \tag{40}$$

where P and Q are traceless and Hermitian matrices depending on $(\alpha^{(1)}, \xi^{(1)})$ and ζ.

In order to prove the above theorem, let us start with the case for which $a = 1$ and let us expand around $\varepsilon = 0$. In that case the Taylor truncated development of Eq. 31 reads:

$$\tilde{\Psi}(t_j) + \varepsilon \partial_t \tilde{\Psi}(t_j) = e^{-i\sigma_z k} C^{(0)} e^{-i\sigma_z k} C^{(0)} + \varepsilon^b \{e^{-i\sigma_z k} C^{(1)}, e^{-i\sigma_z k} C^{(0)}\} \tilde{\Psi}(t_j) + o(\varepsilon^{2b}). \tag{41}$$

Since the orderth zero cancels, we get:

$$\partial_t \tilde{\Psi}(t_j) = \varepsilon^{b-1} \{e^{-i\sigma_z k} C^{(1)}, e^{-i\sigma_z k} C^{(0)}\} \tilde{\Psi}(t_j) + o(\varepsilon^{2b-1}), \tag{42}$$

which constraint b to be equal to 1 to avoid divergences. Taking the formal limit for $\varepsilon \to 0$, we recover the following equation in continuous time and discrete space:

$$\partial_t \tilde{\Psi}(t_j) = \{e^{-i\sigma_z k} C^{(1)}, e^{-i\sigma_z k} C^{(0)}\} \tilde{\Psi}(t_j) \tag{43}$$

using the zeroth orders and Fourier transform we get

$$\partial_t \tilde{\Psi}(t_j) = i\theta\sigma_y e^{-i\sigma_z(\zeta^{(0)}+\xi^{(0)})} \left(S^2 + e^{-2i\sigma_z \xi^{(0)}}\right) \tilde{\Psi}(t_j). \tag{44}$$

proving the above Theorem for $a = 1$.

Now let us explore the case for which $a \neq 1$. The expansion of the Eq. 31 around $\varepsilon = 0$ leads to:

$$\tilde{\Psi}(t_j) + \varepsilon \partial_t \tilde{\Psi}(t_j) = \Big((\mathrm{Id} - i\sigma_z k \varepsilon^{1-a})(C^{(0)} + \varepsilon^b C^{(1)}) \Big)^2 \tilde{\Psi}(t_j) + o(\varepsilon^2). \tag{45}$$

After few simplifications and using the fact that the zeroth order constraint equations 33 are satisfied, we get:

$$\begin{aligned} \partial_t \tilde{\Psi}(t_j) = (&-ik\varepsilon^{-a}\{\sigma_z C^{(0)}, C^{(0)}\} + \varepsilon^{b-1}\{C^{(0)}, C^{(1)}\} \\ &- i\varepsilon^{-a+b} k[\{\sigma_z C^{(0)}, C^{(1)}\} + \{\sigma_z C^{(1)}, C^{(0)}\}])\tilde{\Psi}(t_j) + o(\varepsilon^{2(1-a)-1}) + o(\varepsilon^{2b-1}). \end{aligned} \tag{46}$$

From the above equation we deduce that if $\{\sigma_z C^{(0)}, C^{(0)}\} \neq 0$, $a = 0$ to avoid divergences. Consequently, we will study the coefficients of the above development for each case of the zeroth- order constraints equation. Let us start with C1: in this case $\{\sigma_z C^{(0)}, C^{(0)}\} = 0$ then in order to recover the spatial derivative we need $a = b$. Because $0 \leq a < 1$, $\{C^{(0)}, C^{(1)}\}$ has to be 0, otherwise $b - 1$ would be negative and we would have a divergence in the limit for $\varepsilon \to 0$. This implies the supplementary condition:

1. $\alpha^{(1)} = 0$ and $\theta^{(1)} = 0$,
2. $\alpha^{(1)} = 0$ and $\xi^{(0)} = \pm\frac{\pi}{2}$.

The second one of the above conditions is the only one for which $[\{\sigma_z C^{(0)}, C^{(1)}\} + \{\sigma_z C^{(1)}, C^{(0)}\}] \neq 0$. Plugging it in 48 for the first condition C1, together with the formal limit for $\varepsilon \to 0$, leads us to:

$$\begin{aligned} \partial_t \psi^0 &= 2e^{i\zeta}\theta^{(1)}(\xi^{(1)}\psi^1 + i\partial_x \psi^1), \\ \partial_t \psi^1 &= -2e^{-i\zeta}\theta^{(1)}(\xi^{(1)}\psi^0 + i\partial_x \psi^0). \end{aligned} \tag{47}$$

Notice that the above equations are the continuous space limit of Eqs. 40.a.

Now let us consider the condition C2 given above, for which $\alpha^{(0)} = \pi/2$ and $\xi^{(0)} = \pi/2$. For these values $\{\sigma_z C^{(0)}, C^{(0)}\} \neq 0$, thus we can explore separately the case for $a = 0$. The Eq. 48 becomes:

$$\partial_t \tilde{\Psi}(t_j) = (-ik\{\sigma_z C^{(0)}, C^{(0)}\}\tilde{\Psi}(t_j) + \varepsilon^{b-1}\{C^{(0)}, C^{(1)}\}\tilde{\Psi}(t_j) + o(\varepsilon^1) + o(\varepsilon^b) \tag{48}$$

and for $b = 1$, it follows, after Fourier transform:

$$\begin{aligned} \partial_t \psi^0 &= e^{i\zeta}\sin(2\theta)(i\partial_x \psi^1 + \xi^{(1)}\psi^1) + 2i\cos^2(\theta)(i\partial_x u + \xi^{(1)}\psi^0) + 2i\alpha^{(1)}\psi^0 \\ \partial_t \psi^1 &= -e^{-i\zeta}\sin(2\theta)(i\partial_x \psi^0 + \xi^{(1)}\psi^0) - 2i\cos^2(\theta)(i\partial_x 1 + \xi^{(1)}\psi^1) + 2i\alpha^{(1)}\psi^1. \end{aligned} \tag{49}$$

The case of $a < 1$ requires that $\{\sigma_z C^{(0)}, C^{(0)}\} = 0$, which leads to $\theta^{(0)} = \pm\pi/2$, coming back to **??**.C1.

The last case, C3 has to be split in two sub-cases: (a) $q = q' = 1$ and $q" = 0$ that is $\alpha^{(0)} = \xi^{(0)} = \frac{\pi}{2}\pi$ and $\theta^{(0)} = 0$ and (b) $q = q' = 0$ and $q" = 0$ that is $\alpha^{(0)} = \xi^{(0)} = \theta^{(0)} = 0$. For $a = 0$ we obtain in inverse Fourier basis:

$$\begin{aligned} \partial_t \psi^0 &= -2\partial_x \psi^0 + 2i(\alpha^{(1)} + \xi^{(1)}) \\ \partial_t \psi^1 &= 2\partial_x \psi^1 + 2i(\alpha^{(1)} - \xi^{(1)}) \end{aligned} \tag{50}$$

Notice that there is no limits for $0 < a < 1$ because for $\theta^{(0)} = 0$, $\{\sigma_z C^{(0)}, C^{(0)}\}$ is always non vanishing. Case (b) leads to

$$\begin{aligned} \partial_t \psi^0 &= -2\partial_x \psi^0 + 2i(\alpha^{(1)} + \xi^{(1)}) + 2e^{i\zeta}\theta^{(1)}\psi^1 \\ \partial_t \psi^1 &= 2\partial_x \psi^1 + 2i(\alpha^{(1)} - \xi^{(1)}) - 2e^{-i\zeta}\theta^{(1)}\psi^0 \end{aligned} \tag{51}$$

As in the previous case $\theta^{(0)} = 0$ will make $\{\sigma_z C^{(0)}, C^{(0)}\}$ always non vanishing. Finally all Eqs 47, 49 and 51 can be recasted as $\partial_t \Psi = P\partial_x \Psi + Q$ where P and Q are Pauli matrices or combinations of them and then Hermitian and traceless matrices.

In conclusion we can resuming all the above results, with the following Theorem distinguish three families of PQW:

Plastic Quantum Walks in 1D If $\tau = 2$ and $d = 1$ and one of the following conditions is satisfied

1. $\alpha^{(0)} = \frac{\pi}{2} + q\pi$ and $\theta^{(0)} = \frac{\pi}{2} + q'\pi$, $\xi^{(0)} = \frac{\pi}{2} + q"\pi$, $\alpha^{(1)} = 0$ $[\mathcal{S}]$
2. $\alpha^{(0)} = \frac{\pi}{2} + q\pi$, $\xi^{(0)} = \arccos(\cos(\xi')\varepsilon^{1-\alpha})$, and $\theta^{(0)} = \arccos(\cos(\theta')\varepsilon^{\alpha})$ $[\mathcal{P}'_{1a}]$
3. $\alpha^{(0)} = \frac{\pi}{2} + q\pi$, $\xi^{(0)} = \frac{\pi}{2}q"$, and $\theta^{(0)} = \arccos(\cos(\pi q')\varepsilon^{\alpha})$ $[\mathcal{P}"_{1a}]$

where ξ' and $\theta' \in [0, 2\pi]$, then the QW is Plastic. In particular we will refer to the first PQW as that one with *strong plasticity*.

3.2 Convergence

In numerical analysis, in order to evaluate the quality of a numerical scheme model, the most important criterion for quality is *convergence*. From an intuitive point of view it requires that, after an arbitrary time x_0, and if ε, the discretisation step, has been chosen small enough, the discrete model approximates the solution to a given order of ε. Arrighi, Nesme, Forets [73], proved rigorously that the probability of observing a discrepancy between the iterated quantum walk and the analytical solution of the Dirac equation in arbitrary dimension converge, *i.e.*, goes to zero, quadratically as the discretisation step ε goes to zero. The convergence was already argued in [74] and numerically in [75]. Di Molfetta and Debbasch [76] proved numerically the convergence in a case where the operator was neither invariant for translations nor homogeneous. To ensure convergence, we will assume throughout the entire manuscript that ε could be always chosen arbitrarily small.

3.3 Discussion and open problems

In this section we introduced the concept of plasticity. This characteristic reveals the fundamental property of different QWs to adapt to the anisotropy of the space-time grid. This elasticity, in its strong version, makes the QW itself able to formally follow both limits, in continuous time and discrete space time. It offers a class of QWs that have the ability to unify in a single mathematical representation, the main simulation schemes in both continuous time (Hamiltonian evolutions) and in discrete time (QWs or more generally QCA). Although such a result already lends itself to a wide range of applications, there is still much to do, certainly in at least three directions: (i) the generalization of the results obtained in 1D to higher dimensions; (ii) an extension of the concept of plasticity to arbitrary simplicial complex. In fact Plastic QWs is likely to prove more powerful in a space where not only there is anisotropy, but the very concept of grid is missing, suggesting a coupling

between plasticity and the intrinsic topology of the simplicial complexes. (iii) Finally, there is the question of symmetries: it is well known that continuous time computation models, although widely used, often suffer from the violation of some important symmetries in nature such as Lorentz- covariance; the bounded speed of light can only be approximately recovered e.g. via Lieb-Robinson bounds. This also creates more subtle problems such as *fermion doubling*, where spurious particles are created due to the periodic nature of the momentum space on a lattice. This latter problem is not present in QW. It remains therefore to be investigated whether PQW can finally solve such problems in continuous time, inheriting the good properties of QW in discrete time. In this thesis we will not develop any of these points that we will leave for future research.

3.4 QW over triangulations

In this section we depart from the grid and we will introduce a new family of QW, which relies on triangulations. The motivation is to model discrete transport in all sorts of topologies as simplicial complexes. The interest is of a very large scientific community ranging from the use of new carbon-based materials and their topological properties, to algorithmics and some quantum gravity theories. More and more new technologies make use of materials such as graphene or fullerene or even compounds with crystalline structures such as triexhagonal tessalation, namely Kagome lattice. In each of these structures, the simplest tile is triangular in shape. To ask how quantum information can be transmitted on such topologies is one of the most immediate applications of appropriate QW defined on triangular structures. There have been researches in this direction and in many of them it has been understood how such QWs are able to capture the topological properties of such materials, allowing also a classification. In all previous models of QWs on triangles, the most serious problem was to use three-state systems, which from a technological point of view made their implementation very complicated and costly. In this chapter we will show how, despite these structures are spanned by three base state vectors, defining the three possible directions of displacement, a QW with a physical system with only two internal states, such as a qubit, is possible and can be defined. The idea is similar to the one that led to the introduction of the AQW, but to solve this problem we will have to modify the definition of the walker itself and his configuration space. At the end we will prove that a special family of Triangular QW converge to the Dirac equation.

In the following we will introduce the model.

3.4.1 The model

Our triangles are equilateral with sides $k = 0, 1, 2$, see Fig. 1. Albeit the drawing shows white and gray triangles, these differ only by the way in which they were laid — they have the same orientation for instance. The QW Hilbert space is $\mathcal{H} = \mathcal{H}_e \otimes \mathcal{H}_2$ where $\mathcal{H}_e$ is spanned by the basis states $|e\rangle$ with e an edge of the grid and $\mathcal{H}_2$ is spanned by the usual coin basis states $|0\rangle$ and $|1\rangle$. Differently from the QW on the grid, here the QW lies on the edge of the simplex. Notice that each triangle hosts a $\mathbb{C}^3$ vector, e.g. $(\psi^{0,v}_{j,k})_{k=0\ldots2}$ and $(\psi^{1,v}_{j,k})_{k=0\ldots2}$. For two triangles v and v' sharing an edge, this edge contains twice the information (one for each triangle). This issue is addressed by associating each coin state to a specific triangle. Let us label each triangle with (0 or 1) such that any two adjacent triangles have different internal state. Moreover, if v is a triangle and $k \in \{1, 2, 3\} \cong \mathbb{Z}/3\mathbb{Z}$, the generic state $|e\rangle \equiv |k_v\rangle$ is uniquely defined by the number v and the number k. The generic state of the walker at a given time j' reads:

$$\Psi_{j'} = \sum_{v,k} \left(\psi^{0,v}_{j',k} |0, k_v\rangle + \psi^{1,v}_{j',k} |1, k_v\rangle \right). \tag{52}$$

The dynamics of the Triangular QW is the composition of two operators. The first operator, R, simply rotates every triangle anti-clockwise. Phrased in terms of the hosted $\mathbb{C}^3$ vectors, the component at side k hops to side $(k+1 \bmod 3)$, as shown in Fig. 1. Equivalently each rotation may be seen as the synchronous application of the translation operator S_{u_i} defined as follows:

$$\widehat{S}_{u_k} \begin{pmatrix} \psi_{j,k}^{0,v} \\ \psi_{j,k}^{1,v} \end{pmatrix} = \begin{pmatrix} \psi_{j,k+1\bmod 3}^{0,v} \\ \psi_{j,k+1\bmod 3}^{1,e(v,k)} \end{pmatrix} \tag{53}$$

where $e(v,k)$ represents the neighbor along the k^{th}-edge of the triangle v. Notice that we can rely the displacement on the triangular grid on the vector basis u_x and u_y spanning the square Euclidean grid. Let us introduce the position $r \equiv r(x,y)$, which corresponds to the mean value of each edge k of a triangle v, then the two components wave fonction $(\Psi_{j,k}^{v}) = \Psi_{j,k}(r)$ represent the vector at position r, on the edge k at time j. Notice that although r characterizes completely the position of the walker, the shift is still k-dependent and will always need both informations. Finally the displacement operator will read:

$$\tilde{S}_{u_k} \begin{pmatrix} \psi_{j,k}^{0}(r) \\ \psi_{j,k}^{1}(r) \end{pmatrix} = \begin{pmatrix} \psi_{j,k+1\bmod 3}^{0}(r - \Delta \hat{u}_k) \\ \psi_{j,k+1\bmod 3}^{1}(r + \Delta \hat{u}_k) \end{pmatrix} \tag{54}$$

where Δ is the lattice discretisation step of the triangle grid. Now the basis vector $u_i, \;\; i = 0,1,2$ are given by

$$u_i = \cos(i\frac{2\pi}{3})u_x + \sin(i\frac{2\pi}{3})u_y = R^s u_s, \tag{55}$$

where $s = x, y$ and R is the coordinates change matrix, and finally the shift operators can be written as a convex combination of the usual displacement $\widehat{S}_{u_x}$ and $\widehat{S}_{u_y}$ we introduce in Chap. **??** :

$$\tilde{S}_{u_k} = \cos(i\frac{2\pi}{3})\widehat{S}_{u_x} + \sin(i\frac{2\pi}{3})\widehat{S}_{u_y}.$$

The second operator is the application of the usual 2×2 quantum coin $\hat{C}$ over each two-components vector state lying on every edge shared by two neighboring triangles, but now the coin will be in general different for each edge k. Altogether, the Triangular QW dynamics is given by the following recursive relations:

$$\Psi_{j+1,k}(r) = \Pi_{i=0,1,2}\tilde{S}_{u_k+i\bmod 3}C_{k+i\bmod 3}\Psi_{j,k}(r). \tag{56}$$

The above equation is a very general one.In the next corollary we are going to show that there exists a sub set of quantum coins C, which does not depend on the edge k and for which the Eq 58 admit a continuous limit.

Continuous Limit of a Triangular QW Let consider the Eq. 58 driving an Alternate Quantum Walk over a triangular lattice. Admit that the quantum coins $\hat{C}$ doesn't depend on its position. If $\theta_{0,u_1} = \theta_{0,u_2} = \theta_{0,u_3} = (1-s)\pi + 2q\pi$, $\xi_{0,u_1} = \xi_{0,u_2} = \xi_{0,u_3} = \frac{\pi}{3} + q'\pi$ and $\alpha_{0,u_1} = \alpha_{0,u_2} = \alpha_{0,u_3} = \frac{\pi}{3} + s\pi + 2q"\pi$, where $s \in \mathbb{B}$ and $\{q, q', q"\} \in \mathbb{Z}$, then the Eq. 58 admits as continuous limit the following PDE:

$$\partial_t \Psi = P(\partial_x + \partial_y)\Psi \equiv P\nabla\Psi \tag{57}$$

where P is a Hermitian and traceless matrix.

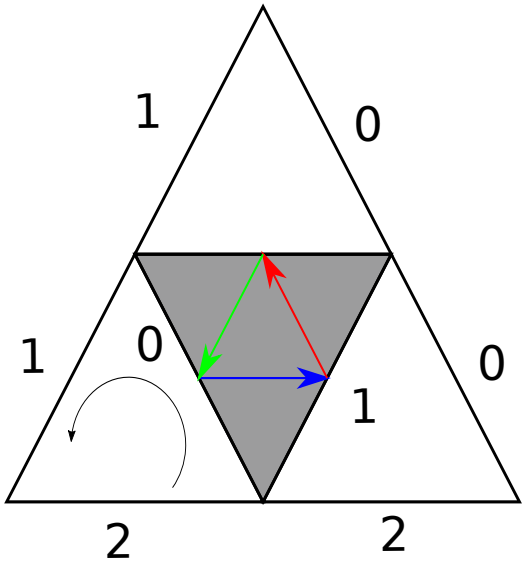

Figure 1: The Triangular QW. Starting at the edge $k = 0$. The circle line represents the counter-clockwise rotation operator.

Proof. By hypothesis C doesn't depend on the walker position, then $C^{(0)}$ is also homogeneous. If we introduce in the Eq. 58 the discretization parameters $\Delta = \varepsilon$, for the spatial dimensions and $\Delta_t = \varepsilon$ for the time dimension, and we develop the same equation around ε then we get up to the first order :

$$\begin{aligned}\Psi_k(t,r) + \varepsilon\partial_t\Psi_k(t,r) = (C^{(0)})^3\Psi_k(t,r) + \varepsilon((C^{(0)})^2\sigma_z C^{(0)}\partial_{u_0}\Psi_k(t,r) \\ +C^{(0)}\sigma_z(C^{(0)})^2\partial_{u_1}\Psi_k(t,r) + (C^{(0)})^3\sigma_z\partial_{u_2}\Psi_k(t,r))\end{aligned} \tag{58}$$

Then in order to consider the formal limit $\varepsilon \to 0$, we need to satisfy:

$$(C^{(0)})^3 = Id \tag{59}$$

from which we derive the following conditions

$$\begin{aligned}\cos(2\theta_0) + 2\cos^2(\theta_0)\cos(\xi_0) = 0 \\ e^{3i\alpha - i\xi}\cos(\theta)\left(e^{4i\xi}\cos^2(\theta) - \left(1 + 2e^{2i\xi}\right)\sin^2(\theta)\right) = 1\end{aligned} \tag{60}$$

The above equations are satisfied if $\theta_0 = (1-s)\pi + 2q\pi$, $\xi_0 = \frac{\pi}{3} + q'\pi$ and $\alpha_0 = \frac{\pi}{3} + s\pi + 2q"\pi$. For theses zeroth conditions

$$C^{(0)} = e^{i\frac{\pi}{3}}R_z(\frac{2\pi}{3}). \tag{61}$$

Then the Eqs. 58 read:

$$\partial_t\Psi_k(t,r) = (\sigma_z\partial_{u_0} + \sigma_z\partial_{u_1} + \sigma_z\partial_{u_2})\Psi_k(t,r) \tag{62}$$

where we used the fact that $(C^{(0)})^2\sigma_z C^{(0)} = C^{(0)}\sigma_z(C^{(0)})^2 = \sigma_z$.

Notice that the PDE obtained above, although defined in 2D is effectively in one spatial dimension. In fact, it is sufficient to define a new variable $v = x + y$ to reduce the Eq 57 to the one dimensional DE obtained in

40. In order to extend the DE to a proper 2D transport we need a different non commuting Hermitian matrix in front to each spatial derivative, e.g. σ_x and σ_y. Using the **??** we can prove that this is possible by mean of a basis change on the coin states.

Dirac Quantum Walk over triangulation Consider the AQW described in 58 where

$$C^{(0)} = \left(e^{i\frac{\pi}{3}} R_z(\tfrac{2\pi}{3})\right) \tag{63}$$

If $\tilde{\Psi}_k(t,r) = U\Psi_k(t,r)$, $C'^{(0)} = UC^{(0)}U^\dagger$ and $U = e^{-i\alpha\sigma_y/2}C^\dagger$ where $\alpha = -\arccos(\sqrt{5}/3)$, then the AQW 58 reads as:

$$\tilde{\Psi}_{j+1,k}(r) = \Pi_{i=0,1,2}\tilde{S}_{u_k+i\text{mod}3}UCU^\dagger\tilde{\Psi}_{j,k}(r). \tag{64}$$

and it admits as continuous limit in spacetime the following PDE:

$$\partial_t\Psi(t,x,y) = (\sigma_x\partial_x + \sigma_y\partial_y)\Psi(t,x,y) \tag{65}$$

Proof. We know that 58 admits a continuous limit iff the zeroth order of the coin is given by the Eq. 63. Notice that a generic basis change applied to the coin states $\{|0\rangle, |1\rangle\}$ and implying that $C'^{(0)} = UC^{(0)}U^\dagger$ and $\tilde{\Psi}_k(t,r) = U\Psi_k(t,r)$ don't change the zeroth order conditions, in fact:

$$\Psi_k(t,r) = U^\dagger(C'^{(0)})^3U\Psi_k(t,r) \tag{66}$$

is satisfied because $U^\dagger U = Id$.
Let us now Taylor expand up to the first order the equation 58 in the new basis:

$$\partial_t\Psi_k(t,r) = \left(\tau_2\partial_{u_2} + \tau_1\partial_{u_1} + \tau_0\partial_{u_0}\right)\Psi_k(t,r) + o(\varepsilon) \tag{67}$$

where

$$\begin{aligned}\tau_0 &= (C^{(0)})^2U^\dagger\sigma_zUC^{(0)}\\ \tau_1 &= C^{(0)}U^\dagger\sigma_zU(C^{(0)})^2\\ \tau_2 &= U^\dagger\sigma_zU\end{aligned} \tag{68}$$

To prove the theorem we need :

$$\sum_{i=0,1,2}\tau_i\partial_{u_i} = (\sigma_x\partial_x + \sigma_y\partial_y). \tag{69}$$

Notice that, using the Eq. 55 in the above equation, we can derive a relation between the τ_i and the σ^s:

$$R_i^s\tau^i = \sigma^s. \tag{70}$$

To solve the system 69, we first translate the $(\partial_{u_i})_{i=0,1,2}$ in terms of the coordinates (x,y), using the Eq. 56

$$\partial_{u_k} = \cos(i\frac{2\pi}{3})\partial_x + \sin(i\frac{2\pi}{3})\partial_y.$$

and then the conditions 69 lead to unique (τ_i) matrices, up to a sign:

$$\begin{aligned}\tau_0 &= \frac{2}{3}\sigma_x + \kappa\sigma_z \\ \tau_1 &= -\frac{1}{3}\sigma_x + \frac{\sqrt{3}}{3}\sigma_y + \kappa\sigma_z \\ \tau_2 &= -\frac{1}{3}\sigma_x - \frac{\sqrt{3}}{3}\sigma_y + \kappa\sigma_z.\end{aligned} \tag{71}$$

with $\kappa = \pm\frac{\sqrt{5}}{3}$. Choose $\kappa = \frac{\sqrt{5}}{3}$, and notice that

$$\sum_i \tau_i = \frac{\sqrt{5}}{3}\sigma_z. \tag{72}$$

and finally from Eq. 71 and the Eq. 68, we can derive $U = e^{-i\alpha\sigma_y/2}C^\dagger$, where $\alpha = -\arccos(\sqrt{5}/3)$ and thus, after the formal limit $\varepsilon \to 0$, the Eq 67 is the following DE in (2+1) dimensions :

$$\partial_t\Psi(t,x,y) = (\sigma_x\partial_x + \sigma_y\partial_y)\Psi(t,x,y). \tag{73}$$

4.0 QUANTUM LATTICE BOLTZMANN AS QUANTUM WALK

It is well known that under an adiabatic assumption the Boltzmann equation reduces to the Navier-Stokes equations in kinetic theory. Analogously the Shrödinger equation can be derived from the Dirac equation under a formally similar condition. This made possible establish a formal parallel between the kinetic lattice Boltzmann equation (LBE) and the relativistic Dirac equation, leading to the modern definition of Quantum Lattice Boltzmann. Such correspondence has been first made by Sauro Succi and collaborators and well discussed, e.g. in [16]. Therefore, the QLB techniques to discretize the Dirac equation has to fall within the class of quantum walks, whose continuum limit delivers Dirac quantum wave equations, as we proved in the previous sections. This one-to-one correspondence between QW and QLB, makes such lattice Boltzmann schemes suitable to be implemented on actual quantum computers. In the following we will review the main steps to justify such correspondence, following mainly [16].

4.1 Operator splitting versus Quantum Walk for the Dirac equation

In the previous section we proved, in the most general framework, that families of QWs admit as continuous limit quantum transport equations, in particular the Dirac equation. Here we would like to move in the other way around. Starting from the Dirac equation, we will show that the first order discretization numerical scheme can be casted in a Quantum Walk. Let us start with the Dirac equation in the Majorana form in (1+1)-spacetime dimension, namely :

$$\partial_t\Psi = [-i\sigma_z\partial_x + M(x,t)]\Psi \tag{74}$$

where Ψ is a two-component wave function and $M(x,t) = IdM_0(x,t) + \sigma\cdot\mathbf{M}$ is an Hermitian matrix encoding the mass term or some spacetime dependent potential, e.g. the electric field. After a simple and straightforward calculation the solution of the above equations reads :

$$\Psi(x,t) = \hat{T}\exp\left[-\Delta t\sigma_z\partial_x - i\int_{t_0}^{t} M(x,t')dt'\right]\Psi(x,t_0) \tag{75}$$

where $\hat{T}$ is the time-ordering operator. Now, if Δt is sufficiently small the above equation can be approximated by:

$$\Psi(x,t) = \exp\left[-i\Delta t M(x,t_0)\right] \exp\left[-\Delta t \sigma_z \partial_x\right] \Psi(x,t_0) + O(\Delta t^2). \tag{76}$$

From the above equation we can recognize essentially two terms : the first exponentially, which acts in the internal space of the wave-function, making possible the 'collisions' between the two components of the state. This term also introduces an inertial term due to the mass and the potential encoded in M. Remark that such exponential is unitary and can be easily map, term by term to a quantum coin operator of the kind :

$$e^{-i\xi_{j,n}} \begin{pmatrix} e^{i\alpha_{j,n}} \cos\theta_{j,n} & e^{i\beta_{j,n}} \sin\theta_{j,n} \\ -e^{-i\beta_{j,n}} \sin\theta_{j,n} & e^{-i\alpha_{j,n}} \cos\theta_{j,n} \end{pmatrix} \tag{77}$$

where

$$\xi_{j,n} = M_{0,j,n}\Delta t \tag{78}$$

$$\tan(\alpha_{j,n}) = -\frac{M_{z,j,n}}{|\mathbf{M_j, n}|} \tan(|\mathbf{M_{j,n}}|\mathbf{\Delta t}) \tag{79}$$

$$\tan(\beta_{j,n}) = \frac{M_{x,j,n}}{M_{y,j,n}} \tag{80}$$

$$\tan(\theta_{j,n}) = \tan(|\mathbf{M_{j,n}}|\mathbf{\Delta t}) \sqrt{\frac{\mathbf{M^2_{x,j,n}} + \mathbf{M^2_{y,j,n}}}{|\mathbf{M_{j,n}}|^2 + \mathbf{M^2_{z,j,n}} \tan^2(|\mathbf{M_{j,n}}|\mathbf{\Delta t})}} \tag{81}$$

The second exponential acts in the position space without mixing the internal components of the wave function. From here, and after the general and detailed introduction on quantum walks we had, it is clear the identification of such operator to the standard conditioned translation operator typical for quantum walk. Indeed its actions explicitly moves the upper component to the left and the lower component to the right :

$$\exp\left[-\Delta t \sigma_z \partial_x\right] \Psi(x,t_0) = \begin{pmatrix} \psi^1(x-\Delta t) \\ \psi^2(x+\Delta t) \end{pmatrix}. \tag{82}$$

This suggests to use the Courant-Friedrichs-Lewy condition, introducing $\Delta x = \Delta t$, which means that we discretized space and time on the same foot. Notice that this would correspond to the isotropy condition in the Plastic QW, as introduced in the last section. In conclusion, without any surprises, the discretization scheme of the Dirac equation, based on operator splitting coincides with the QW formulation. But inevitably, this would bears a close relation with the lattice Boltzmann scheme, because the latter has been proved to encompass the operator splitting of the Dirac equation in the Majorana representation. In the following section we will shortly try to convince the reader, recalling the main steps of the proof.

4.2 Quantum Lattice Boltzmann scheme from the Dirac equation to QWs

The non-relativistic limit of the Shroedinger equation has been proved to admit an hydrodynamical interpretation, noticed first by Erwin Madelung back in 1927. Indeed the homonym Madelung transformations map the Shroedinger equation into the hydrodynamic equation of a compressible, inviscid fluid. Recentlly, Di Molfetta and collaborators have been proved that a new relativistic generalization of the Madelung transform maps this Dirac equation into a 2D dispersive hydrodynamics for relativistic quantum fluids. In the non relativistic limit, the two component spinor which obeys the Dirac equations degenerates into a single wave-function which obeys

the Schrödinger equation, connecting the relativistic Madelung transformations to the former non relativistic ones. From a formal point of view this result is not surprising because the Dirac equation is the discret analogue as a special form of Boltzmann kinetic equations [77]. This also means in other words that a QLB scheme can be seen as a unified computational framework to simulate both relativistic and non-relativistic quantum wave equations.

In this section we review how to derive a QLB scheme starting from the Dirac equation. Again, let us start with the Dirac equation in (1+1)-spacetime dimension :

$$[\partial_t + v_a \partial_x]\psi_a = -i \sum_b M_{ab}(x,t)\psi_b(x,t) \tag{83}$$

where this time we wrote the equation explicitly component by component. Notice that v_a, as pointed out before, can get two discret values, respectively $+1$ for the upper component and -1 for the lower component. In a LB dictionary, these velocities can be considered as 'microscopic velocities' and M would coincide with the 'collision term'. If we assume the each field is at least twice differentiable, we can Taylor expand the above equation around $\Delta t = 0$ and we recover, following [16], the lattice Boltzmann equation:

$$\psi_i(x + v_a \Delta t, t + \Delta t) = \psi_a - i\Delta t \sum_b M_{ab}\psi_b + O(\Delta t^2). \tag{84}$$

Now using an implicit Crank-Nicolson discretization scheme, we can integrate the collision term as :

$$iM(x,t)\begin{pmatrix}\psi_1(x,t)\\ \psi_2(x,t)\end{pmatrix} = \frac{i}{2}M_{j,n}\left\{\begin{pmatrix}\psi^1_{n+1,j+1}\\ \psi^2_{n+1,j-1}\end{pmatrix} + \begin{pmatrix}\psi^1_{n,j}\\ \psi^2_{n,j}\end{pmatrix}\right\} \tag{85}$$

and together with the Eq. 83, we recover the second order QLB scheme :

$$\begin{pmatrix}\psi^1_{n+1,j+1}\\ \psi^2_{n+1,j-1}\end{pmatrix} = T_{j,n}\begin{pmatrix}\psi^1_{n,j}\\ \psi^2_{n,j}\end{pmatrix} + O(\Delta t^2) \tag{86}$$

where the transfer matrix $T_{j,n}$ is given by:

$$T_{j,n} = \left[I_2 + i\frac{\Delta t}{2}M_{j,n}\right]^{-1}\left[I_2 - i\frac{\Delta t}{2}M_{j,n}\right] \tag{87}$$

Using explicitely the definition of $M_{j,n}$ and after few simplification we get for $T_{j,n}$:

$$T_{j,n} = \frac{1}{C_{j,n}}\begin{pmatrix}1 - i\Delta t M_{z,j,n} & -\Delta t(iM_{x,j,n} + M_{y,j,n})\\ -\Delta t(iM_{x,j,n} - M_{y,j,n}) & 1 + i\Delta t M_{z,j,n}\end{pmatrix} \tag{88}$$

where $C_{j,n} = 1 + i\delta t M_{0,j,n}$. As the reader could have already remarked the above matrix is unitary, then is norm-preserving. Moreover we can identify each coefficient of the above matrix with the quantum coin coefficient in Eq. 78, revealing finally the hidden QW-structure of the QLB scheme. In fact, the QLB scheme is nothing but, again, a composition of a conditioned shift operator and a coin operator, playing this time the role of a collision term. These two last section helped us to see clearly the one-to-one correspondence between the QLB scheme and a QW and this correspondence is absolutely general in the linear case. However reversibility and linearity constraints inevitably the phenomena we can simulate by mean of a single particle quantum walk.

Let us justify this statement.
The discrete Boltzmann equation in the most general framework reads as follows :

$$\partial_t f + v_i^a \nabla_a f_i = \Omega_{ij}(f_j - f_j^e) \tag{89}$$

where $f_i = f(x, v_i, t)$ is the probability density of finding the particle i around position x, at time t with discrete velocity v_i. The LHS of the equation is the particle free-streaming, which we already had at the beginning of this section. In absence of mass or external forces, this is the only term which really counts. The RHS, instead, represents the collision term, steering the distribution function towards a local equilibrium f_i^e. Obviously in the quantum case, the real probabilities will be replaced by probabilities amplitudes and the dynamics has to be kept reversible, which also means that there is no equilibrium distribution for an arbitrary initial Ψ_0. However, we can always formally introduce a local equilibrium in the Eq. 83, $\Psi_{eq} := U\Psi$, where U is a unitary which may depend on M. Notice that this unitary does not correspond to a global rotation because it depends on the spacetime grid. Therefore our Dirac equation can be recasted in the following form :

$$[\partial_t + \sigma_z \partial_x]\Psi = \Omega(\Psi - \Psi_{eq}) \tag{90}$$

where $\Omega = iM[I + U]^{-1}$. Now the Dirac equation looks as the most general discrete Boltzmann equation, at least formally, where the dynamics can be seen as a propagation-relaxation process in imaginary time, where the collision term Ω, cause oscillations around the local equilibrium. This should not surprise the attentif reader convinced in the reversibility of quantum mechanics. In fact, the only possible equilibrium in the linear, one particle, case, is the vacuum state, namely here $\Psi_{eq} = 0$. This is somehow obvious because, due to the reversibility of the process, we cannot have limiting equilibrium distribution.

However, this result should not disappoint because it actually represents the fundamental building block for constructing Boltzmann schemes for systems with N interacting quantum bodies. There are essentially two directions that can be taken to generalise this result to interacting systems. The first, simpler, is to *introduce non-linear terms* into the Dirac equation. The strategy is the same as we have described so far: discretizing the non-linear Dirac equation by means of unitaries coincides with introducing non-linear phases in the standard QW. Non-linear terms should introduce in the above equation, non-trivial solutions. Also this should not be surprising, because from the physical point of view it would coincide with the symmetry breaking of the vacuum state.

Another way, less marked than the previous one, is to model the interaction through a *quantum cellular automata*. This time the interaction would be taken into account at the microscopic level and not at the actual level by non-linear phases, handily included in the evolution operator. This way, I believe, is certainly the most promising, because it is richer from the phenomenological point of view: localisation, ergodicity breaking and fragmentation of Hilbert space, quantum chaos and classical limit are only a part of what still needs to be explored and understood in this framework. Moreover, the introduction of non-linear terms in the evolution operator does not represent a great computational advantage (only polynomial) over a classical simulator. On the contrary, quantum cellular automata allow an exponential advantage over classical machines.

As a conclusion of this part, it is interesting to explore more precisely, with some examples, how a quantum walk can simulate hydrodynamic behaviour, even in the absence of interaction or non-linearity. As we have already mentioned, the Dirac equation admits its hydrodynamic interpretation, via Madelung transformations.

4.3 An example : Quantum Simulation of Hydrodynamics shocks

Let us consider the simplest but non trivial quantum walk on the line, where the evolution is controlled by the standard unitary operator U and the coin (the collision) operators is $C = e^{-i\theta\sigma_1}$. The explicit evolution equation of the walk reads:

$$\begin{bmatrix} \psi^1(j+1,n-1) \\ \psi^2(j+1,n+1) \end{bmatrix} = \begin{bmatrix} \cos\theta & -i\sin\theta \\ -i\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \psi^1(j,n) \\ \psi^2(j,n) \end{bmatrix} \tag{91}$$

where the index j represents the iteration or discrete time. In the second section we studied how to compute the continuous limit of this walk, when the discretisation step of the spacetime grid goes to zero. And in the last section we saw that such a QW coincides with a QBL scheme where the coin plain the role of the scattering operator and the conditioned shift plays the role of the streaming term. Taking the formal continuous limit the Dirac equation can be recasted as follows

$$i\gamma^\mu\partial_\mu\psi - m\psi = 0\,, \tag{92}$$

where $\psi = (\psi^1, \psi^2)^T$, $\gamma^0 = \sigma_1$, $\gamma^1 = i\sigma_2$ (σ_2 is the second Pauli matrix) and $\hbar = c = 1$ for simplicity.

Now we know that the Dirac equation (92) can be obtained from the Lagrangian density

$$\mathcal{L} = \frac{i}{2}\left(\overline{\psi}\gamma^\mu\partial_\mu\psi - \partial_\mu\overline{\psi}\gamma^\mu\psi\right) - m\overline{\psi}\psi \tag{93}$$

where $\overline{\psi} = \psi^\dagger\gamma^0$. The associated particle current is $j^\mu = \overline{\psi}\gamma^\mu\psi$ and the stress energy tensor reads $T^{\mu\nu} = \frac{i}{4}[\overline{\psi}\gamma^\mu\partial^\nu\psi - \partial^\nu\overline{\psi}\gamma^\mu\psi + (\mu \leftrightarrow \nu)]$. Both j and T are conserved *i.e.* $\partial_\mu T^{\mu\nu} = 0$ and $\partial_\mu j^\mu = 0$. In order to apply the Madelung transformation we have to split the wave fonction Ψ into the density j^μ and the phase of $\Psi_{L/R}$. In a relativistic framework the covariant current is given by:

$$j^0 = |\psi^2|^2 + |\psi^1|^2 \tag{94}$$

$$j^1 = |\psi^2|^2 - |\psi^1|^2 \tag{95}$$

The overall Madelung transformation over the spinor is given by In particular, the spinor ψ now reads

$$\psi(\mathbf{x},t) = \frac{1}{\sqrt{2}}e^{i\varphi_+/2}\begin{bmatrix} \sqrt{j^0 - j^1}e^{i\varphi_-/2} \\ \sqrt{j^0 + j^1}e^{-i\varphi_-/2} \end{bmatrix} \tag{96}$$

where $\varphi_\pm = \varphi^1 \pm \varphi^2$ and $\varphi_+/2$ can be viewed as the global phase of ψ.

In terms if these new variables, the Lagrangian density and the stress energy tensor read

$$\mathcal{L} = -m(j_\mu j^\mu)^{1/2}\cos\varphi_- - \frac{1}{2}\left(j^\mu\partial_\mu\varphi_+ - \epsilon^{\mu\nu}j_\nu\partial_\mu\varphi_-\right) \tag{97}$$

and

$$T^{\mu\nu} = -\frac{1}{4}\left(j^\mu\partial^\nu\varphi_+ - \epsilon^{\mu\alpha}j_\alpha\partial^\nu\varphi_- + (\mu \leftrightarrow \nu)\right), \tag{98}$$

where $\epsilon^{\mu\nu}$ denotes the completely antisymmetric symbol of rank two, with the convention $\epsilon^{01} = -\epsilon^{10} = 1$.

The dynamical equations derived from $\mathcal{L}(j^0, j^1, \varphi_+, \varphi_-)$ are

$$\epsilon^\mu{}_\alpha\partial_\mu j^\alpha = 2m(j_\mu j^\mu)^{1/2}\sin\varphi_- \tag{99}$$

$$m\cos\varphi_-\, j^\mu = -\frac{1}{2}(j_\mu j^\mu)^{1/2}\left(\partial^\mu\varphi_+ + \epsilon^{\mu\nu}\partial_\nu\varphi_-\right) \tag{100}$$

$$\partial_\mu j^\mu = 0. \tag{101}$$

where the density n of the $(1+1)$D Dirac fluid is given by $n = (j_\mu j^\mu)^{1/2}$. Notice that we can express the above equation (100) in terms of the density n and the velocity u^1 *i.e.* the density and the spatial part of the fluid 2-velocity:

$$m \cos\varphi_- \, u^\mu = -\frac{1}{2}\left(\partial^\mu \varphi_+ + \epsilon^{\mu\nu}\partial_\nu \varphi_-\right) \tag{102}$$

and, in this form, brings to mind the standard relation $\frac{w}{n}u^\mu = -\partial^\mu\varphi$ which links the velocity u of a relativistic potential flow to its potential φ, the enthalpy per unit volume w and the particle density n.

We thus retain $w = mn\cos\varphi_-$ as the enthalpy per unit volume of the $(1+1)$D Dirac fluid.

The velocity field u then derives from two potentials. One is $\varphi_+/2$ *i.e.* the global phase of the spinor ψ and contributes to u in the standard way. The other potential is the phase differential $\varphi_-/2$ and contributes to u in a non-standard way, by contraction of its gradient with the $(1+1)$D completely antisymmetric symbol.

Using (100), one then finds that

$$T^{\mu\nu} = wu^\mu u^\nu + \frac{n}{2}\left(\epsilon^{\mu\alpha}u_\alpha \partial^\nu\varphi_- + u^\mu\epsilon^{\nu\alpha}\partial_\alpha\varphi_-\right), \tag{103}$$

to be compared with the stress-energy tensor $T^{\mu\nu} = wu^\mu u^\nu - p\eta^{\mu\nu}$ of a relativistic perfect fluid of pressure p. The pressure of the Dirac fluid thus vanishes. This is not surprising because pressure in spin 0 superfluids is generated by interaction terms and there is no interaction in the free Dirac equation derived above. The last two terms on the right-hand side of (103) depend on the gradient of φ_- and, thus, on the gradient of w/n. Indeed, the definition of w leads to $\sin^2\varphi_- = 1 - (\frac{w}{mn})^2$ and $\sin\varphi_- d\varphi_- = -d(\frac{w}{mn})$, so that, if $w \neq nm$,

$$\partial_\mu\varphi_- = -\sigma\frac{\partial_\mu(\frac{w}{mn})}{\left(1-(\frac{w}{mn})^2\right)^{1/2}} \tag{104}$$

where σ is the sign of $\sin\phi_-$. As for relativistic spin 0 superfluids, the two extra-terms in the above expression of the stress-energy tensor thus depend on the gradient of a thermodynamic function (the enthalpy per particle w/n) and are therefore best viewed as generalized 'quantum pressure' terms. As shown in [7] the two component spinor which obeys Dirac equation degenerates, in the Galilean limit, into a single wavefunction which obeys the Schrödinger equation and the relativistic hydrodynamics degenerates into the usual Madelung hydrodynamics. The above generalization of the Madelung transform strongly suggests that the original QW can be used to simulate quantum flows. First note that a general positive energy plane wave solution of (92) can be written as (see (96)-(101)) $j^0 = n\sqrt{1+q^2}$, $j^1 = nq$, $\varphi_+/2 = -m\left(\sqrt{1+q^2}t - qx\right)$, $\varphi_- = 0$, where q denotes both wave-number and momentum in unit of m (remember $\hbar = c = 1$). The spinor $\psi^1 = \sqrt{\sqrt{1+q^2}-q}e^{im\phi}/\sqrt{2}$, $\psi^2 = \sqrt{\sqrt{1+q^2}+q}e^{im\phi}/\sqrt{2}$ thus describes, at $t=0$, a unit density fluid ($n=1$) in motion with constant velocity u^1 given by $u^1 = q = \partial\phi/\partial x$. In order to simulate quantum flows, we now select the initial data

$$\phi = \frac{q_{\max}}{m}\left[\cos(x) + \frac{1}{3}\cos(3x) + \frac{1}{2}\cos(2x+0.9)\right], \tag{105}$$

which, with $q_{\max} = mu_{\max}$ corresponds to the velocity field $u^1 = u_{\max}(-\sin(x) - \sin(3x) - \sin(2x+0.9))$. The evolution of this initial condition through the QW for various values of m and constant $q_{\max}$ (the larger the mass, the less relativistic the propagation) is displayed in Fig.2.

Note that a similar (but somewhat simpler) type of initial condition $\phi = q_{\max}\cos(x)/m$ has already been used in the cosmological context to simulate the dynamics of (i) a non-quantum cosmological fluid through

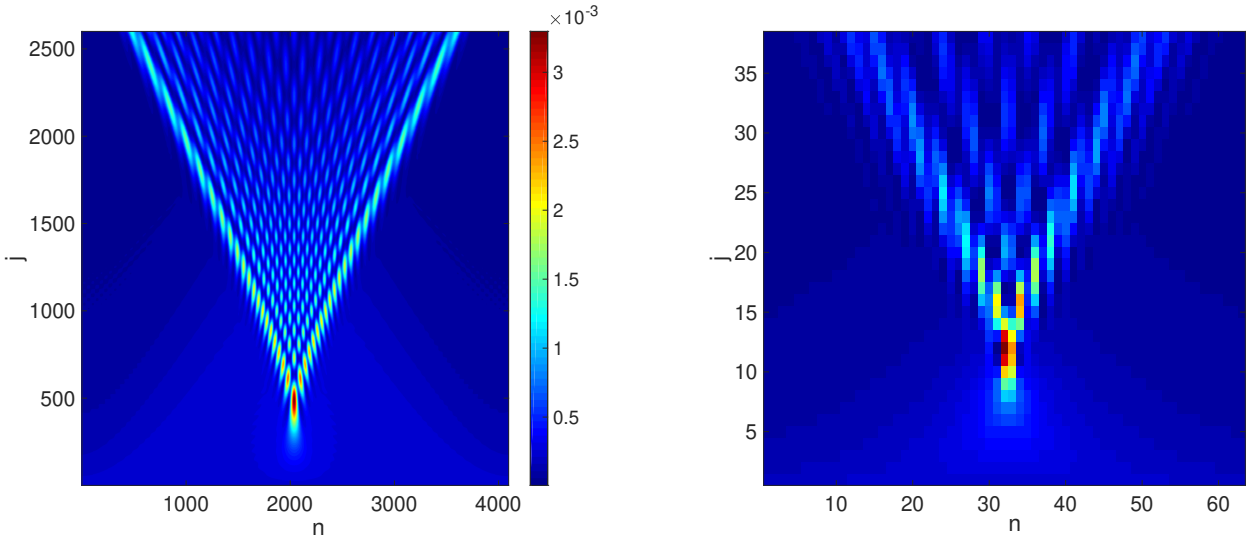

Figure 2: (color online) a) DTQW with initial data $\cos(x) + \frac{1}{3}\cos(3x) + \frac{1}{2}\cos(2x + 0.9)$ (same as Fig.?? but $u_{\max} = 0.2$) b) Same as (a), but initial data: $\cos(x)$; c) Approximation by Pearcey's integral in (x, t) space with $\varepsilon = 0.05$

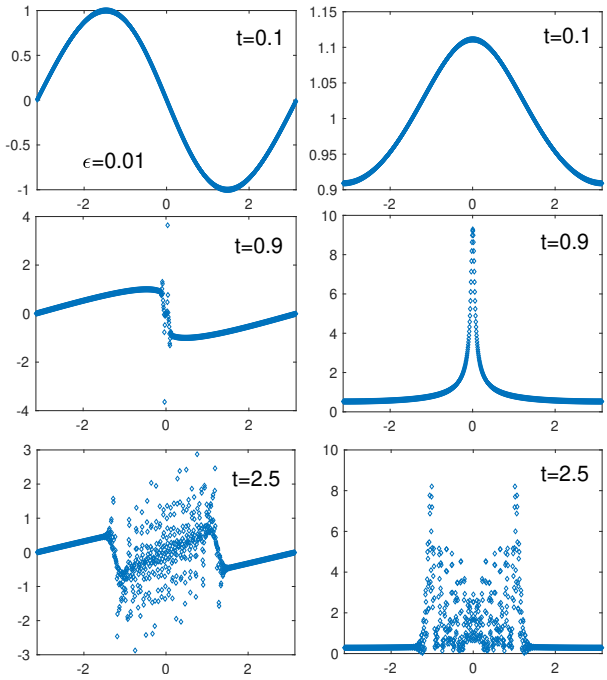

Figure 3: (color online) Evolution of velocity $v = m^{-1}\partial_x\varphi$ (left) and density n (right) for 3 values of time and $m^{-1} = 0.01$ obtained from a numerical solution of Schrödinger equation $i\partial_t\psi = -\frac{1}{2m}\partial_{xx}\psi$, with $\psi = n^{1/2}\exp i\varphi$ and initial data $\varphi = m\cos x$ and $n = 1$.

the non-linear Schrödinger equation [78] (ii) a Bose-Einstein condensates of axions [79]. Fig.2 shows that this simpler initial data generates a single symmetric shock.

The figures below show that the QW can indeed be used to simulate hydrodynamical shocks in a quantum fluid [80, 81], and indeed they are able to reproduce the analytical solution (Fig.2.b) we calculated starting from the continuous dynamical equations.

Again, such a result should come as no surprise, having shown that a quantum walk is nothing more than a linear QLB. The absence of pressure terms in the Dirac fluid dynamics equations is a consequence of the absence of interaction in the model. In the next section we will briefly discuss how we can introduce nonlinear terms into the QW equations and thus effectively model microscopic interaction.

5.0 INTRODUCING EFFECTIVE NONLINEARITIES

Here we show how we can account non-linearities in the QW definition. This is usually done by introducing in the quantum coin operator, namely the collision terms, a quadratic dependency on the probability amplitude. However this is only a choice determined by the phenomenon we would like to simulate. For example, let us consider the following nonlinear Dirac equation:

$$(\mathbb{I}\partial_t - \sigma_z\partial_x - i\kappa\tilde{\mathcal{M}})\Psi(t,x) = 0 \tag{106}$$

where

$$\tilde{\mathcal{M}} = \begin{pmatrix} s_0 & -i\frac{s_3}{3} \\ i\frac{s_3}{3} & s_0 \end{pmatrix} \tag{107}$$

where $s_0 = |\Psi|^2$ and $s_3 = \Psi^*_{j,m}\sigma_2\Psi_{j,m}$. The constant κ can be interpreted as the coupling factor. The above equation in the covariant form is the Nambu and Jona-Lasinio equation, i.e. the Dirac equation with a quartic interaction. As discussed in the previous two sections, including a non linear terms would make appear in the QLB scheme a non trivial equilibrium distribution and in the Dirac fluid a non vanishing quantum pression term. But how do we include such terms in the QW definition ?

Let consider again a QW on a line. Consider for all $(n,j)\in \mathbb{N}^2$, the collection $W^n_j = (\Psi_{k,m})_{k=nj,m\in\mathbb{Z}}$. This collection represents the state of the QW at 'time' $k = nj$. For any given n, the collection $S^n = (W^n_j)_{j\in\mathbb{N}}$ thus represents the entire history of the QW observed through a stroboscope of 'period' n. The evolution equations for S^n are those linking W^n_{j+1} to W^n_j for all j. We need to introduce a time-scale τ and a length-scale λ and an $\epsilon \in \mathbb{R}$ such that $\tau\epsilon \ll 1$ and $\lambda\epsilon \ll 1$. Define $\Delta t = \tau\epsilon$, $\Delta x = \lambda\epsilon$ and:

$$\begin{aligned} x_m &= \Delta x\, m \\ t_j &= \Delta t\, j \end{aligned} \tag{108}$$

Consider the map $\mathcal{F}$ as follows:

$$\mathcal{F} : \mathcal{F}[\phi(t_j,x_m)] \to e^{ig|\phi(t_j,x_m)|^2}\phi(t_j,x_m) \tag{109}$$

Now if we apply the above mapping to the a simple Hadamard walk the finite difference equations read:

$$\psi^-(t_j+\Delta t,x_m) = \frac{1}{\sqrt{2}}[\mathcal{F}[\psi^-(t_j,x_m+\Delta x)] + \mathcal{F}[\psi^+(t_j,x_m+\Delta x)]] \tag{110}$$

$$\psi^+(t_j+\Delta t,x_m) = \frac{1}{\sqrt{2}}[\mathcal{F}[\psi^-(t_j,x_m-\Delta x)] - \mathcal{F}[\psi^+(t_j,x_m+\Delta x)]] \tag{111}$$

If Ψ is at least twice differentiable we can Taylor expand the equations defining S^n and in particular 111 in powers of ϵ. The formal continuous limit is obtained letting both Δt and Δx to zero, i.e. letting ϵ to zero. For the limit to exist, all zeroth order terms of the Taylor expansion must identically cancel each other and the differential equations describing the limit is then obtained by equating to zero the non identically vanishing, lowest order contribution.
If we consider S^1 we can easily deduce from (111) that the continuous limit doesn't exist because the zeroth order doesn't identically cancel. As we already saw in the second section of these lectures, we have to turn our attention on S^2 which admits a formal continuous limit. The S^2 reads:

$$\psi^-(t_j+2\Delta t,x_m)=\frac{1}{2}[\mathcal{F}[\phi^-(t_j,x_m+\Delta x)]+\mathcal{F}[\phi^+(t_j,x_m-\Delta x)]$$
$$\psi^+(t_j+2\Delta t,x_m)=\frac{1}{2}[\mathcal{F}[\phi^-(t_j,x_m-\Delta x)]-\mathcal{F}[\phi^+(t_j,x_m+\Delta x)]$$

where

$$\phi^{\mp}(t_j,x_m) \quad = \quad e^{ig|\psi^-(t_j,x_m+\Delta x)|^2}\psi^-(t_j,x_m+\Delta x) \pm e^{ig|\psi^-(t_j,x_m+\Delta x)|^2}\psi^+(t_j,x_m+\Delta x). \quad (112)$$

Indeed a straightforward computation and letting ϵ to zero, delivers the following equation obeyed by the wave function $\Psi(T,X)$:

$$(\mathbb{I}\partial_T-\mathcal{P}\partial_X-i\kappa\mathcal{M})\Psi=0 \quad (113)$$

where

$$\mathcal{P}=\frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \qquad \mathcal{M}=\begin{pmatrix}s_0 & i\frac{s_3}{3}\\ -i\frac{s_3}{3} & s_0\end{pmatrix} \quad (114)$$

and $T=t/\tau$ and $X=x/\lambda$. The operator P is self-adjoint and its eigenvalues are -1 and $+1$. Two eigenvectors

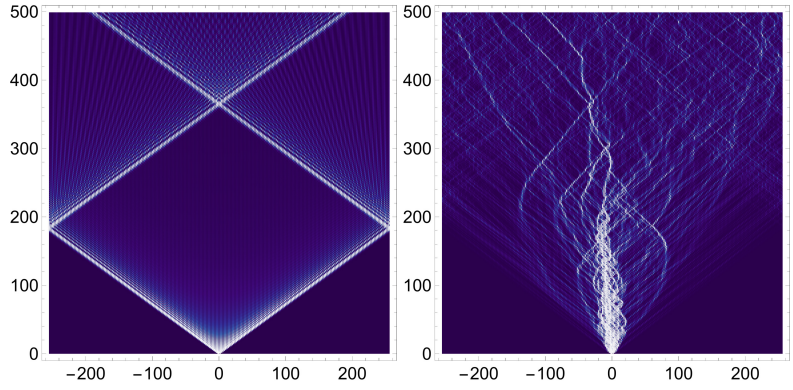

Figure 4: (Color online) Time evolution of the probability density $\Pi_{j,m}$ for (a) an Hadamard QW (ω=0) and (b) NL-QW (ω=5) with a symmetric initial condition $\Psi_{0,m}=\frac{\delta_{0,m}}{2}(b_-+ib_+)$.. The grid points N = 256.

associated to these eigenvalues are

$$\mathcal{B}_-=\left(\cos\frac{\theta}{8}\right)b_-+\left(\sin\frac{\theta}{8}\right)b_+, \quad (115)$$

$$\mathcal{B}_+=\left(\sin\frac{\theta}{8}\right)b_--\left(\cos\frac{\theta}{8}\right)b_+. \quad (116)$$

The family $(\mathcal{B}_-, \mathcal{B}_+)$ forms an orthonormal basis of the two dimensional spin Hilbert space. If we re-write equation 113 on this new spin basis the result is:

$$(\mathbb{I}\partial_T - \sigma_3\partial_X - i\kappa\tilde{\mathcal{M}})\tilde{\Psi} = 0. \tag{117}$$

The family of the above QW exhibits a very complex dynamics. As shown in Fig. 4.b, the DNS (Direct Numerical Simulations) of the probability density's evolution is very different from the standard Hadamard walk in Fig. 4.a and such behavior depends in general on the constant g. Notice that the symmetry breaking in the simulation is entirely due to the round-off noise.

6.0 HINTS FOR A QLB ON CURVED SURFACE

The last topic I would like to deal with here is the simulation of a fluid on a curved surface. In line with what has been said so far, I will only suggest formal models, in the linear case, because these can then easily be extended to the case with interaction, either by introducing non-linear phases, or by extending the model to the multi-particle sector.

In the previous chapter we have proven that some family of QWs admits as continuous limit in spacetime an equation of the form:

$$\partial_t\Psi(t,\mathbf{x}) = \sum_{i=1}^{d} P_i\partial_{x_i}\Psi(t,\mathbf{x}) \tag{118}$$

where C may be seen as a constant and uniform velocity matrix for the continuous field $\psi(t, \boldsymbol{d}x)$. Any function of the form $\omega(\boldsymbol{d}x - ct)$ is a solution of the above equation and it describes the transport of the function ω at constant speed v. In other words the evolution operator which drives the field is homogeneous at every point of the space. What does it happen if we consider the same equation on an arbitrary manifold? Such a PDE in an arbitrary dimension d can be written as follows:

$$\partial_t\Psi(t,\boldsymbol{d}x) = \sum_{i=1}^{d}\left(P_i(\boldsymbol{d}x)\partial_{x_i}\Psi(t,\boldsymbol{d}x) + \Psi(t,\boldsymbol{d}x)\frac{1}{2}\partial_{x_i}P_i(\boldsymbol{d}x)\right). \tag{119}$$

where each $P_i(\boldsymbol{d}x)$ is a Hermitian matrix, such that $|P_i(\boldsymbol{d}x)| \leq Id$. Notice that the space dependent coefficients in front of the derivatives may be seen as component of a non-homogeneous velocity tensor. This suggests that the mechanism now driving the walker needs to be non homogeneous, in particular the quantum coin parameters. Our goal in the following is to build a quantum scheme such that, given a particular PDE of the form 119 we wish to simulate, we are able to retro-engineer the corresponding QW. To illustrate the main idea let us start by a the simple academic case of the infinite line.

6.1 Mimicking curved transport on the grid

Let us consider a QW over the line, e.g. that one introduced in the previous chapter. We already proved that it formally converges, in the continuous spacetime limit, to the Eq. 47 which is of the form 118, where the velocity corresponds to the real constant $\bar{\theta}$. Our conjecture is that, to simulate a non-homogenous velocity field, we would wish to make $\bar{\theta}$ dependent on each point of the spacetime grid:

$$\theta(t,x) = \theta_0 + \varepsilon^b\bar{\theta}(t,x). \tag{120}$$

Then coming back to the results of the second section, for $a = 1$ we can see that the coefficients $\varepsilon\partial_x[\{\sigma_z C^{(0)}, C^{(1)}(t,x)\}+\{\sigma_z C^{(1)}(t,x), C^{(0)}\}]$ leads now to a spatial derivative of $C^{(1)}(t,x)$, due to the inhomogeneity introduced in the jet 120. Computing the formal limit for $\varepsilon \to 0$, leads to recover the following couple of inhomogeneous PDEs:

$$\begin{aligned}\partial_t\psi^0 &= 2ie^{i\zeta}(\bar{\theta}(t,x)\partial_x\psi^1 + \psi^1\frac{1}{2}\partial_x\bar{\theta}(t,x))\\ \partial_t\psi^1 &= -2ie^{-i\zeta}(\bar{\theta}(t,x)\partial_x\psi^0 + \psi^0\frac{1}{2}\partial_x\bar{\theta}(t,x))\end{aligned} \tag{121}$$

The above equations are of the required form in 119. Indeed, fixed by hand a specific metrics leads to define the $\bar{\theta}(t,x)$ and thus, to retro-engineer the corresponding QW just encoding the metric coefficients into the definition of the quantum coin. In order to show how it works, we propose the following example:

Example: Quantum Walking in and around a black hole

The Eq. 119 includes the massless Dirac equation (DE) coupled to a $(d+1)$-dimensional spacetime. In $(1+1)$-spacetime and synchronous frame, the massless DE can be written as follows:

$$i\partial_t\chi + \frac{i}{2}\{B^x, \partial_x\}\chi = 0, \tag{122}$$

and where $B^x = \gamma^1 e^x{}_1$. In particular, one can make the choice $\gamma^1 = \sigma_x$. Here we are not discussing the physics behind this equations. We are only interested in formally simulating them on the lattice by means of local unitaries.
Let us fix in 121 ζ to $-\pi/2$ so that it coincides with Eq. 122 and by identification we can set $e_1^x = \bar{\theta}(t,x)$. Now we assume that the spacetime fonction B^x, which defines the spacetime metrics coefficients, is externally fixed by hand, i.e. the corresponding curvature is external and not dynamical. As exemple, we choose the spherically symmetric solution of Einstein equation in vacuo, a Schwarschild black hole. In a special coordinates frame, called Lemaître coordinates, the Eq. 122 reads:

$$i\partial_t\chi - \frac{i}{2}\{\frac{r_g}{r}\sigma_x, \partial_x\}\chi = 0, \tag{123}$$

where $r(t,x) = \left[\frac{3}{2}(x-t)\right]^{2/3} r_g^{1/3}$, r_g is constant and called the gravitational radius. The event horizon is located at $r = r_g$ *i.e.* $x = t + (2/3)r_g$, and the singularity is located at $r = 0$ *i.e.* $x = t$. The exterior of the black hole is the domain $r > r_g$ and finally the trajectory of the quantum particle, i.e. the geodesics the particle would follow in this metrics, are analytically computed by $dt = \pm\left(r_g/r(t,x)\right)^{1/2} d\rho$.

Now, again, by identification

$$\bar{\theta}(t,x) = \sqrt{\frac{r(r,x)}{r_g}} \tag{124}$$

and thus we can prepare our local unitaire W, in particular the quantum coin C to simulate the transport of a quantum particle in and around the radius of Schwarschild black hole.

6.2 A Quantum Walk over a generic 2D spatial triangulation

Now let us depart from the grid and let us consider a QW over an equilateral triangles as introduced in the first section. Due to the high malleability of triangles to pave any curved surface in two spatial dimensions, we may argue that triangles could open the doors to an other way to simulate a transport equation with inhomogeneous velocity as in 119: for instance we can start to stretch the distances between the point of the grid in an inhomogeneous way, deforming continuously the surface over which the QW propagate. Such a deformation will introduce locally a metrics which is not simply recoverable by a change of coordinates. However this operation, which is already known as a standard technique to triangulated curved manifold, is not unitary and then cannot be accounted in our quantum numerical scheme. However we may be luckier than that and find out that such deformation may be absorbed by local non homogeneous unitary as we did on the grid. We will see how in the following, but first we will explore the idea introducing a global homogeneous deformation of the lattice. Immagine that such transformation Λ exists, the basis vector u_i, introduced in 3.4.1, which span the Euclidean plane will transform as follows:

$$u_i' = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix} u_i \equiv \Lambda u_i. \tag{125}$$

where λ_{ij} are position independent, although they are eventually allowed to depend on time. The derivative ∂_{u_i} will also transform as

$$\partial_{u_i'} \equiv \Lambda \partial_{u_i} \tag{126}$$

and then using the definition of the triangular QW and computing the formal continuous limit we arrive to the following equation:

$$i\partial_t \psi = \left[\left(\lambda_{11}\sigma^x + \lambda_{12}\sigma^y \right) \partial_x + \left(\lambda_{21}\sigma^x + \lambda_{22}\sigma^y \right) \partial_y \right] \psi, \tag{127}$$

which describes the Dirac equation on a flat geometry, in fact the velocity still remain homogeneous in space time and comparing with Eq. (122) gives

$$B^x = \lambda_{11}\sigma^x + \lambda_{12}\sigma^y \tag{128}$$

$$B^y = \lambda_{21}\sigma^x + \lambda_{22}\sigma^y. \tag{129}$$

or $B^s = \Lambda_i^s \sigma^i$ and using the equation 70

$$B^s = \Lambda_i^s R_j^i \tau^j. \tag{130}$$

Notice that the homogeneous transformation Λ may also help us to redefine the matrices τ_i. In fact from Eq 67 we get:

$$\partial_t \Psi_k(t,r) = \left(\tau_2' \partial_{u_2} + \tau_1' \partial_{u_1} + \tau_0' \partial_{u_0} \right) \Psi_k(t,r) \tag{131}$$

where

$$\tau_i' = \Lambda \tau_i. \tag{132}$$

It is now clear that in order to simulate an inhomogeneous velocity field we need to choose a space-time dependent $\Lambda(t,x,y)$ transformation. Because such a transformation is not unitary, from Equation 130, we will explore an equivalent way to retro-engineer the deformation playing with our local unitaries.

Instead of introducing a distortion $\Lambda(t,x,y)$ on the lattice via the modification of the u_i vectors, the unitary matrices τ^i can be transformed to produce the same effect. In other words, we seek for a set of matrices $\beta^i(t,x,y)$ that fulfill the following conditions:

- (C1) We impose that
$$\Lambda^j_k(t,x,y)R^k_i\tau^i = R^j_i\beta^i(t,x,y). \tag{133}$$
- (C2) Each of them has $\{-1,1\}$ as eigenvalues, i.e. at any time step and at any point (x,y) of the lattice there exist three unitaries $U_i(t,x,y)$ such that
$$\beta^i(t,x,y) = U^\dagger_i(t,x,y)\sigma^z U_i(t,x,y). \tag{134}$$

Notice that condition (C1) implies that the coordinate transformation dictated by $\Lambda^j_k(t,x,y)$ is transferred to the unitary operations $\beta^i(t,x,y)$, instead of the original τ^i. Additionally, condition (C2) will allow us to rewrite the QW evolution in terms of the usual state-dependent translation operators.

To alleviate the notations, in what follows we will omit the spacetime dependence both in these matrices and in the $U_i(t,x,y)$, and write simply β^i and U_i. The above conditions allow to calculate the β^i matrices, which can be written as a combination of Pauli matrices, i.e. $\beta^i = \vec{n}^i\cdot\vec{\sigma}$, where each $\vec{n}^i$ must be a real, unit vector $\vec{n}^i = (\sin\theta_i, 0, \cos\theta_i)$ for some angles θ_i (that are time and position dependent).

In this way
$$\beta_i = U^\dagger_i\sigma_z U_i = \begin{pmatrix}\cos\theta_i & \sin\theta_i\\ \sin\theta_i & -\cos\theta_i\end{pmatrix}, \tag{135}$$
and each U_i can be obtained by diagonalization of the corresponding β^i. We finally write them as
$$U_i = \begin{pmatrix}\cos\frac{\theta_i}{2} & \sin\frac{\theta_i}{2}\\ -\sin\frac{\theta_i}{2} & \cos\frac{\theta_i}{2},\end{pmatrix}. \tag{136}$$

The most naif way to implement such a walk is alternating the unitaries U_i and the shift operators. However, although different, the unitaries will be three different ones, one of them depending on a different parameter θ_i, this strategy is not sufficient because Λ depends on four real free parameters. Thus, in order to recover this local deformation we need at least one more internal parameter in the QW evolution. Moreover because we want to get terms like $\partial_j\lambda_{ij}$, as we have seen in the previous section, we have to iterate twice each unitary operator. All this considerations lead to build the following operator:
$$\Psi_{j+2,k}(r) = Z_2Z_1\Psi_{j,k}(r). \tag{137}$$
where
$$\begin{aligned} Z_1 &= H\Pi^2_{i=0}\bar{V}_iV_iH\\ Z_2 &= Q\Pi^2_{i=0}\bar{K}_iK_iQ, \end{aligned} \tag{138}$$
and
$$\begin{aligned} V_i &= U_iS_{u_i}U^\dagger_i\\ \bar{V}_i &= U^\dagger_iS_{u_i}U_i\\ K_i(\theta_{i+3}) &= U_{i+3}S_{u_i}U^\dagger_{i+3}\\ \bar{K}_i(\theta_{i+3}) &= U^\dagger_{i+3}S_{u_i}U_{i+3} \end{aligned} \tag{139}$$
where
$$H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \qquad Q = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\\ 1 & i\end{pmatrix}. \tag{140}$$

Let us discuss this choice. Each Z_i iterates twice the triangular QW as seen in the definition of the Dirac triangular QW, choosing a different unitaries for each edge k of the triangle in order to get in the continuous limit spatial derivatives of the unitaries U_i. Notice that for the second iteration we have chosen the conjugate transpose of the unitaries U_i. This is justified from the fact that, in the end we wish to recover spatial derivatives of the form $\partial_j \beta_i = (\partial_j U_i^\dagger)\sigma_z U_i + U_i^\dagger \sigma_z \partial_j U_i$. Iterating twice the same operator V or K would not be sufficient to recover the total derivative and we would have twice $U_i^\dagger \sigma_z \partial_j U_i$. Finally H and Q ask for a change of basis in the coin state basis to recover in the continuous limit a true 2D propagation. In conclusion, two of the Z_i are necessary to have enough free parameters for the deformation Λ. As in the previous section, we have chosen $\theta(r)_i = \pi + \varepsilon^{1/2} l_i(r)$ and $\Delta_x = \varepsilon^{1/2}$.

By expanding this equation up to first order in ε, after a tedious but straightforward computation, which we spare the reader from detailing here, one arrives to the following equation in the continuum limit:

$$\begin{aligned}\partial_t \Psi = [\partial_{u_2}(l_2\sigma_x + l_5\sigma_y) + \partial_{u_1}(l_1\sigma_x + l_4\sigma_y) + \partial_{u_0}(l_0\sigma_x + l_3\sigma_y)]\,\Psi + \\ + [(l_2\sigma_x + l_5\sigma_y)\partial_{u_2} + (l_1\sigma_x + l_4\sigma_y)\partial_{u_1} + (l_0\sigma_x + l_3\sigma_y)\partial_{u_0}]\,\Psi\end{aligned} \tag{141}$$

Notice that $\beta_i \simeq \lambda_i + o(\varepsilon)$. Now using the Eq. 56 we can reformulate the above equation in terms of ∂_x and ∂_y:

$$\begin{aligned}\partial_t \Psi = \partial_x(\lambda_{00}\sigma_x + \lambda_{01}\sigma_y)\Psi + 2(\lambda_{00}\sigma_x + \lambda_{01}\sigma_y)\partial_x\Psi \\ +\partial_y(\lambda_{10}\sigma_x + \lambda_{11}\sigma_y)\Psi + 2(\lambda_{10}\sigma_x + \lambda_{11}\sigma_y)\partial_y\Psi,\end{aligned} \tag{142}$$

where

$$\begin{aligned}\lambda_{00} &= -\frac{1}{2}(l_2 + l_1) + l_0 \\ \lambda_{01} &= -\frac{1}{2}(l_5 + l_4) + l_3 \\ \lambda_{10} &= -\frac{\sqrt{3}}{2}(l_2 - l_1) \\ \lambda_{11} &= -\frac{\sqrt{3}}{2}(l_5 - l_4),\end{aligned} \tag{143}$$

which is a neat generalisation of the Eq. 127 to an inohomogeneous Λ. Notice that we have a system of linear equations which is overdetermined and which leaves us enough freedom to recover the deformation matrix we wish. For instance a good choice to gauge away this ambiguity is: $l_5 = -l_4$ and $l_2 = -l_1$ which leads to the unique choice:

$$\lambda_{00} = l_0 \quad \lambda_{01} = l_3 \quad \lambda_{10} = \sqrt{3} l_1 \quad \lambda_{11} = \sqrt{3} l_4. \tag{144}$$

We thus proved that a non homogeneous deformation of the triangulation can be simulated by local unitaries keeping the triangulation regular.

6.3 Discussion and perspectives

In this last section we proved that the QW hereby constructed over a general triangulation recovers, in the continuum limit, the Dirac equation in curved $(2+1)$–dimensional spacetime. We also noticed that the equation

between changes of metric, aka $\Lambda-$deformations, and changes of local unitaries $\tau-$matrices enables us to absorb any continuous spatial deformations of the triangulation in the very fabric of the QW itself keeping the metrics flat (i.e. paved by equilateral triangles). Besides being very powerful, this duality seems to be profound and deserves further development. It is worth mentioning that some physical theories provides a language to describe the quantum geometry of space using spin foam which are particular types of 2-complex, i.e. triangles. The principle of duality could therefore suggests new discrete symmetries underlying the continuous texture of space-time. Instead, from a technological point of view, the applications that the results presented in this chapter might have are many: for example, to mimic the transport on a carbon structure would mean to take into account its imperfections, the ripples, which would be simulated by a network of inhomogeneous local units, nowadays easily achievable with various technologies. But more generally any curved surface can be reproduced if the local deformation matrix is known. Other possible extensions are currently being developed: an extension to larger dimensions and the generalization to dynamic triangulations. Finally, a recent result showed how the QW may be used to look for topological defects, which are properties of the configuration space itself [15]. We wonder if this suggests to target more general topological classification problems - *e.g.* seeking to characterize homotopy equivalence over configuration spaces that represent manifolds as CW-complexes.

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