



Discrete-time quantum walks and gauge theories

Pablo Arnault

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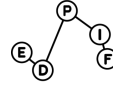
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Discrete-time quantum walks and gauge theories

by Pablo Arnault

PhD thesis in Theoretical Physics
based on four scientific publications [1, 2, 3, 4]

Director: Fabrice Debbausch (LERMA, UPMC)
Co-director: Marc Brachet (LPS ENS, CNRS)

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at the Université Pierre et Marie Curie, in front of the following jury:

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Mr. Pablo Arrighi	Professor	Rapporteur
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“ Trachte ich denn nach *Glücke*? Ich trachte nach meinem *Werke*! ”

In *Also sprach Zarathustra*, by F. Nietzsche, last chapter, “Das Zeichen”.

A mis padres

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Enfin, mon esprit se pose sur Sophie Elzière.

Abstract

A quantum computer, i.e. utilizing the resources of quantum physics, superposition of states and entanglement, could furnish an exponential gain in computing time. A simulation using such resources is called a quantum simulation [5, 6, 7, 8]. The advantage of quantum simulations over classical ones is well established at the theoretical, i.e. software level [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 4]. Their practical benefit requires their implementation on a quantum hardware. The quantum computer, i.e. the universal one (see below), has not seen the light of day yet, but the efforts in this direction are both growing and diverse. Also, quantum simulation has already been illustrated by numerous experimental proofs of principle, thanks too small-size and specific-task quantum computers or simulators [21, 22, 23, 24, 25, 26]. Quantum walks (QWs) are particularly-studied quantum-simulation schemes, being elementary bricks to conceive any quantum algorithm, i.e. to achieve so-called universal quantum computation [11, 12, 9, 10]. Eventually, at a purely theoretical level, quantum simulation already provides a broad understanding of many quantum dynamics in terms of (quantum) information-theoretic principles.

The present thesis is a step more towards a simulation of quantum field theories based on discrete-time QWs (DTQWs). First, it is indeed shown, in certain particular cases, how DTQWs can simulate, in the spacetime-continuum limit, the action of a Yang-Mills gauge field on fermionic matter, and the retroaction of the latter on the gauge-field dynamics [1, 2, 3]. The suggested schemes preserve gauge invariance on the spacetime lattice, i.e. not only in the continuum. In the (1+2)-dimensional Abelian case, lattice gauge-invariant equivalents to Maxwell's equations are suggested, which are consistent with the current conservation on the lattice; also, outside the continuum limit, tight-binding phenomenology is recovered. In the (1+1)-dimensional non-Abelian case, a lattice gauge-covariant version of the non-Abelian field strength is suggested; also, short-time agreement with classical (i.e. non-quantum) trajectories is shown. Second, it is shown how this DTQWs-based fermionic matter can be coupled to relativistic gravitational fields of the continuum, i.e. to curved spacetimes, in 1+2 dimensions [4]; an application is presented, where the 2-dimensional space is the polarization plane of a linear plane gravitational wave.

Résumé

Un ordinateur quantique, i.e. utilisant les ressources de la physique quantique, superposition d'états et intrication, pourrait fournir un gain exponentiel de temps de calcul. Une simulation utilisant ces ressources est appelée simulation quantique [5, 6, 7, 8]. L'avantage des simulations quantiques sur les simulations classiques est bien établi au niveau théorique, i.e. software [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 4]. Leur avantage pratique requiert leur implémentation sur un hardware quantique. L'ordinateur quantique, sous-entendu universel (cf. plus bas), n'a pas encore vu le jour, mais les efforts en ce sens sont croissants et variés. Aussi la simulation quantique a-t-elle déjà été illustrée par de nombreuses expériences de principe, grâce à des calculateurs ou simulateurs quantiques de taille réduite et à tâche spécifique [21, 22, 23, 24, 25, 26]. Les marches quantiques (MQs) sont des schémas de simulation quantique particulièrement étudiés, étant des briques élémentaires pour concevoir n'importe quel algorithme quantique, i.e. pour le dénommé calcul quantique universel [11, 12, 9, 10]. À un niveau purement théorique, la simulation quantique fournit déjà une large compréhension de nombreuses dynamiques quantiques à partir de principes de théorie de l'information (quantique).

La présente thèse est un pas de plus vers une simulation des théories quantiques des champs basée sur les MQs à temps discret (MQTD). Dans un premier temps, il est en effet montré, dans certains cas particuliers, comment les MQTD peuvent simuler, à la limite au continuum d'espace-temps, l'action d'un champ de jauge Yang-Mills sur de la matière fermionique, et la rétroaction de cette-dernière sur la dynamique du champ de jauge [1, 2, 3]. Les schémas proposés préservent l'invariance de jauge au niveau du réseau d'espace-temps, i.e. pas seulement au continuum. En dimension 1+2 d'espace-temps et dans le cas abélien, des équations de Maxwell invariantes de jauge sur réseau sont proposées, compatibles avec la conservation du courant sur le réseau ; on retrouve aussi, en dehors de la limite au continuum, de la phénoménologie de liaisons fortes. En dimension 1+1, une courbure non-abélienne, définie et covariante de jauge sur le réseau, est proposée. Dans un deuxième temps, il est montré comment cette matière fermionique à base de MQTD peut être couplée à des champs gravitationnels relativistes du continuum, i.e. à des espaces-temps courbes, en dimension 1+2 [4] ; une application est présentée, où l'espace de dimension 2 est le plan de polarisation d'une onde gravitationnelle linéaire plane.

Notes on the typography used in the manuscript

Books, scientific memoirs or reports, Master or PhD theses, are noted in italic font.

The doubled quotation marks, “...”, are used either to quote somebody else’s words, or the name of a scientific paper, and are always associated to a reference – unless sufficiently well-known –, while the non-doubled ones, ‘...’, are used for two different – although obviously non-orthogonal – purposes: (i) to stress that the quoted word or group of words is being explained, or (ii) to stress that the quoted entity is not used in its most-used meaning, and/or to warn the reader not to understand this linguistical entity too rigorously or formally, because it is merely used to give some intuition of what is being explained. The reader should be able to determine, from the context, in which situation we are.

The word ‘ N -dimensional’ will be abbreviated ‘ ND ’ throughout the manuscript.

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Introduction

The guideline of the research work on which this thesis is based is the discretization of relativistic quantum¹ field theories (QFTs) with discrete-time quantum walks (DTQWs). The research field known as lattice gauge theories (LGTs), now established for several decades since the seminal work of Wilson on the confinement of quarks in 1974 [27], already provides an extensive framework to discretize QFTs², which have found numerous applications [28]. One may then wonder about the purpose of DTQWs-based discretizations of QFTs. A way to answer this question is to first introduce DTQWs and, more generally, quantum walks (QWs), as well as quantum computing and quantum simulation.

0.1 Feynman’s checkerboard and very brief history of quantum computing

The history of DTQWs is usually traced back to Feynman’s attempts to build a fermionic path integral. We refer the reader to Schweber’s historical review on the subject, where notes on the discretization of the Dirac equation, taken by Feynman in 1946, are reproduced [29]; these discretizations are a particular family of nowadays standard DTQWs³. These attempts, however, did not succeed above one spatial dimension. In the 60’s, Berezin [30] was able to formulate path integration for fermions, as functional integration over Grassmann variables, and this method became standard [31]. Several answers to Feynman’s original attempts have been given, but all have drawbacks that make them, if not marginal, at least non-standard, see Subsection i.3.1 for more details.

Generally speaking, QWs model quantum transport on graphs. Seminal formulations in discrete [32, 33] and continuous [34] time, appeared in the 90’s⁴. The first connection between both formulations was made in 2006 [35]. QWs are a topic at the crossing between quantum computing and quantum simulation⁵, as their history reveal. Quantum computing is the conception of algorithms with, instead of the logical bits, i.e. two-state variables, used by classical algorithms, two-state variables that behave quantumly, i.e. that can actually be in any (normalized) linear superposition of the two states; such two-state quantum variables are called *logical* qubits. A quantum algorithm uses the coherence and entanglement between logical qubits as a mathematical resource to speedup a given computational task. We shall discuss the meaning of quantum simulation further down. QWs were identified as suitable

¹The research work presented in this thesis deals only with *first-quantized* field theories, which are actually often referred to as *classical*. The second quantization of our schemes is certainly one of the next steps to take.

²LGTs exist in a full second-quantized framework.

³The DTQWs that appear in Feynman’s work have weakly coupled spin components, since he was focused on their continuum limit. This is explained in Subsection i.1.4. We refer the reader to Subsection i.3.1 for more details on Feynman’s work, and that which followed.

⁴The scientific papers on which this thesis is based deal only with DTQWs.

⁵The intuitive difference between computing and simulation is elaborated on and usefully phrased in terms of a few key concepts by Johnson, Clark and Jaksch [8]; we shall review such concepts further down.

elementary schemes to build quantum algorithms in the late 90's [34] and early 2000's⁶ [39]. They enabled, then, to build faster versions of key classical algorithms, such as database search [40] or element distinctness [41], and were eventually understood, in the 2010's, as being a possible elementary basis to conceive *any* quantum algorithm [9, 10], that is, a basis for so-called universal quantum computation. For them to be useful, quantum algorithms must run on a universal quantum computer, i.e. hardware, in which quantum coherence and entanglement between *physical* qubits, i.e. two-state physical quantum systems, is ensured. The idea of quantum computers was seminally developed by Feynman, who pointed out in 1982 [42] the potential exponential computing speedup provided by such a hypothetical device. Feynman's original paper is written in the perspective of using such computations to study physical phenomena, more precisely local phenomena⁷. A convenient way to define local phenomena in a very broad sense, is to demand that they can be described by partial differential equations^{8,9} (PDEs), or discrete versions of such equations. That being said, such mathematics can account for different physical types of locality.

0.2 Two notions of locality: mesoscopic near-neighbors locality, and relativistic locality

Let us introduce two physical notions of locality. Before the birth of relativity, many physical laws were constructed as local, in the following meaning: they modeled, thanks to PDEs, little-by-little transport resulting from near-neighbors interactions between tiny samples of

⁶The first milestone quantum algorithms such as Shor's [36, 37] or Grover's [38] appeared, if not before, at least independently of the rise of quantum-walk schemes, in the mid 90's.

⁷An important answer to Feynman's conjecture was given by Lloyd's (digital) "universal quantum simulators" in 1996 [43]. In that work, it is shown that a quantum computer would indeed furnish an exponential gain in the computing time needed to simulate any *local Hamiltonian*. It is said that a quantum computer would simulate *efficiently* this local Hamiltonian, while it is strongly believed that a classical computer cannot. Note however that, as mentioned in Ref. [44], Lloyd's result is only valid for a non-vanishing spatial-lattice step, i.e. the result does not imply that the continuous-space theory can be simulated efficiently. In Ref. [44], DTQWs converging faster towards their continuum limit are suggested. A local Hamiltonian is a Hamiltonian $H = \sum_{k=1}^l H_k$, where H_k acts on a Hilbert space of finite dimension m_k (spatial lattice) which does not grow with the size of the input (locality). The typical example is tight-binding Hamiltonians.

⁸Differential calculus, developed in the 17th century by Newton and Leibniz, provided the appropriate tool to describe local phenomena, described further down in the main text, and is a key historical step in the development of physics. Physics as a scientific discipline, in the terms science is understood today, is indeed usually traced back to Galileo, that is, not much before the advent of differential calculus. Galileo already pointed out the primordially of mathematics in the study of natural sciences, and his famous (rephrased) quote, namely, that "the book of Nature is written in the language of mathematics", is always to meditate. The ambiguity of the preposition 'of' in 'of Nature' underlines the metaphorical question of whether the author of this book is (i) Nature itself, in which case the human being would rather be a rune unraveler with a small interpretative part in the translation, or (ii) in fact nobody but the human being, who would then rather be a writer whose work results from an anthropomorphic and rational understanding of Nature. In other words, are mathematics a language actually spoken by Nature, i.e. underlying natural phenomena independently of humans, or are they merely our best tool to understand Nature? This is a rough introductory scheme for the epistemological debate between realism and idealism. It is amusing to note that Galileo's year of death coincides with Newton's birth.

⁹Non-localities may be used to model some phenomena, which translate mathematically as *integro*-differential terms in the PDE.

matter, which have a typical so-called mesoscopic¹⁰ length scale, and are considered point particles on macroscopic scales. We will refer to such a locality notion as the *mesoscopic near-neighbors locality*¹¹. Example of such laws are the Navier-Stokes equation [45, 46] in fluid mechanics, or the heat equation in thermodynamics¹². With the advent of special relativity around 1905, and then general relativity around 1915, it emerged what we will call *relativistic locality*, which has the following meaning: in these theories, the speed of light is an upper bound for the speed of any physical phenomenon or interaction; in the standard continuous spacetime, this translates into the need to consider, instead of the pre-relativistic Galilean spacetime transformations, Lorentz transformations to relate, and thus define, inertial frames. We will clarify this simple picture further down.

Both locality notions have the following common feature, which is often implied by the word ‘locality’: both define a causal neighborhood around each point in space. In Appendix A, we elaborate on these two types of causal neighborhood, which are of a very different nature. Now, it is no surprise that the above-mentioned pre-relativistic mesoscopic-transport equations do not verify relativistic locality, i.e. neither these equations are Lorentz invariant, nor the speed of the mesoscopic particles is bounded. That being said, this is not a problem for all applications of these equations in which the maximum reachable speed is much smaller than the speed of light, which is the case for most macroscopic phenomena on Earth¹³.

Let us now consider relativistic locality and non-relativistic limits. Maxwell’s equations, which were precisely the starting point of relativity, verify relativistic locality. However, the pre-Maxwellian versions of Coulomb’s force between electric charges and Ampère’s force between electric currents, do not verify relativistic locality. These two laws were thought as resulting from some instantaneous so-called “action at a distance”, already evoked by Newton to refer to his gravitational law, which also does not verify relativistic locality. Such an action at a distance was in astonishing contrast with the intuitive mesoscopic near-neighbors locality of everyday’s life. First with Maxwell’s equations and then parallelly to the advent of special relativity, the electromagnetic interactions were eventually understood to be mediated at the speed of light. The pre-Maxwellian Coulomb’s and Ampère’s laws were derived as non-relativistic limits of relativistic counterparts derived from Maxwell’s equations, namely the forces derived from the so-called “retarded potentials”. Similarly, the gravitational interaction was understood, parallelly to the advent of general relativity,

¹⁰A mesoscopic scale is a scale much smaller than the macroscopic scale, i.e. that of everyday-life objects, but still much bigger than the microscopic scale, i.e. that of atoms and molecules. At mesoscopic scales, one can often consider that a given physical medium made of atoms and molecules, is actually a continuous medium, whose physical properties can thus often be described thanks to PDEs. See http://s2.e-monsite.com/2010/03/16/02/meca_flu.pdf, Chapter 1, for a short explanation on the possibility to distinguish clearly these three scales.

¹¹Of course, even though we use the word ‘mesoscopic’, this notion of locality is exactly that accounting for contact interactions in everyday life, often with solid objects, which are particular type of continuous media.

¹²The original *Analytic theory of heat*, written by Fourier in French, and published in 1822, is available at <https://archive.org/details/thorieanalytiq00four>.

¹³Note that these equations we are mentioning do not exhaust all possible types of mesoscopic transport, i.e. they do not always apply. For example, there are some phenomena which actually exhibit relativistic effective features, such as, typically, an upper bound speed, which is usually much smaller than the speed of light and depends on the properties of the medium. The conception of such equations can demand and/or lead to an understanding of the mathematics of relativity. Examples of such equations are relativistic diffusion equations [47], which can govern, e.g., heat transport in some media, or the sine-Gordon equation [48], which can model, e.g., wave transport in long biological molecular chains or membranes.

to be mediated at the speed of light¹⁴. The relativistic electromagnetic and gravitational laws, and the associated non-relativistic limits, are said ‘fundamental’ in the sense that – as linked to the nature of spacetime – they are considered scale-independent, at least above the smallest length scale experimentally probed, which is much below the microscopic scale¹⁵.

Now, several of the pre-relativistic mesoscopic-transport equations were also, since the advent of relativity, gradually made compatible, through certain non-relativistic limits, with relativistic locality. Such connections are, however, difficult ones to make, and they are still the subject of current research. Indeed, building relativistic counterparts to the pre-relativistic mesoscopic-transport equations often requires, not only implementing fundamental non-relativistic limiting procedures, but also conceiving approximations, for the fundamentally-relativistic microscopic collisional dynamics, which preserve, at the mesoscopic scale, relativistic locality. Two relevant examples of such relativistic laws are (i) relativistic diffusion equations [49], and (ii) relativistic versions of the Navier-Stokes equation [50], which may eventually be derived from relativistic versions of the Boltzmann equation [51]. Ultimately, one must perform *ab initio* computations of quantum molecular dynamics to derive the microscopic collision rules. The possibility to view pre-relativistic mesoscopic-transport equations as non-relativistic limits of relativistic counterparts is thus strongly underlaid by all these attempts to preserve relativistic locality, which is valid at the microscopic scale, along the several approximation steps made to capture only the effects which are relevant at macroscopic scales.

As a sum up, we may say that many pre-relativistic physical laws, either fundamental, i.e. considered scale-independent above the smallest length scales experimentally probed, or effective, i.e. emergent only at macroscopic scales, and depending on the smoothing of the microscopic dynamics, were, with the advent of relativity, derived as non-relativistic limits of relativistic laws, and were thus made subject to standard relativistic locality. Also, most of the conclusive theories that developed afterwards, up to nowadays, can be made compatible with standard relativistic locality^{16,17}, as well as information theories¹⁸.

¹⁴When such a result was obtained, the Newtonian gravitational law had, obviously, already been derived as a non-relativistic limit of the general-relativistic gravitational law. (Otherwise the gravitational interaction is simply instantaneous.)

¹⁵The smallest length scale that can be probed is often considered to be 10^{-18} m. This length scale can be probed at the LHC, with beam collisions involving an initial kinetic energy of the order of $hc/10^{-18} \simeq 4$ TeV.

¹⁶Lorentz covariance is still taken as a principle in many current theoretical works, since experimental tests on the violation of Lorentz covariance are overwhelmingly seen as disproving such a violation, and any new physical theory must anyways reproduce the – possibly merely effective – relativistic locality that rules the many phenomena which have been tested, which is a strong constraint. However, nothing prevents, theoretically, from actually forgetting about relativistic locality, or at least its standard version that we have been referring to and which is associated to Lorentz invariance, at small spacetime scales still unprobed, provided we recover this standard relativistic locality at higher, probed scales. See further down for more details.

¹⁷See Appendix C for a discussion on so-called *quantum non-locality*.

¹⁸The fact that the transmission of information must involve physical processes, and should thus, among other properties, not be superluminal, has become a paradigm in information theory; see e.g. [52] and <http://adamilab.msu.edu/wp-content/uploads/Reprints/2011/Adami2011.pdf>. Quantum mechanics shows that information can be *encoded* non-locally, but cannot be *transmitted* faster than light, a result known as the no-communication, or no-signaling theorem [53].

0.3 Extending the ideas of relativity: locality principle on networks

Now, the previous simple picture used to define relativistic locality actually results from the interplay between three ingredients: two distinct principles, namely (i.a) the relativity principle, i.e. that all physical laws must be the same in all inertial frames, which are postulated to exist, and (i.b) the requirement that the speed of light be the same in all inertial frames, and (ii) assumptions on spacetime, namely isotropy and homogeneity¹⁹. In special relativity, inertial frames are indeed related, and in a way thus defined by Lorentz transformations, but in general relativity, Lorentz transformations are replaced by generic diffeomorphisms which must be Lorentzian only locally, i.e. at each spacetime point. Now, although the upper-bound property of the speed of light results from the interplay between these three ingredients, it can be tempting to infer a *locality principle*, i.e. to *postulate* the upper-bound property, since it is an easy way to (i) ensure causality in physical phenomena, and (ii) avoid the need to make assumptions on the properties of spacetime. In a broad sense, such a locality principle requires the existence of *any type* of bounded causal neighborhood. The upper bound for the speed of phenomena and interactions is typically the speed of light in the context of fundamental physics. This upper bound can also take other values if we wish to model other types of finite-speed interactions on graphs.

Several research works, aiming at grounding physics on quantum-information principles, are based on such a locality principle. These works have suggested derivations of standard relativistic locality, i.e. Lorentz transformations in continuous spacetime, from *local evolution rules on an abstract network*. The network is then typically mapped to a discrete spacetime. In addition to verifying the locality principle, these evolution rules also have a flavor of the aforementioned other notion of locality: they are formulated as near-neighbors interactions between the nodes of the network, which is in conceptual and technical analogy with, (i) indeed, the near-neighbors interactions between the mesoscopic samples of matter which form fluids, or, even more, between the cells of their lattice-gas versions [55, 56, 57, 33, 58], but also with (ii) tight-binding condensed-matter models. These discrete schemes also satisfy a kind of relativity principle, i.e. they are invariant under changes of observer, at the network level, in a meaning which is necessarily different from the standard relativistic one, and also specific to each work [59, 60]. We will briefly comment on such works further down.

Eventually, let us make a remark before coming back to our initial topic: relativistic locality is, as mesoscopic near-neighbor locality, also reflected by the use of PDEs, but in a field-theory framework. As an example for this, consider any fundamental-fields dynamics, such as Maxwell's equations, already mentioned, the Klein-Gordon equation, or the Dirac equation, among others^{20,21}.

¹⁹For a derivation of the upper-bound property of the speed of light from these assumptions, see, e.g., [54].

²⁰The locality, in terms of PDE description, of the Schrödinger equation, is to be seen as a residue of the fundamental relativistic locality of the Dirac or the Klein-Gordon equation.

²¹By the way, since we are speaking of fields, another remark is in order: the non-localizability of fields does, in a sense, a priori not necessarily affect locality, since, if localizability is a property related to a quantity A , locality is a property related to the variations ΔA of A .

0.4 On digital and analog quantum simulation

The idea of discretizing physical laws described by PDEs naturally appeared with the development of computers since the Turing machine. Cellular automata (CA), initially developed by Ulam and Neumann in the 40's, were designed for this purpose²², and were then quantized²³ [42, 61]. Meyer's seminal paper on DTQWs [33], in which he introduces them as a particular family of single-particle unitary quantum cellular automata²⁴ (QCA), namely partitioned (or staggered) QCA, and which is, rather than quantum-computing, quantum-simulation oriented, became a reference in the aforementioned quantum-computing arena. That being said, since the 70's and 80's, i.e. already before the raise of quantum computing, and then still rather independently from this new subject in the 90's and 2000's, many CA and QCA schemes were developed for simulation purposes. Around the 2010's, Arrighi and Grattage demonstrated the intrinsic universality of partitioned QCA, i.e. QWs, in the design of quantum-simulation schemes [69, 11, 12], a topic that will be discussed further down. In 2015, the well-known quantum lattice Boltzmann equation was eventually explicitly identified as a QW by Succi [18]. Now, as built out of QWs, these numerical schemes are naturally implementable by quantum algorithms that a quantum computer would naturally run. But these QCA schemes are still implemented, nowadays, with classical algorithms on classical computers, which eventually brings us back to the topic of quantum simulation, on which we shall now comment more lengthily.

As defined by many, quantum simulation is the simulation of physical phenomena with a system utilizing these features of quantum mechanics which are absent from the so-called classical world, such as quantum coherence and entanglement [5, 6, 8]. I shall use this definition. The other obvious definition is that of simulating a system which displays such quantum features [7]. This second definition does thus not focus on the computing power of quantumness to simulate *any* physical phenomena, although both definitions often 'interact', simply because simulating systems where all elementary entities are described by functions, as quantum mechanics requires, instead of a few coordinates, as in classical physics, is, generically, computationally way more costly, as Feynman seminally discussed [42]. Before digging into the notion of quantum simulation, let us first make it clear that of simulation.

Linguistically, the word simulation is close to that of mimic. Does the simulation mimic something? A simulation is aimed at obtaining information about a physical system of interest, that we shall sometimes merely call 'system' for brevity. It does so through a mathematical *model*, namely, a mathematical object which is thought to describe the system.

²²In addition to be local in their standard definition, CA are also often homogeneous, i.e. the local rules that are applied at each time step are the same everywhere. One can however relax this constraint. The general question of (i) whether a given CA might be associated a continuum counterpart, i.e. a PDE (the reverse is usually feasible), and of (ii) the generality of such a PDE, has been extensively studied, and is not straightforward; for a review, see <https://arxiv.org/pdf/1003.1983.pdf>.

²³Feynman explicitly mentions cellular automata in his seminal paper on quantum simulation, but "[doesn't] want to force" [42] such a vision, i.e. his work should not be merely regarded as a way to quantize CA, but also algorithms that are not phrased as CA.

²⁴There is a substantial literature on two-particle DTQWs [62, 63, 64], including experiments [65]. Now, we know that the framework of second quantization is, on the one hand, useful to describe quantum systems with large numbers of particles [66], and, on the other hand, fundamentally necessary in a relativistic framework [31]. In the sense that such second-quantized formulations of DTQWs are still lacking, as well as works on many-particle DTQWs, current works on DTQWs should still currently rather be seen as *single-particle* unitary QCA. The work led by Boettcher and Portugal on the non-perturbative renormalization of DTQWs [67, 68], is certainly to be used in future second-quantization developments.

The model is meant for being tested, i.e. its ‘behavior’ must be compared to that of the system. This is done by comparing data provided by a so-called *simulation of the model* – i.e. a computation associated to a particular realization of the model, which is literal – to data provided by an experimental measure on the system; this comparison enables to state up to which accuracy the model describes the system. The data out of the simulation are, ultimately, numbers, but they are not ‘produced’ the same way whether this simulation is digital or analog, terms that will be defined below.

It is useful to introduce the concept of hypothetical physical system, or *ideal system*, which is induced by the mathematical model. In the case where this mathematical model is a dynamical PDE, the simulation will typically explore, starting from an input initial state, the state of the ideal system at successive instants. Epistemologically, the simulation, as an isolated task, gives results only on the ideal system described by the model, and not on the actual system. To obtain results on the latter, one must, as mentioned, compare the results of the simulation to that of experiments on the actual system. For it to be part of the scientific method, quantum simulation must, as classical simulation, be subject to this rule.

A simulation performed thanks to a computer is called a digital simulation, see further down for more details. There exist another type of simulation, called analog simulation. We shall discuss the differences between both. Note that, although classical analog simulation is currently maybe less topical (at least it is not the topic of the present work), since the computing power of current classical computers often makes them better tools for simulating physical phenomena, the digitality or analogy of a simulator are features which are independent from its quantumness.

Before clarifying the concept of digital simulation, one must make it clearer that of computation and computer. A computation is a series of operations with *numbers*, aimed at delivering a numerical result. This means any entity carrying out the computation must be able to represent, manipulate, and output *integers*, whatever its functioning may be. This entity can be a human being, but one can envisage a device that carries out these computations. Such a device is called a *computer*, or *digital device* (the ‘digits’ are the symbols with which we write integers, and hence any number, at least approximatively). There relies the difference between a digital and an analog device: the latter is not designed to perform operations between integers, and its output is a certain *physical quantity* that often belongs to a certain physical continuum. The ‘numerical output of an analog simulation’, mentioned above²⁵, is thus indirect, via a *physical measurement*^{26,27}. Now, what we often refer to as ‘computers’ in current everyday-life, are *universal* computers, i.e. able to carry out so-called *universal* (classical) computation. Vaguely speaking, this means they can run any program. More fundamentally – but at this stage not less vaguely – this means a universal computer is able to realize any type of ‘automatic task’ if we

²⁵We must test the mathematical model and thus extract numbers from the analog simulation.

²⁶The result of a physical measurement is typically interpreted as a real number which cannot be known exactly but only up to some *accuracy*, which depends, among other things, on the analog device.

²⁷Note that an analog device may be used only for its physical output, i.e. the measurement of the physical output is needed for certain purposes only.

give it the instructions in an ‘appropriate way’²⁸. Universal computation is achieved by (i) implementing well-chosen series of *elementary operations* (called *primitives*), which (ii) belong to a certain well-chosen finite set, and which can often be viewed as equivalent to logical operations, also called *logical gates*. A digital device, or computer, always implements, at least implicitly, certain logical gates, but is not always universal²⁹, in which case its computational limitations are often manifest³⁰.

Now, on the one hand, a digital simulation is simply a computation that ‘explores’ a mathematical model, i.e., typically, that provides a particular numerical realization of this literal model. The physical functioning of a digital simulator has, a priori³¹, nothing to do with that of the ideal system, and thus of the actual system. On the other hand, if an analog simulator, also called emulator, cannot explore the mathematical model by performing computations, as the digital simulator does, what does it do? The analog simulator is a machine that directly *mimics* the ideal system. To sum up, before digging into the concept of analog simulation, while both analog and digital simulation, on the one hand, are used to learn about a physical system, and, on the other hand, only provide, epistemologically, results on an ideal system induced by a mathematical model, they work differently: analog simulation directly mimics the ideal system while digital simulation explores the mathematical model thanks to an algorithm. However, what does mimicking an ideal system actually mean?

The analog simulator is built out of elementary physical devices and implements interactions between those devices. Now, by interacting between themselves, the elementary devices usually mimic, this time, *actual* elementary systems, i.e. systems, such as atoms, that have been scientifically proved to behave *effectively* – i.e. in the way they interact with each other – as the devices. These elementary devices are then assembled according

²⁸This statement obviously calls for mathematical definitions of the notions of ‘automatic task’ and ‘appropriate way’. The first answer historically given to such questions is that of Turing, with his now-called *Turing machine*, conceived in the late 30’s [70, 71], and which is still a reference, at ‘least’ pedagogical, and at ‘most’ fundamental through the Church-Turing thesis. In Appendix B, we briefly elaborate on the notions of computation, computers, and computational universality, both the standard classical notions and their quantum counterparts.

²⁹Vaguely speaking, this means that either the set of elementary operations is not well chosen, or so is the way of chaining them, or both.

³⁰All current quantum computers are non-universal, essentially because of the too poor scalability of current quantum technologies. Achieving the construction of a universal quantum computer thus demands to meet scalability challenges. This is briefly elaborated on at the end of Appendix B.

³¹If one is able to reproduce all physical phenomena with a universal computer, one is actually naively tempted to say that nature might be ruled, not only mathematically, but even physically, by processes similar to that which happen in a hardware, up to some accuracy. Such statements can be given a scientific meaning. They inspire, among others, Arrighi [69] and D’Ariano [59], works which fall within the broader subject of natural computing, in which the computing rules are inspired by physical phenomena. We briefly pursue such questions further down in the present introduction.

to the mathematical model of interest, in order to mimic the related *ideal* system³². We have stated above that, before comparing the data out of the analog simulator to that out of the physical system of interest, the simulation only provides information about the ideal system. If the experimental test is passed by the simulator, one can eventually say that it mimics, not only the ideal, but the *actual* system of interest.

While this protocol must indeed be followed, the way it has just been formulated might give a naive picture of, not only analog simulation, but also, more broadly, of empirical sciences. Indeed, there is sometimes, rather than a final series of tests after the simulator is built, a feedback loop between the ongoing construction of the simulator and the physical system of interest. In other words, the reliability of the analog simulator as a tool to mimic the *actual* system of interest, i.e. the validity of the mathematical model to describe this system, is sometimes tested, at increasing levels of detail, *along the way* in the construction of the analog simulator. By this feedback process we build confidence on the analog simulator, so as to use it as a starting point for future experiments, and not to have to start from scratch, i.e. from the elementary devices. Because many of the elementary devices have often been very well tested with respect to previous physical systems of interest, one may want to set up the feedback loop at a (conceptual) scale which is intermediate between the elementary devices and that of the final machine, and eventually large with respect to that of the elementary device; to give a naive pedagogical example, one may want to test (i) the whole unfinished simulator every, let's say, to give a number, five devices assembled, if we have to assemble one hundred, or (ii) only the devices on which one has less confidence from the above-mentioned past tests.

The characteristics of an analog simulator may be summed up in the following sentence: an analog simulator is a simulator that works by analogy, that is, a mapping which is not, at least explicitly, underlaid by logic, but is instead a phenomenal copy of the ideal system. This mapping a priori depends on the ideal system, so that, in this sense, one has to build,

³²A widely used (digitally-simulated) analog simulator is the electronic-circuit simulator SPICE, i.e. the Simulation Program with Integrated Circuit Emphasis. SPICE can be used on the online platform Part-Sim: https://www.google.fr/search?client=safari&rls=en&q=spice+simulator&ie=UTF-8&oe=UTF-8&gfe_rd=cr&ei=80FWfPkJ4jAaJj_qsAL. It is used by companies to check the performances of microelectronic circuits to be built. This (digitally-simulated) analog simulator is classical, i.e. it does not use quantum superposition and entanglement as a resource to simulate an ideal system. A class of developing classical analog simulators, this time actual (i.e. not digitally-simulated), are the so-called synthetic molecular motors, which are synthesized (macro)molecules that mimic natural (macro)molecules which convert chemical energy of the living being they belong to, into mechanical energy, in order (i) to perform certain operations, such as DNA transcription and RNA translation, or DNA replication, or (ii) to transport other molecules (these are the so-called “cargo proteins”). Natural molecular motors are usually chemically driven. The synthetic ones can also be light driven. Synthetic molecular motors can be used for nano-technologies, and not necessarily to simulate and study natural molecular motors. A widespread type of analog quantum simulators are cold-atom optical-lattice simulators. The lattice is formed by laser-induced standing waves. Atoms usually jump from one site to a neighboring one by quantum tunneling, and this dynamics can mimic electron transport in condensed matter. The following review by Jaksch and Zoller may be consulted: <https://arxiv.org/abs/cond-mat/0410614>.

roughly speaking, a machine for each ideal system³³.

We can now come back to our first question: does the simulation, in its most general meaning, mimic something? Since the analog simulator is said to mimic (i) the ideal system, (ii) the actual systems that have inspired the latter and, eventually, if experiments are conclusive, (iii) the actual system of interest, can we similarly say that the digital simulator mimics, first the ideal system, and then, if the experimental test is passed, the actual system? This reveals that the notion of mimic still demands to be clarified.

The digital simulator does the following: it runs an algorithm which reproduces the behavior of an ideal system, but *only* through the associated mathematical model. Now, one can envisage a machine ruled by this digital simulator, that *effectively* mimics the ideal system. Such a digitally-ruled machine is called a *robot*³⁴. Now, if, regarding the scientific method, some digital simulator is, effectively, i.e. via a hypothetical associated robot, as good a simulator as some analog simulator, should we less speak of ‘mimic’ for the digital simulator, i.e. for the *internal functioning* of the robot, than for the mimic of the ideal system’s internal functioning which is realized by the analog simulator? Shouldn’t we rather conclude that the digital simulator is as good a mime as the analog simulator, regarding, if not the ‘metric’, i.e. the position of each physical component of the internal ‘machinery’ of the actual system of interest, at least the ‘topology’ of this internal machinery, i.e. the way its physical components interact with each other, e.g. which ones are connected, and which ones are not? This series of linguistic questions underlines both (i) the scale dependence of the notion of mimic, and (ii) the question of whether the mimic refers to objects, the ‘metric’, or to relations between these objects, the ‘topology’. The difficulty is that these two questions intertwine. To be made scientific, the eventual question of whether logic might rule any extra-human phenomenon should be formulated in terms of measurement of physical quantities, and, because the notion of extra-humanity and that of measurement are difficultly compatible, the question is, stated as such, rather metaphysical³⁵. Note that natural computing, i.e. the design of algorithms inspired by natural phenomena, is a growing field of research. The previous lines aim at illustrating that linguistic and metaphysical questions can (i) be used as a source of inspiration for science, and (ii) eventually be formulated in scientific terms³⁶.

In their review on quantum simulation, Johnson, Clark and Jaksch [8] note that it would be unreasonable to demand to a quantum simulator more accuracy in its accordance

³³This is ‘roughly speaking’ because there are many intermediate scales. One can indeed think of an analog simulator that would be able to simulate a given physical theory, but which would still not be universal. Can we push this further and think of a universal analog quantum simulator, e.g., an analog equivalent to Lloyd’s universal digital quantum simulator? On the one hand, digital simulation focuses on the mathematical model, so that it is scale independent, i.e., typically, it can simulate any type of PDE or Hamiltonian, regardless of the associated physical scales. On the other hand, analog simulation focuses on the ideal system induced by the mathematical model, so that it is a priori more likely to depend more strongly on the scale, which might be a brake on its universality potential.

³⁴Although the purpose of such a machine is to be a phenomenal copy of some existing phenomenon, so that the machine is, *in such an external point of view*, an analog machine, it is obviously *not* an analog simulator, because it is ruled by a *digital* simulator, i.e. its *internal functioning* is digital, while the internal functioning of the analog simulator is *also* analog. Generally speaking, an analog device can either rule or be ruled by digital device.

³⁵The current scientific approach to make these notions compatible is that of decoherence in quantum mechanics [72, 73].

³⁶While the – at least intuitive – knowledge of Popperian epistemology is certainly needed to practice science, it is, by construction, explicitly not sufficient, by excluding from the start, from the analysis, human inductive cerebral processes.

with the mathematical model it simulates, than with the system of interest, which requires comparing data out of the simulator with experimental data out of the system of interest. While this remark obviously also holds in the case of simulations with classical computers, it is particularly topical in the context of quantum simulation, in a sense given by the following two reasons: first, current quantum simulators can handle at most a few tens, or hundred of physical qubits³⁷, so that the typical *accuracy* that can be achieved if one wants to perform the simulation in a reasonable time can be a limiting factor, while accuracy is not a limiting factor for many standard tasks demanded to classical computers³⁸, and second, quantum *error* correction is not standard in current quantum simulation, but rather an intensively-developing research field³⁹, while errors on current classical computers are rather extremely rare⁴⁰.

0.5 On the quantum simulation of quantum field theories

Since the possibility of universal quantum computation, although recently established theoretically, is currently limited by the size of the quantum hardware, and is rather seen as a long-term aim, analog quantum simulation attracts much attention for short- and mid-term research, and is the subject of an increasing number of works. In such a context, several theoretical works on the quantum simulation of QFTs, have been carried out. Let us first mention two research groups which are very active in this research field, and whose approaches are essentially the same: on the one hand, the collaboration between Cirac, Zohar and Reznik, and on the other hand, Zoller's team⁴¹. These two groups have carried out intensive theoretical and experimental work on the quantum simulation of standard LGTs, in a strong short- and mid-term experimental perspective. These works eventually yielded seminal experimental evidence several months ago; the title of the paper reporting the results, namely "Real-time dynamics of lattice gauge theories with a few-qubit quantum computer" [24], already gives some additional precisions on the setup, which simulates the Schwinger mechanism. Let us also mention the theoretical work led by D'Ariano on the quantum simulation of standard continuum QFTs [59]. The general aim of this work is (i) to recover QFT from quantum-information principles, in the perspective that (ii) such rules might further account for sub-Planckian physics, i.e. phenomena below the

³⁷One can speak of physical qubit even if the simulator is analog and not digital, since a physical qubit is merely a two-level quantum system, and analog simulators are often built out of such elementary systems.

³⁸The 'good question' may be, regarding this matter, merely the naive one: can current quantum computers fulfill the job of classical computers faster? A still up-to-date answer to this question is that the few quantum computers which are currently used are specific-task quantum computers.

³⁹Because keeping coherence and entanglement between an increasing number of physical qubits is nowadays, essentially, the major technological problem faced in the design of a quantum computer, quantum error correction is a topic of major importance.

⁴⁰Note that we have here, very naturally, and without, I think, bothering the reader, opposed quantum simulation, which can be analog or digital, to classical computation, which is digital, and this for two reasons: on the one hand, as we mentioned above, classical analog simulators are a *much*-less-used tool to study physics than classical computers, while on the other hand, analog quantum simulators are sometimes – i.e. essentially when it comes to focusing on a specific problem for which the analog simulator has been designed –, better tools than classical computers, thanks to their quantumness.

⁴¹These two groups involve other researchers than those mentioned.

Planck length – and, of course, deliver known super-Planckian physics⁴² –, i.e. might be a setup to overcome the “logical clash” [59] between general relativity and QFT. A notable step has been made in this direction: *free* QFT is recovered as a continuum limit of a certain family of QCA, essentially DTQWs for fermions, and entangled pairs of such DTQW-fermions for bosons. Second quantization is evoked. Einstein’s relativity principle, ensured in the continuum, is replaced, at the discrete level, by requiring the “invariance of the eigenvalue equation of the automaton/walk under the change of representations” [59], without needing to refer to spacetime. Recall that the aim of this work is to get free of as many physical principles as possible in the formulation of the theoretical setup, i.e. to axiomatise QFT with mathematical quantum-information constraints. The work led by Arrighi is in the same vein, and it moreover suggests discretizations for curved spaces. By nature, this work goes much further in the mathematical analysis of the suggested PDE-discretization schemes⁴³. As well as the work by D’Ariano, this work includes recovering continuous-spacetime relativistic transformations in the continuum limit of underlying unitary transformations acting on logical qubits [60]. Eventually, note that non-Abelian gauge theories have recently been phrased in the quantum-information tensor-network language⁴⁴ [75, 16]. The reader may want to have a look at the following two presentations, respectively by D’Ariano and Chandrashekar, which review current results on the DTQW-based simulation of (free) QFT: <http://www.qubit.it/people/dariano/> and <http://www.iopb.res.in/~iscqi2016/slides/conference/d4/chandrasekhar.pdf>; the presentation by Chandrashekar includes recent results on the topology of such schemes. Several original works coauthored, among others, by Di Molfetta and Pérez, and dealing with quantum simulations, with DTQWs, of phenomena related to high-energy physics, have been published within the last months [76, 77, 78]; these include the DTQW-based quantum simulation of neutrino oscillations [77] and DTQW-based Kaluza-Klein-like frameworks and phenomenology, by Bru et al. [79].

The topic of quantum simulation, however, goes well beyond the quantum simulation of quantum field theories in the narrow sense. Quantum simulation is, in particular, now widely used to study condensed-matter phenomenology [80, 81].

0.6 Outline of the thesis

This thesis is organized as follows. It is divided into two parts. Part I is devoted to the in-progress construction of DTQWs-based lattice Yang-Mills gauge theories, while Part II presents DTQWs able to simulate, in the continuum limit, Dirac dynamics in curved spacetime. Each part is preceded by some introductory material.

Part I contains two chapters. Chapter 1 is based on two publications, Refs. [1] and [2], dealing with the coupling of 2D DTQWs to 2D electromagnetic fields, while Chapter 2 is based on a single publication, Ref. [3], dealing with the coupling of 1D DTQWs to a generic

⁴²The smallest length scale ever probed is often considered to be 10^{-18} m, thanks to particle-physics experiments led at the Large Hadron Collider (LHC). The scale of the Planck length being 10^{-35} m, there are actually, above the Planck length, still $35 - 18 = 17$ orders of magnitude to be probed before reaching the Planck length. Known super-Planckian physics thus lies above 10^{-18} m.

⁴³In Ref. [74], for example, the observational convergence of the homogeneous (i.e. free) Dirac DTQW in arbitrary spacetime dimension, is rigorously proven.

⁴⁴Tensor networks were introduced by Penrose, see <http://homepages.math.uic.edu/~kauffman/Penrose.pdf>.

non-Abelian $U(N)$ Yang-Mills gauge field. All together, these three papers should enable the reader to visualize the in-progress construction of DTQWs-based lattice Yang-Mills gauge theories.

The aim of Introductory Material [i](#) is twofold. First, several well-established results on 1D homogeneous and inhomogeneous DTQWs, are presented, in Sections [i.1](#) and [i.2](#), respectively; this allows to set up the notations that will be used in the rest of the manuscript. Second, several results established by seminal works related to DTQWs, are reviewed and discussed: Section [i.3](#) deals with Feynman’s checkerboard and Aharonov’s quantum random walks, while Section [i.4](#) aims at situating quantum walks in the interrelations between several relativistic and non-relativistic physical systems related by analytical continuation.

Before presenting, in Section [1.2](#), the two publications [[1](#), [2](#)], Chapter [1](#) begins with Section [1.1](#), which is a relatively detailed chronological review of historical milestone results on quantum walks, quantum computing and quantum simulation. The quantum-information era that we enter every day a little more, relies on the power of such results.

The reader is strongly invited, before taking a close look, in Section [1.2](#), at Publications [[1](#)] and [[2](#)], to read the first introductory subsection, namely Subsection [1.2.1](#), which is a state-of-the-art ‘recap’ on 1D DTQWs coupled to electric fields, and their interpretation as such, which is threefold.

Publication [[1](#)] is presented in Subsection [1.2.3](#). A new family of DTQWs is presented, which coincides, in the continuum limit, with the Dirac dynamics of a relativistic spin-1/2 fermion coupled to a constant and uniform magnetic field. Standard relativistic Landau levels are extended from the continuum Dirac dynamics to the lattice situation, where the walker is indeed ‘sensitive’ to the non-vanishing step of the spacetime lattice. Such Landau levels for DTQWs are built perturbatively in the step, around the continuum situation. We eventually demonstrate, through numerical simulations, that the parameter interpreted as the magnetic field in the continuum limit, has, beyond both (i) the continuum limit and (ii) perturbative effects of the step, qualitatively the same confining properties as a standard magnetic field, if small compared to 2π , the size of the Brillouin zone. The possibility of quantum simulating condensed-matter systems by DTQWs is also discussed.

Publication [[2](#)] is presented in Subsection [1.2.4](#). A new family of DTQWs is presented, which coincides, in the continuum limit, with the Dirac dynamics of a relativistic spin-1/2 fermion coupled to a generic electromagnetic field in dimension 2. We extend the electromagnetic interpretation beyond the continuum limit, by showing the existence of (i) a lattice gauge invariance, (ii) a lattice invariant quantity, and (iii) conserved currents on the lattice. This allows us to suggest lattice equivalents to Maxwell’s equations. Summing-up, we build a DTQW-based Abelian $U(1)$ lattice gauge theory, in 1+2 dimensions. We recover, through numerical simulations, known phenomenology, both a standard one, associated to standard electromagnetic fields [[82](#), [83](#), [84](#)], and a less standard one, associated to periodically-driven systems [[81](#), [85](#), [86](#)], which, in particular, matches qualitatively with recent results on DTQWs, both in one [[87](#), [88](#)] and two [[89](#), [79](#)] dimensions.

Before presenting, in Section [2.2](#), Publication [[3](#)], Chapter [2](#) begins with Section [2.1](#), which is a compact but in-detail referenced chronological review of the historical steps which led to non-Abelian Yang-Mills gauge theories, from the discovery of electricity and magnetism, to chromodynamics and standard lattice gauge theories.

The reader might be, on the one hand, interested in Subsection [2.2.1](#), and is strongly suggested, on the other hand, to read Subsection [2.2.2](#) before taking a close look at

Publication [3], which is commented and then reproduced in Subsection 2.2.3. Indeed, Subsection 2.2.1 tries to give a schematic picture of non-Abelian gauge theories, without equations, while Subsection 2.2.2 shows how the DTQW on which Publication [3] is grounded, is a very natural extension of its Abelian counterpart [90].

Publication [3] is introduced in Subsection 2.2, but commented and reproduced in Subsection 2.2.3. A new family of 1D DTQWs is presented, which coincides, in the continuum limit, with the unidimensional Dirac dynamics of a relativistic spin-1/2 fermion coupled to a generic non-Abelian $U(N)$ Yang-Mills gauge field. The gauge-theory interpretation is extended beyond the continuum limit, by showing the existence of, (i) not only a $U(N)$ gauge invariance on the lattice, but also (ii) an associated lattice gauge-covariant quantity, which delivers, in the continuum, the field strength associated to a standard $U(N)$ Yang-Mills gauge field. We show, through numerical simulations, that classical, i.e. non-quantum phenomenology, is recovered at short times.

Part II contains solely Chapter 3, which is based on Publication [4]. It is preceded by Introductory Material ii, which aims at giving a pedagogical, general, and essential view of the results of Refs. [91, 90], that is, of how to make a DTQW propagate in a (1+1)D curved spacetime, to speak in vague but pointful terms, that are clarified in this Introductory Material ii. The publication on which Chapter 3 is based, is an extension of the results presented in this introductory material.

Chapter 3 directly presents and comments Publication [4]. A new family of 2D DTQWs is presented, which coincides, in the continuum limit, with the Dirac dynamics of a relativistic spin-1/2 fermion propagating in a generic (1+2)D curved spacetime. The particular case where this spacetime corresponds to the polarization plane of a gravitational wave (GW), is focused on. We show how the probability of presence of the DTQW in this plane is affected by a pure shear GW. In the continuum limit, the GW modifies the eigen-energies of the walker by an anisotropic factor which is computed exactly. For wavelengths close to the spacetime-lattice step, the probability of presence is modified non trivially; the minimal comment on such an influence is that the net effect of the GW is maximal, by far, for short wavelengths, comparable to two or three spacetime-lattice step.

Eventually, the conclusion opens the present work to various related works and possible further studies.

Part I

DTQWs interacting with Yang-Mills fields

One-dimensional DTQWs

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MOTIVATIONS

The aim of this introductory material to the first part of the manuscript, is twofold. First, we discuss some well-established results on (1D) DTQWs, which allows us to set up the notations that will be used in the rest of the manuscript. Second, we review some of the material contained in seminal works related to DTQWs.

i.1 Homogeneous DTQWs

i.1.1 Notations

In this first paragraph, we set up the notations for the standard DTQW on a 1D graph. Consider a graph whose vertices (also called nodes) are countable, so that one can label each vertex by an integer p , and which is two-regular, i.e. for which each vertex p has two neighbors, $p - 1$ and $p + 1$. Such a graph is called ‘1D graph’ because the p ’s can be viewed as coordinates on a curve, either (i) a line when the number of vertices is infinite, which in practice corresponds to the situation where the walker never reaches the boundaries, or (ii) a circle with a periodic boundary condition in the opposite case; one might also think of a segment but then the graph is not two-regular at the extremities, and one must set

different evolution rules at these boundaries, such as, for example, absorbing or reflecting boundaries. A vertex p will thus also be referred to as a position on the curve, or a site. Unless otherwise mentioned, we consider the case of a line, that we orient in the direction of growing p 's to the right. The evolution of the walker on the graph is labelled by a discrete time $j \in \mathbb{N}$. Since the walker is quantum, its state belongs to a Hilbert space \mathcal{H} on the field of complex numbers; we denote this state $|\Psi_j\rangle$, in a Schrödinger picture and using Dirac notations. The Hilbert space is the tensorial product $\mathcal{H} = \mathcal{H}_{\text{spin}} \otimes \mathcal{H}_{\text{position}}$ of the Hilbert space $\mathcal{H}_{\text{position}}$ spanned by the position basis $(|p\rangle)_{p \in \mathbb{Z}}$, and of a finite-dimensional Hilbert space $\mathcal{H}_{\text{spin}}$ accounting for an internal degree of freedom that we call spin¹; the spin (Hilbert) space is also called ‘coin space’, the word ‘coin’ being used in analogy with the coin tossing of classical random walks, and the elements of $\mathcal{H}_{\text{spin}}$ are sometimes called ‘coins’. The minimal dimension for the coin space of a DTQW on a 1D graph is two, and we consider this case from now on, unless otherwise mentioned. Each element of the coin space can be identified to its components on a certain basis $(|\uparrow\rangle, |\downarrow\rangle)$ that we call up-down basis; these components form a couple of complex numbers, that we will note as a column vector so as to perform matrix operations properly. The state of the walker can be decomposed on what we may call the up-down position basis of \mathcal{H} , $(|s\rangle \otimes |p\rangle)_{s \in \{\uparrow, \downarrow\}, p \in \mathbb{Z}}$:

$$|\Psi_j\rangle = \sum_{\substack{s \in \{\uparrow, \downarrow\} \\ p \in \mathbb{Z}}} \psi_{j,p}^s |s\rangle \otimes |p\rangle = \sum_{p \in \mathbb{Z}} \left(\psi_{j,p}^{\uparrow} |\uparrow\rangle + \psi_{j,p}^{\downarrow} |\downarrow\rangle \right) \otimes |p\rangle. \quad (1)$$

The probability for the walker to be located at time j on site p with spin s is $|\psi_{j,p}^s|^2$.

The evolution of the walker on the graph is governed by a one-step evolution operator \hat{W} , also called walk operator,

$$|\Psi_{j+1}\rangle = \hat{W} |\Psi_j\rangle, \quad (2)$$

which is the composition of two operators \hat{S} and \hat{U} ,

$$\hat{W} = (\hat{U} \otimes \hat{I}_{\mathcal{H}_{\text{position}}}) \hat{S}, \quad (3)$$

where $\hat{I}_{\mathcal{H}_{\text{position}}}$ is the identity operator acting on $\mathcal{H}_{\text{position}}$.

The operator \hat{S} is a spin-dependent shift of the walker to the neighboring sites. We note by S_{position} its representation on the up-down position basis of \mathcal{H} . S_{position} acts on the two-component ‘wavefunction’² $\Psi_j : p \mapsto \left(\psi_{j,p}^{\uparrow}, \psi_{j,p}^{\downarrow} \right)^{\top}$, where \top denotes the transposition, as

$$(S_{\text{position}} \Psi_j)_p = \begin{pmatrix} \psi_{j,p+1}^{\uparrow} \\ \psi_{j,p-1}^{\downarrow} \end{pmatrix}, \quad (4)$$

so that the upper spin component moves left in time, and the lower moves right. A key feature of this operator is that it is entangling; in formal terms, this means it cannot be factorized, i.e. written as the tensorial product of an operator acting on the position space

¹The word ‘spin’ is used, a priori, *solely* because we deal with a *two-state* quantum mechanical degree of freedom, i.e. this degree of freedom is, a priori, and a fortiori in a 1D context, *not* the standard spin in 3D space, which is associated to the behavior of the quantum system under 3D rotations, i.e. elements of $\text{SO}(3)$. However, this does not preclude from using the mapping $\text{SU}(2) \rightarrow \text{SO}(3)$ to *visualize* the behavior of the two-state degree of freedom we are dealing with under $\text{SU}(2)$ operations. See below for information on this mapping. One often speaks of *pseudo-spin*.

²We put quotation marks because Ψ_j is only defined on the spatial (1D) lattice, i.e. it is rather a sequence than a function of p . It will indeed become a standard wavefunction in the continuum limit, see Subsection i.1.4.

and another acting on the spin space.

The operator \hat{U} , which acts on $\mathcal{H}_{\text{spin}}$, is a rotation of the walker's spin up to a global phase, and is called 'coin operator' (or operation). Written in a particular basis of the coin space, the coin operation is represented by a 2×2 unitary matrix, the unitarity being (in particular) needed for the total occupation probability of the walker, $\Pi_j \equiv \sum_{p \in \mathbb{Z}} (|\psi_{j,p}^\uparrow|^2 + |\psi_{j,p}^\downarrow|^2)$, to be preserved in time, i.e. Π_j independent of j . The set $U(2)$ of 2×2 unitary matrices is a Lie group, and admits several parametrizations. In particular, any matrix U of $U(2)$ can be written as the product of a global phase³ $e^{i\alpha} \in U(1)$ by a matrix \bar{U} of $SU(2)$, the subgroup of $U(2)$ whose matrices have unit determinant⁴. To each matrix of $SU(2)$, one can associate a rotation matrix belonging to $SO(3)$ ⁵ (this is why I said above that \hat{U} is a rotation up to a phase); this mapping accounts for the classical representation of the spin, that is, an orientation in the 3D (Euclidean) space, i.e. a point on the so-called Bloch sphere. $SU(2)$ can thus be parametrized with the Euler angles of $SO(3)$: we write the matrix representation of \hat{U} on basis $(|\uparrow\rangle, |\downarrow\rangle)$ as

$$U^{\text{Euler}}(\alpha, \theta, \xi, \zeta) = e^{i\alpha} \underbrace{\begin{bmatrix} e^{i\xi} \cos \theta & e^{i\zeta} \sin \theta \\ -e^{-i\zeta} \sin \theta & e^{-i\xi} \cos \theta \end{bmatrix}}_{\bar{U}^{\text{Euler}}(\theta, \xi, \zeta) \in SU(2)} \quad (5)$$

to match with the notations of Refs. [92, 93, 90], where

$$\{(\alpha, \theta, \xi, \zeta) \in \Sigma = [0, \pi[\times [0, \pi/2] \times [0, 2\pi[^2\} \quad (6)$$

is a possible set⁶ to map the whole Lie group $U(2)$ one to one^{7,8}, a result proved in Appendix F, Section F.2, Subsection F.2.1, for another possible parametrization set⁹, namely

$$\{(\alpha, \theta, \xi, \zeta) \in \Sigma' = [0, \pi[\times [-\pi/2, 0] \times] - 2\pi, 0] \times [0, 2\pi[\}, \quad (7)$$

which is more appropriate to link θ , ξ and ζ to standard Euler angles of $SO(3)$ for an active rotation, as shown in Subsection F.2.2. In the following, we will either use the first set, Σ , or forget to choose the angles within this set when such details are not needed. Note that $U^{\text{Euler}}(\alpha, \theta, \xi, \zeta)$ is in $SU(2)$ if and only if $\alpha = k\pi, k \in \mathbb{Z}$. The well-known Hadamard coin operation, or Hadamard transform, which transforms a spin up or down into an equal

³The word 'phase' will be used either for the angle or the associated complex exponential, but the proper meaning should be obvious from the writing.

⁴For a proof of this result in the general case of $U(N)$, see Appendix F, Section F.1.

⁵The mapping $SU(2) \rightarrow SO(3)$ is not one to one but two to one, $\pm U \in SU(2) \mapsto R(U) \in SO(3)$, which reflects different topologies: $SU(2)$ is simply connected, while $SO(3)$ is doubly connected, which can be seen by the fact that $SO(3)$ is topologically (i.e. homeomorphic to) a 3D ball with antipodal points identified – this is the 3D equivalent of identifying the ends of a real interval, which yields a circle, which is doubly connected. $SU(2)$ is the universal covering group of $SO(3)$, and it covers $SO(3)$ twice. This accounts for the fact that the spin does not behave exactly as a vector under rotations.

⁶This set is natural given the parametrization used.

⁷Except when $\theta = 0$ or $\pi/2$, for which this parametrization is not unique.

⁸Note that this set is not what we call a 'chart' (or, rather, 'chart codomain', the 'chart domain' being the space subset which is being mapped), because it is not open. In particular, this set gives no information about the topology of $U(2)$. Only an atlas, i.e. an open cover of $U(2)$ (collection of open sets whose union contains $U(2)$) together with its corresponding mapping functions to the codomains, namely the charts, can describe the topology of $U(2)$. Because this topology is not trivial, i.e. not that of a cartesian product, but yet simple enough, any atlas of $U(2)$ is made of at least two charts (not more).

⁹One can easily adapt the proof to the above set.

superposition of spin up and down¹⁰, is obtained for $\theta = \pi/4$ and $\alpha = \xi - \pi = \zeta - \pi = \pi/2$, and is thus not in $SU(2)$. It is useful to have in mind the following expression:

$$\bar{U}^{\text{Euler}}(\theta, \xi, \zeta) = e^{i\frac{\xi+\zeta}{2}\sigma_3} e^{i\theta\sigma_2} e^{i\frac{\xi-\zeta}{2}\sigma_3}, \quad (8)$$

having introduced two of the three Pauli matrices,

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (9)$$

The DTQW is said homogeneous in space (resp. time) when the coin operation does not depend on space (resp. time), i.e. when the parameters of the coin operation, namely α , θ , ξ and ζ in the parametrization we use, do not depend on p (resp. j). The DTQW is said homogeneous when both homogeneities are satisfied (hence the title of the present subsection).

After n time steps, the walker catches a global phase $n\alpha$ which does not affect the different occupation probabilities, typically the spin-traced one $||\psi_{j,p}||^2 \equiv |\psi_{j,p}^\uparrow|^2 + |\psi_{j,p}^\downarrow|^2$, or the two spin-dependent ones involved in the latter, $|\psi_{j,p}^\uparrow|^2$ and $|\psi_{j,p}^\downarrow|^2$.

An explicit practical way to write the one-step evolution equation, (2), is

$$\begin{pmatrix} \psi_{j,p}^\uparrow \\ \psi_{j,p}^\downarrow \end{pmatrix} = e^{i\alpha} \begin{bmatrix} e^{i\xi} \cos \theta & e^{i\zeta} \sin \theta \\ -e^{-i\zeta} \sin \theta & e^{-i\xi} \cos \theta \end{bmatrix} \begin{pmatrix} \psi_{j,p+1}^\uparrow \\ \psi_{j,p-1}^\downarrow \end{pmatrix}. \quad (10)$$

A widespread convention for this one-step evolution equation is to apply the coin operation before the shift, and to make the upper (lower) spin component move right (left) in time. This convention is equivalent to ours up to a time-reversal operation, as detailed in Appendix G. We used our convention rather than this widespread one because it is simpler in the following sense: when the coin operation depends on position, applying the shift after the coin operation shifts the parameters of the coin operation and makes the equations more cumbersome.

i.1.2 Solution of the homogeneous DTQW on the line by Fourier transform

From Eq. (2), we obtain

$$|\Psi_n\rangle = \hat{W}^n |\Psi_0\rangle. \quad (11)$$

Since the positions p are discrete, the representation W_{position} of \hat{W} on the up-down position basis of \mathcal{H} is a matrix. This matrix has a finite dimension which is easy to determine, as explained in the next paragraph. Hence, solving the previous equation reduces to computing powers of the finite-dimensional matrix W_{position} , which can formally always be done.

The kind of spatial transport we consider, namely, the spin-dependent shift operation given in Eq. (4), implies that the maximal position p_{max} that a walker localised at $j = 0$ on $p = 0$ can reach, is constrained by $|p_{\text{max}}| \leq n$. Hence, to evolve an arbitrary initial wavefunction $\Psi_{j=0}$ up to time n , one needs in the end a Hilbert space \mathcal{H} with dimension $D(n) = 2(2n + \Delta)$, where the overall factor 2 is the dimension of the coin space, $\Delta \in \mathbb{N}$ is the support of $\Psi_{j=0}$, and the factor 2 in front of n is because the walker moves both left

¹⁰By ‘equal superposition’, we mean as usual a superposition whose coefficients have equal modulus. The Hadamard transform is not the only equally-weighting operation, since the phases in front of the equal-modulus coefficients can be modified.

and right at each time step. One should thus compute, to evolve the walker from time $j - 1$ to j , the $D(j)$ -dimensional matrix product $W_{\text{position}} \times W_{\text{position}}^{j-1}$. It is computationally faster to first diagonalize the $D(n)$ -dimensional matrix W_{position} and then to compute the $D(n)$ -dimensional matrix power, which reduce to scalar powers; this diagonalization is always possible since this matrix is unitary by construction.

The operation $U^{\text{Euler}}(\alpha, \theta, \xi, \zeta)$ is a 2×2 matrix with non-vanishing determinant, whose diagonalization is straightforward. The shift operation \hat{S} is already diagonal in the up-down basis of the coin space: indeed, its ‘components’ on this basis, that we denote by $S = [\hat{S}^{ab}]$, $(a, b) \in \{\uparrow, \downarrow\}^2$, are¹¹

$$S = \begin{bmatrix} \sum_p |p-1\rangle\langle p| & 0 \\ 0 & \sum_p |p+1\rangle\langle p| \end{bmatrix}. \quad (12)$$

S is manifestly non-diagonal in the position basis, for example $\langle p-1|S|p\rangle = \text{diag}(1, 0) \neq 0$. When $D(n)$ is big, and in the case where the coin operation involves no parameters¹² but only numbers, one can perform the diagonalization of W_{position} numerically, within some finite numerical precision, in a reasonable time, provided that $D(n)$ is not too big. If we ask for an infinite numerical precision or if the coin operation contains parameters, the diagonalization can be done with a formal-computation software, but this task rapidly becomes very demanding when $D(n)$ increases, and the resulting expressions for the eigenvalues and eigenvectors are often unpractical, i.e. extracting valuable information from them can be difficult¹³.

Now, for homogeneous walks, the coin operation does not depend on the position p , so that we can give a simple analytical solution to our problem by Fourier transform. The previous discussion is still useful because it holds in the case of spatially inhomogeneous walks, where going to Fourier space does not simplify the problem analytically. Taking the Fourier transform of Eq. (10) yields a simple eigenvalue problem for a 2×2 matrix, whose solution we give in the next paragraph. The Fourier transform of a sequence s on \mathbb{Z} takes as an argument a wavevector $k \in \mathbb{R}$ belonging to an interval of length 2π . We choose the interval to be $[-\pi, \pi[$, in order to have a simple mapping between this wavevector and the notion of momentum of standard quantum mechanics¹⁴. The wavevector k will be referred to as the quasimomentum. See Appendix E for a discussion on the use of such a terminology. In the continuum limits considered further down in this work, the quasimomentum is replaced by the standard notion of momentum. The wavelength of the modes is by definition $\lambda = 2\pi/|k|$ ¹⁵. We can write this Fourier transform as

$$\tilde{s}_k = \sum_{p \in \mathbb{Z}} s_p e^{-ikp}, \quad (13)$$

¹¹We also define $U = [\hat{U}^{ab}]$, independently of any parametrization of $U(2)$, and then U^{Euler} is the function that maps $(\alpha, \theta, \xi, \zeta)$ to $U = U^{\text{Euler}}(\alpha, \theta, \xi, \zeta)$. In the case of \hat{S} , the ‘components’ on the spin basis are operators acting on the position Hilbert space.

¹²By parameters, I mean numerically-undetermined literal quantities, i.e. variables belonging to \mathbb{R} .

¹³This is even more the case if the coin operation depends on time or position.

¹⁴In standard quantum mechanics, one typically integrates over *components of the momentum on some axis*, which can be positive or negative, hence the use of this symmetric interval, although any interval of length 2π can be chosen.

¹⁵This wavelength is bounded by 2 from below and goes up to infinity. One should not be surprised that it is possible to generate any function on a lattice with a superposition of modes having wavelengths which cannot go below 2, because the smallest length scale on which a sequence can vary on a lattice or, equivalently, the smallest period of a periodic sequence on this lattice, is 2.

so that the inverse transform reads

$$s_p = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \tilde{s}_k e^{ikp}. \quad (14)$$

More formally, this corresponds to introducing the quasimomentum basis $(|k\rangle)_{k \in [-\pi, \pi)}$ and the quasimomentum operator \hat{k} which acts on the quasimomentum basis as $\hat{k}|k\rangle = k|k\rangle$ and satisfies $e^{i\hat{k}} = \sum_{p \in \mathbb{Z}} |p-1\rangle\langle p|$, so that the shift operation, which reads

$$S = \begin{bmatrix} e^{i\hat{k}} & 0 \\ 0 & e^{-i\hat{k}} \end{bmatrix}, \quad (15)$$

is diagonal in the quasimomentum basis. We note

$$S_k \equiv \langle k|S|k\rangle = \text{diag}(e^{ik}, e^{-ik}). \quad (16)$$

One is thus led to the diagonalization of the 2×2 unitary matrix $W_k(\alpha, \theta, \xi, \zeta) \equiv U^{\text{Euler}}(\alpha, \theta, \xi, \zeta) S_k$, which is straightforward. A priori, one can deduce from Eqs. (8) and (16) that the eigenvalues of $W_k(\alpha, \theta, \xi, \zeta)$ do not depend on ζ . Since α is just a global phase with no effect on the spatial dynamics, we set it to zero. Computing the eigenvalues of $W_k(\alpha = 0, \theta, \xi, \zeta)$ yields

$$\lambda_k^{\pm}(\theta, \xi) = \cos \theta \cos(k + \xi) \mp i \sqrt{1 - \cos^2 \theta \cos^2(k + \xi)}. \quad (17)$$

One can easily compute the eigenvectors [94].

Let us give more details about the role played by the angles ζ and ξ . Using Eq. (8), the one-step evolution equation can be written (with $\alpha = 0$) as

$$\Psi_{j+1} = e^{i\frac{\xi+\zeta}{2}\sigma_3} e^{i\theta\sigma_2} e^{i\frac{\xi-\zeta}{2}\sigma_3} S \Psi_j, \quad (18)$$

where S is given by Eq. (12). One can rewrite the former equation as

$$\Psi'_{j+1} = e^{i\frac{\xi}{2}\sigma_3} e^{i\theta\sigma_2} e^{i\frac{\xi}{2}\sigma_3} S \Psi'_j, \quad (19)$$

where

$$\Psi' = e^{-i\frac{\zeta}{2}\sigma_3} \Psi. \quad (20)$$

This means that choosing an angle $\zeta \neq 0$ is equivalent to the change of spin basis given by the previous equation¹⁶, with manifestly no effect on the spatial dynamics. This can be understood on the Bloch sphere: ζ performs rotations in the plane of the Bloch sphere which is orthogonal to the axis corresponding to the up-down spin basis, called quantization axis¹⁷; since the DTQW dynamics couples the spatial degree of freedom to the spin components on the up-down spin basis, the choice of basis in the plane orthogonal to the quantization axis is irrelevant to the dynamics. For ξ , the situation is a bit different: Eq. (18) can be written

$$\Psi''_{j+1} = e^{i\frac{\zeta}{2}\sigma_3} e^{i\theta\sigma_2} e^{-i\frac{\zeta}{2}\sigma_3} \begin{bmatrix} e^{i(\hat{k}+\xi)} & 0 \\ 0 & e^{-i(\hat{k}+\xi)} \end{bmatrix} \Psi''_j, \quad (21)$$

¹⁶To be fully explicit, the $SU(2)$ matrix $e^{-i\frac{\zeta}{2}\sigma_3}$ corresponds to the $SO(3)$ active rotation (we rotate the spin) of axis \mathbf{e}_z (vertical unit vector, oriented from bottom to top) and angle ζ , if the counterclockwise, i.e. trigonometric rotation direction, is counted positively, which is the standard convention. Equivalently, it is a rotation of the spin *basis* by the opposite angle $-\zeta$.

¹⁷This was pointed out to me by A. Alberti.

where

$$\Psi'' = e^{-i\frac{\xi}{2}\sigma_3}\Psi. \quad (22)$$

Choosing an angle $\xi \neq 0$ is thus equivalent to both (i) the change of spin basis given by the previous equation¹⁸, which has no effect on the spatial dynamics, and (ii) a shift of the wavevector by ξ , which appears in the expression of the eigenvalues, Eq. (17).

Let us now focus on the angle θ , which is the only one that induces superpositions of spin up and down¹⁹, and hence entangles the spatial and spin degrees of freedom through the alternance of repeated spin-dependent shifts and coin operations. We will call it *mixing angle*, *spin coupling* or simply *coupling*.

i.1.3 Energy spectrum and Hamiltonian of the DTQW

Because $W_k(\alpha, \theta, \xi, \zeta)$ is unitary, its eigenvalues have unit modulus, so that we can write

$$\lambda_k^\pm(\theta, \xi = 0) = e^{-iE_k^\pm(\theta)}, \quad (23)$$

where we have introduced the *eigenenergies*²⁰

$$E_k^\pm(\theta) = \pm f_k(\theta) = \pm 2 \arctan \frac{\sqrt{1 - \cos^2 \theta \cos^2 k}}{1 + \cos \theta \cos k}. \quad (24)$$

Because of symmetry properties of $f_k(\theta)$, it is enough to study this function for $k \in [0, \pi/2]$ (recall that $\theta \in [0, \pi/2]$). One can easily show using trigonometric formulae that

$$f_k(\theta) = \arccos(\cos \theta \cos k) \quad \text{for } (k, \theta) \in [0, \pi/2]^2, \quad (25)$$

so that, for example, $f_k(\theta = 0) = k$ and $f_{k=0}(\theta) = \theta$. As functions of k , the eigenenergies are called *dispersion relations*, *energy spectrums* or *energy bands*, the last denomination being widely used in condensed-matter physics. Here, we have two bands, $E^+(\theta)$ and $E^-(\theta)$. The *energy gap* is the minimum value of the difference between the two bands, $\min_k \{E_k^+(\theta) - E_k^-(\theta) = 2f_k(\theta)\}$. This gap is then a function of θ . It occurs at $k = 0$ and is given by $2f_{k=0}(\theta) = 2\theta$. The gap then only vanishes when $\theta = 0$, i.e. when the coin operation is the identity: this is the trivial situation where the upper and lower spin components of the wavefunction do not interfere; the upper is transported left and the lower right, at opposite constant speeds (one space step every time step) and without deformation. When $\theta = \pi/2$ (resp. $k = \pi/2$), the eigenenergies do not depend on k (resp. θ) and equal $\pm\pi/2$.

¹⁸Corresponding to the SO(3) active rotation of axis \mathbf{e}_z and angle ξ .

¹⁹ $\theta \neq 0$ produces non-diagonal elements in $U^{\text{Euler}}(\alpha, \theta, \xi, \zeta)$.

²⁰These quantities are ‘mathematically’ eigenfrequencies. In this quantum-mechanical context, one would associate to these frequencies an energy through the Planck-Einstein relation, i.e. energy = $\hbar \times$ frequency. Since we work with the natural units, energy and frequency have the same value. One could also envisage a notion of energy ‘simply’ related to signal processing; essentially, this means that the proportionality constant between energy and frequency would have a different value than \hbar . I don’t know to which extent the DTQW scheme could model classical propagation with complex notations. The following 2000 paper by Spreeuw, <https://arxiv.org/pdf/quant-ph/0009066.pdf>, constructs a classical analog to quantum-information processing with classical wave optics; one must note, however, that the scaling of the suggested scheme is very poor, i.e. it is basically a classical scaling (exponential growth), which is precisely what one wishes to avoid with quantum simulation. In the present thesis, DTQWs are rather used for their quantumness than for their classical-simulation potential, but the quantumness of our schemes should certainly be investigated in depth.

One can formally define the Hamiltonian \hat{H} associated to the walk operator by

$$\hat{W} = e^{-i\hat{H}} . \quad (26)$$

i.1.4 Continuum limit for homogeneous DTQWs

Consider the effect of a weak coupling, $\theta \ll \pi/2$, on the dynamics of the large-wavelength Fourier modes ($\lambda \gg 1$, i.e. $|k| \ll \pi$) of an initial walker $\Psi_{j=0}$. Taylor expanding Eq. (24) at leading order in θ and k yields

$$E_k^\pm(\theta) = \pm \sqrt{k^2 + \theta^2} + \text{higher order terms} , \quad (27)$$

which is a relativistic dispersion relation with mass θ . We say that the dispersion relation (24) has a *Dirac cone* at $k = 0$ when $\theta = 0$. In the following, we are going to show that, in the limit of infinitesimally-small coupling, wavevectors and frequencies, which corresponds to a continuous limit in both space and time, the dynamics of the walker is that of spin-1/2 relativistic particle in free space. We call this limit the continuum limit.

To be coherent with the papers I coauthored and with the litterature of Di Molfetta et al., I will use $\zeta = \pi/2$, keeping $\alpha = \xi = 0$ for the aforementioned reasons. This coin operation reads

$$C(\theta) = U^{\text{Euler}}(\alpha = 0, \theta, \xi = 0, \zeta = \pi/2) = \begin{bmatrix} \cos \theta & i \sin \theta \\ i \sin \theta & \cos \theta \end{bmatrix} . \quad (28)$$

It is *balanced* (or *unbiased*) for $\theta = \pi/4$, i.e. it transforms each spin component, up or down, in an equally-weighted superposition of both, as the Hadamard transform does, but differs from the latter in the sign of the determinant ($C(\theta)$ do belong to $SU(2)$).

Let us come back to the dynamics of the large-wavelength Fourier modes of the walker: one can push this to the continuous-space limit. To handle this limit formally, we introduce a (dimensionless) space step $\epsilon_x \in \mathbb{R}^+$, assume that $\Psi_{j,p}$ coincides with the value taken by a function $\Psi_j : p \mapsto \Psi_j(x_p)$ at space coordinate $x_p = p\epsilon_x$, and let ϵ_x go to zero. Now, *provided that* $\theta \ll \pi/2$, then a small wavenumber implies, from Eq. (27), small eigenenergies i.e. large eigenperiods, which can be pushed to the continuous-time limit, so that we can write derivatives with respect to time and, in the end, describe the evolution of those large-wavelength and large-period time modes by partial differential equations (PDEs). We then also introduce a dimensionless time step $\epsilon_t \in \mathbb{R}^+$, assume that $\Psi_j(x_p)$ coincides with the value taken by a function $\Psi(\cdot, x_p) : j \mapsto \Psi(t_j, x_p)$ at time $t_j = j\epsilon_t$, and let ϵ_t go to zero with ϵ_x .

The condition $\theta \ll \pi/2$ seems necessary to go to the continuous-time limit, as underline above; let us evaluate this formally. We allow θ to read

$$\theta = \theta_0 + \Delta\theta , \quad (29)$$

where θ_0 is the limit of θ when ϵ_t and ϵ_x go to zero, and $\Delta\theta$ goes to zero with them. To handle the continuum limit formally, we write

$$\Delta\theta = \epsilon_m \bar{\theta} , \quad (30)$$

i.e. we *scale* $\Delta\theta$ by some $\epsilon_m \in \mathbb{R}^+$ (the index m will make sense further down) that goes to zero with ϵ_t and ϵ_x , $\bar{\theta}$ being an arbitrary real parameter. Using the coin operation (28), Eq.

(10) reads

$$\begin{pmatrix} \psi^\uparrow(t_j + \epsilon_t, x_p) \\ \psi^\downarrow(t_j + \epsilon_t, x_p) \end{pmatrix} = \begin{bmatrix} \cos(\theta_0 + \epsilon_m \bar{\theta}) & i \sin(\theta_0 + \epsilon_m \bar{\theta}) \\ i \sin(\theta_0 + \epsilon_m \bar{\theta}) & \cos(\theta_0 + \epsilon_m \bar{\theta}) \end{bmatrix} \begin{pmatrix} \psi^\uparrow(t_j, x_p + \epsilon_x) \\ \psi^\downarrow(t_j, x_p - \epsilon_x) \end{pmatrix}. \quad (31)$$

Assume that Ψ is differentiable at least once in both t and x , and that both derivatives are continuous, so that we can Taylor expand the left- and right-hand sides of the previous equation at first order in ϵ_t , ϵ_x , and ϵ_m . The expansion must be valid for any $(\epsilon_t, \epsilon_x, \epsilon_m)$, in particular for $(0,0,0)$, so that the zeroth-order terms of the expansion must balance:

$$\begin{pmatrix} \psi^\uparrow(t, x) \\ \psi^\downarrow(t, x) \end{pmatrix} = \begin{bmatrix} \cos \theta_0 & i \sin \theta_0 \\ i \sin \theta_0 & \cos \theta_0 \end{bmatrix} \begin{pmatrix} \psi^\uparrow(t, x) \\ \psi^\downarrow(t, x) \end{pmatrix}. \quad (32)$$

This is possible only if $C(\theta_0)$ is the identity matrix, i.e. if

$$\theta_0 = 0, \quad (33)$$

actually $\theta_0 = n\pi$ with $n \in \mathbb{Z}$, but considering $\theta \in [0, \pi/2]$ is enough to parametrize any coin operation (see the mapping set for $SU(2)$, 6). This zeroth-order constraint, namely

$$C(\theta) \xrightarrow{\epsilon_x, \epsilon_t \rightarrow 0} \mathbf{1}_2, \quad (34)$$

is the proper formal way to express the informal small-coupling condition, $\theta \ll \pi/2$.

If the zeroth-order constraint is satisfied by the coin operation, then the limit to the continuum is ensured, i.e. the zeroth-order terms of the above-mentioned Taylor expansion cancel each other. The PDE satisfied by Ψ is obtained by retaining, on both sides of this Taylor expansion, the first-order terms corresponding to the small parameter that goes to zero the slower, either ϵ_t , ϵ_x or ϵ_m . We write $\epsilon_t = \epsilon_m^\delta$ and $\epsilon_x = \epsilon_m^\rho$, where the exponents $\delta > 0$ and $\rho > 0$ account for the fact that ϵ_t , ϵ_x and ϵ_m may tend to zero differently. The richest PDE is actually obtained when $\delta = \rho = 1$, i.e. when all three small parameters go to zero at the same ‘speed’, and reads

$$(\partial_0 - \partial_1) \psi^\uparrow = i \bar{\theta} \psi^\downarrow \quad (35a)$$

$$(\partial_0 + \partial_1) \psi^\downarrow = i \bar{\theta} \psi^\uparrow, \quad (35b)$$

where $\partial_0 = \partial_t$ and $\partial_1 = \partial_x$. This equation can be recast as

$$(i \gamma^\mu \partial_\mu - m) \Psi = 0, \quad (36)$$

where (hence the index m in ϵ_m)

$$m \equiv -\bar{\theta}, \quad (37)$$

the index μ is summed over from 0 to 1, and the gamma matrices have been defined as $\gamma^0 \equiv \sigma_1$, $\gamma^1 \equiv i\sigma_2$. This equation is the flat-spacetime Dirac equation, with Lorentzian-

metric convention $[\eta^{\mu\nu}] = \text{diag}(+, -)$, for a relativistic spin-1/2²¹ fermion of mass m . The gamma matrices satisfy the so-called Clifford algebra, $\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\eta^{\mu\nu}$. The weak-coupling limit of large-wavelength and low-frequency modes is thus described by an effective fermionic classical-field equation.

We already mentioned that a choice $\zeta \neq \pi/2$ can be viewed as a spin-basis change with no change in the coin operation $C(\theta)$, namely $\Psi \rightarrow e^{i\frac{-(\zeta-\pi/2)}{2}\sigma_3}\Psi$ (active-rotation presentation), which does not affect the dynamics. If we do not absorb ζ in the spin basis, this results, in the continuum limit, in a complex-valued mass m [90]. A choice $\xi \neq 0$ can be viewed as both a spin-basis change, namely $\Psi \rightarrow e^{-i\frac{\xi}{2}\sigma_3}\Psi$ (active-rotation presentation), and a substitution $k \rightarrow k' = k + \xi$, so that the small-wavenumber condition needed to go to the continuous-time limit becomes $|k + \xi| \ll \pi$ if we keep the variable k , i.e. the Dirac cone obtained for $\theta = 0$ is located at $k = -\xi$.

As a final remark regarding homogeneous QWs (not only DTQWs, but also CTQWs), I would like to mention a publication I like a lot, namely Ref. [95], which I recommend as a concise and big-picture introduction to QWs, that should obviously be completed by more detailed reviews.

i.2 Inhomogeneous DTQWs

i.2.1 Introduction

We are now interested in making the parameters of the coin operation, α , θ , ξ and ζ , time and position dependent: $\alpha_{j,p}$, $\theta_{j,p}$, $\xi_{j,p}$ and $\zeta_{j,p}$. The walker's dynamics on the spacetime lattice can now be determined by Fourier transform only if none of those parameters is space dependent.

i.2.2 Continuum limit for inhomogeneous DTQWs and electric coupling

We have seen previously that the condition for the continuum limit to exist is that the coin operation tends to the identity matrix when ϵ_t and ϵ_x go to zero. This constrains, in addition to the previous condition on θ_0 , i.e. $\theta_0 = 0$, (i) the angles α and ξ to tend to space- and time-independent values in the continuum limit, and (ii) such values to belong to a certain discrete set [90]; the angle ζ , which may depend on j and p , is not constrained [90] (no difference from the homogeneous case, i.e. $\zeta \neq \pi/2$ yields a complex-valued mass,

²¹In the definition of the DTQW, the word ‘spin’ has been used solely because of the two-state (or, more generally, finite-dimension) property of the coin degree of freedom. Now that (i) the 1D space is not a lattice anymore, but *continuous*, and that the walker dynamics is governed by the Dirac equation, one can speak of (*Dirac*) *spinor* in $(1+1)D$, and in this sense use the word ‘spin 1/2’. However, this ‘spin 1/2’ is *not* the usual spin 1/2 that particles ‘living’ in 3D space can have, but actually corresponds to so-called *chirality*, and one often speaks of *chiral fermions*. Indeed, in one spatial dimension rotations do not exist (only reflections), and the $(1+1)D$ spin 1/2 can thus not be associated to the behavior of the system under 3D rotations. For information on spinors and the Dirac equation in $1+1$ dimensions, see, e.g., the following notes, by N. Wheeler, <http://www.reed.edu/physics/faculty/wheeler/documents/Classical%20Field%20Theory/Miscellaneous%20Essays/A.%202D%20Dirac%20Equation.pdf>, and the following, by R. Davies, for the construction of spinors in various dimensions, http://www.rhysdavies.info/physics_page/resources/notes/spinors.pdf. In 2D space, there is no notion of chirality, and the two-state internal degree of freedom of the $(1+2)D$ Dirac wavefunction has another physical status. In 3D space, there is both chirality and standard spin 1/2 associated to 3D rotations, and the $(1+3)D$ Dirac wavefunction has a four-state internal degree of freedom.

but this time ζ can depend on j and p). Let us then, as we did for θ , assume that

$$\alpha_{j,p} = \alpha_0 + \Delta\alpha_{j,p}, \quad \xi_{j,p} = \xi_0 + \Delta\xi_{j,p}, \quad (38)$$

where α_0 and ξ_0 are possible values for the angles in the continuum limit, and

$$\Delta\alpha_{j,p} = \epsilon_A \bar{\alpha}_{j,p}, \quad \Delta\xi_{j,p} = \epsilon_A \bar{\xi}_{j,p}, \quad (39)$$

where we have introduced some $\epsilon_A \in \mathbb{R}^+$ (the index A will make sense further down) that goes to zero with ϵ_t , ϵ_x and ϵ_m , and $\bar{\alpha}$ and $\bar{\xi}$ may have any dependence on time j and position p . For simplicity, let us make the possible [90] choice

$$\alpha_0 = \xi_0 = 0. \quad (40)$$

We assume that $\bar{\alpha}_{j,p}$ and $\bar{\xi}_{j,p}$ coincide with the values $\bar{\alpha}(t_j, x_p)$ and $\bar{\xi}(t_j, x_p)$ taken by continuous functions $\bar{\alpha}$ and $\bar{\xi}$ of time and space. We choose ζ of the form $\zeta = \zeta_0 + \Delta\zeta$, with $\zeta_0 = \pi/2$ to be coherent with the previous example, and $\Delta\zeta = -\Delta\xi$, for at least two reasons, explained below, and which are independent from the continuum limit. The coin operation obtained can be written

$$U^{\text{Euler}}(\alpha, \theta, \xi, \zeta) = U^{\text{Euler}}(\Delta\alpha, \Delta\theta, \Delta\xi, \pi/2 - \Delta\xi) \quad (41a)$$

$$= e^{i\Delta\alpha} C(\Delta\theta) F(\Delta\xi), \quad (41b)$$

where we have introduced the spin-dependent phase-shift operation,

$$F(\omega) = \begin{bmatrix} e^{i\omega} & 0 \\ 0 & e^{-i\omega} \end{bmatrix}. \quad (42)$$

At each time step, not only the walker's spin is rotated by an amount $\Delta\theta$, but the walker also catches a local spin-independent phase $\Delta\alpha_{j,p}$ and a local spin-dependent one, $\pm\Delta\xi_{j,p}$. The PDE obtained in the continuum limit is, setting all four small parameters equal, i.e. $\epsilon_t = \epsilon_x = \epsilon_m = \epsilon_A$,

$$(i\gamma^\mu D_\mu - m)\Psi = 0, \quad (43)$$

where $D_\mu = \partial_\mu - iA_\mu$ is the covariant derivative, with

$$A_0 = \bar{\alpha}, \quad A_1 = -\bar{\xi}, \quad (44)$$

(hence the index A in ϵ_A). This is the same Dirac equation as Eq. (36) but, this time, for a fermion coupled, through a charge $q = -1$, to an electromagnetic potential with covariant components A_μ . The mass m can also depend on time and space, i.e. the angle θ may also depend on j and p through $\bar{\theta}$.

As long as $\Delta\zeta$ goes to zero with the other small parameters, any choice of $\Delta\zeta$ delivers the same continuum limit, because, in the Taylor expansion in the small parameters, the term containing $\Delta\zeta$ is multiplied by ϵ_m , and is then of order more than one in ϵ_m . The reason why we have chosen $\Delta\zeta = -\Delta\xi$ is theoretical, and explained in the next subsection²².

²²In the case one is only interested in simulating the continuum limit, I see a posteriori another reason which leads to choose $\Delta\zeta = -\Delta\xi$, without invoking the theoretical reason explained in the next subsection, and which is both experimental and computational: as manifest in Eq. (8), shifting ξ by $\Delta\xi$ without simultaneously shifting ζ by $-\Delta\xi$ at each time step involves performing *two* spin-dependent phase shifts of the form (42), instead of a single one with the retained choice $\Delta\zeta = -\Delta\xi$.

i.2.3 Lattice gauge invariance of DTQWs

We know that the Dirac equation (43) is invariant under local phase rotations: when we perform the substitution $\Psi(t, x) \rightarrow \Psi'(t, x) = e^{-i\phi(t, x)}\Psi(t, x)$ in (43), where ϕ is some local phase, the equation is kept invariant provided that we also shift the 2-vector potential by the 2-gradient of the local phase,

$$A_\mu \rightarrow A'_\mu = A_\mu - \partial_\mu \phi. \quad (45)$$

The electric field derived from the electromagnetic potential is the same for any function ϕ : this property, which already exists in classical electrodynamics, is called *gauge freedom*, and the potential A_μ is then called *gauge potential*. This so-called *gauge invariance* is that associated to charge conservation through Noether's theorem. We can view this invariance property with the gauge principle²³: the free Dirac equation, (36), is invariant under *global* phase rotations; for it to be invariant under *local* phase rotations, one must introduce a gauge field which transforms as written above under local phase rotations.

One is thus naturally led to evaluating the gauge invariance of 1D DTQWs under local phase rotations on the spacetime lattice. It turns out that the one-step evolution equation, (10), is invariant [90] under the substitution $\Psi_{j,p} \rightarrow \Psi'_{j,p} = e^{-i\phi_{j,p}}\Psi_{j,p}$, provided that we replace the spacetime-dependent angles by

$$\alpha'_{j,p} = \alpha_{j,p} + \Sigma_{j,p} - \phi_{j+1,p} \quad (46a)$$

$$\xi'_{j,p} = \xi_{j,p} + \Delta_{j,p} \quad (46b)$$

$$\zeta'_{j,p} = \zeta_{j,p} - \Delta_{j,p} \quad (46c)$$

$$\theta'_{j,p} = \theta_{j,p}, \quad (46d)$$

where

$$\Sigma_{j,p} = (\phi_{j,p+1} + \phi_{j,p-1})/2, \quad \Delta_{j,p} = (\phi_{j,p+1} - \phi_{j,p-1})/2. \quad (47)$$

The angle θ is manifestly gauge invariant. The sum $\xi + \zeta$ is also gauge invariant. This means that we don't need the variable $\xi + \zeta$ to have a gauge invariant DTQW; we thus set it to zero, i.e. we take $\zeta = -\xi$, which explains the choice made in Subsection i.2.2. Transformations (46) with the choice $\zeta = -\xi$ thus provide a discrete transformation for the phases, which delivers, in the continuum, the standard gauge transformation of the electric 2-potential [90], which is formally made explicit by Eq. (1.5) in Subsection 1.2.1.

i.3 Reviewing seminal papers

i.3.1 Feynman's checkerboard

As far as I know, the first appearance of DTQWs in the literature is due to Feynman. In 1965, the book *Quantum Mechanics and Path Integrals* [97], written by Feynman and Hibbs, was published; it is based on notes taken by the latter while attending lectures of the former. In Problem 2-6 of this book, one considers a particle that, at each time step, can only move one step to left or to the right, at the velocity of light (which is 1 in natural units).

²³A review, by Jackson and Okun, on the historical “roots” of the gauge principle formulated by Weyl in 1929 [96], can be found at <https://arxiv.org/vc/hep-ph/papers/0012/0012061v1.pdf>. The post-Weyl developments are only mentioned. To Weyl, this gauge principle was a first step in the development of a unified theory of electromagnetism and gravity, on which he worked. See the following paper on the spin connection in Weyl space, <http://www.weylmann.com/connection.pdf>.

At each time step, the particle has a probability amplitude $i\epsilon_t m$ of changing its direction, where ϵ_t is the (dimensionless) time step and m the (dimensionless) mass of the particle. In Feynman's work, the time step is $\epsilon = \epsilon_t m = \epsilon_t/(1/m)$, i.e. it is given in units of $1/m$ [97]. This model is known as the Feynman checkerboard (or chessboard), and corresponds to the following particular finite differentiation of the Dirac equation in dimension 1, written by Feynman himself in his notes of 1946 on the "Geometry of Dirac's Equation in 1 dimension", reproduced in Fig. 8 of Ref. [29]:

$$\psi_L(t, x) = \psi_L(t - \epsilon, x - \epsilon) + i\epsilon \psi_R(t - \epsilon, x - \epsilon) \quad (48a)$$

$$\psi_R(t, x) = \psi_R(t - \epsilon, x + \epsilon) + i\epsilon \psi_L(t - \epsilon, x + \epsilon). \quad (48b)$$

The subscript 'L' (resp. 'R') is for 'coming from the left (resp. right)', i.e. 'going to the right (resp. left)'. These equations are those of a DTQW: indeed, they can be recast as

$$\Psi(t, x) = (S_{\text{position}}^s K^s \Psi(t - \epsilon, \cdot))_x, \quad (49)$$

where

$$\Psi(t, x) = \begin{pmatrix} \psi_L(t, x) \\ \psi_R(t, x) \end{pmatrix}, \quad (50)$$

the spin-dependent shift operation acts as

$$(S_{\text{position}}^s \Psi(t, \cdot))_x = \begin{pmatrix} \psi_L(t, x - \epsilon) \\ \psi_R(t, x + \epsilon) \end{pmatrix}, \quad (51)$$

and the coin operation is given by

$$K^s = \begin{bmatrix} 1 & i\epsilon \\ i\epsilon & 1 \end{bmatrix}. \quad (52)$$

The superscript 's' is for standard, because I use in this thesis a different convention for the one-step evolution equation, in which the coin operation is applied *after* the shift, but both conventions are equivalent up to a time-reversal operation, as detailed in Appendix G. See also the last paragraph of Subsection i.1.1 for comments on these two conventions.

This dynamics yields a family of possible zig-zag paths (in the (x, t) plane) taking the particle from a given starting position to a given final one. To each path corresponds a probability amplitude of taking it, and the problem suggests to show that the sum of all these probability amplitudes yields, in the continuous-spacetime (or continuum) limit $\epsilon \rightarrow 0$, the standard (retarded) propagator for the Dirac equation in dimension 1. This propagator is a 2×2 matrix. The discrete-spacetime version suggested in the problem [97] is noted $[K_{\beta\alpha}(\epsilon)]$, $(\alpha, \beta) \in \{L, R\}^2$, and is given by

$$K_{\beta\alpha}(\epsilon) = \sum_R N_{\beta\alpha}(R) (i\epsilon)^R, \quad (53)$$

where $N_{\beta\alpha}(R)$ is the number of paths with R corners whose first (resp. last) step is in the β (resp. α) direction, and $(i\epsilon)^R$ is the probability amplitude of each such path. The problem suggests to find the expressions of the $N_{\beta\alpha}$'s and to take the continuum limit, but no solution is provided in the book.

Narlikar [98] gives expressions for the four $N_{\beta\alpha}$'s, which involve combinatorial factors. Gersch [99] solves the problem without computing the $N_{\beta\alpha}$'s, thanks to a mapping between $K_{\beta\alpha}$ and the partition function of an Ising model. Jacobson and Schulman [100] also provide expressions for the $N_{\beta\alpha}$'s, without citing Narlikar, whose work was probably unknown to

them²⁴. Kauffman and Noyes [102] provide explicit wavefunction solutions for the DTQW-fashion finite-differentiated Dirac equation, which involve the same kind of combinatorial factors as those aforementioned. Kull and Treumann [103] also provide wavefunction expressions in discrete spacetime, similar to those written in [102], and with combinatorial arguments similar but slightly different from those used to derive the $N_{\beta\alpha}$'s in the previous works; they show that the continuum limit of these wavefunctions coincides with solutions of the Dirac equation, but they do not check this at the discrete level, i.e. on a finite-differentiated Dirac equation, as [102] does. While reviewing works [100] and [102], Earle [104] points out some errors they contain, and gives in particular correct expressions for the few-steps paths. All works recover the appropriate continuum limit. Jacobson [105] provides a generalization to (i) 1+3 dimensions, which however requires superluminal motion, as pointed out by Plavchan²⁵, and (ii) to the presence of non-Abelian Yang-Mills couplings. The more recent attempts to properly generalize the Feynman checkerboard to more than one dimension remain inconclusive. A recent (2016) work in that direction, by Foster and Jacobson [106], still requires superluminal motion (although the speed is bounded), and it is moreover non-unitary. A recent (2014) rigorous mathematical formulation of a 3D Dirac-equation checkerboard-like path integral, by W. Ichinose [107], also runs into the problem of superluminal motion (the speed can even be infinite in this case), pointing out that Feynman [108] noted that the same superluminal motion could happen in the path integral of a photon, which is a (massless) *bosonic* particle (with spin 1). An earlier (2005) work by T. Ichinose [109] first treated the same problem in radial coordinates, with distance r to the origin, where there is a possibly-superluminal local speed $c(r) = r$ (in natural units). The following works should also be reviewed for further research: [110, 111, 112].

Let us mention the work of Riazanov [113], prior to the Feynman checkerboard, which already “exploits the tie between spin and translation” [105] to build, thanks to a “fifth parameter” [105] (in addition to the four coordinates of spacetime) which is “integrated out in the end” [105], a propagator for the (1+3)D Dirac equation. Gaveau et al. [114] and then Karmanov [115] investigate the link between the aforementioned continuum-limit propagators and random processes, through analytic continuation, see Subsection i.4.

i.3.2 Aharonov's quantum random walks

In their paper of 1990 entitled ‘Quantum random walks’ [32], Aharonov, Davidovich and Zagury introduce what can be viewed as a standard DTQW in which we measure and reinitialize the spin at each time step. Kempe's review [116] provides details on this work, in particular on the part in which, thanks to the large-wavepacket approximation, the effects of the quantum interferences between the left- and right-going walkers are pedagogically exemplified (Paragraphs 4 and 5 of the original paper). In Appendix D, I give extensive formal material to treat the theoretical part of the original paper (from the beginning up to Paragraph 6, included), adding some physical insights. The conclusions are the following.

The authors show that in the absence of coin operation, their protocol essentially corresponds, effectively, to a classical random walk on the line. Indeed, from a given time step to the next one, the wavefunction is simply shifted one step to the right or to the left

²⁴Jacobson wrote in 1985 a short review on the subject, citing the previous related papers he had coauthored until then [101].

²⁵See his informal paper “Feynman's checkerboard, the Dirac equation and spin”, at http://www.brannenworks.com/plavchan_feynmancheckerboard.pdf. I thank A. Alberti for sending me this reference.

with some probabilities $|c^+|^2$ and $1 - |c^+|^2$, respectively, without deformation (but with a possible phase change).

Introducing an appropriate coin operation enables the following effect to appear: if, after successive spin measurements, the classical counterpart walker, which has followed a classical random path, is at some distance from its original position, it is possible for the quantum-walker *mean position* to be much further away. This applies to any classical path, including single-direction-going ones (example taken by the authors), but this does not mean that the quantum walker can overcome the well-known light-cone position bound of DTQWs (the particularities of Aharonov's scheme with respect to standard non-measured DTQWs change nothing to this essential feature of DTQWs, determined by the spin-dependent shift operation). Indeed, imagine a wavepacket whose initial support is bounded and large with respect to the lattice step; its edges²⁶ will move at the effective speed of light (with opposite directions), but this does not prevent the center of the wavepacket to go faster than the speed of light *for some finite time (not forever)*. A subtlety regarding this matter is that, to show this effect regarding the center of the wavepacket, one does an approximation of non-deformation of the wavepacket, while this deformation is necessary to account for the respect of the light-cone position bound.

i.4 Wick rotations in relativistic and non-relativistic frameworks

It is known that the Schrödinger equation²⁷ [117] can be obtained from the diffusion equation²⁸ [119, 120, 121] by analytic continuation²⁹, as well as the (*fermionic*) relativistic version of the first, the Dirac equation, is obtained, *in the case of one spatial dimension*, by analytic continuation of the telegrapher's equations³⁰ [114]. The discrete-spacetime version of the relativistic mapping is the persistent classical random walk yielding the DTQW³¹. There is also a discrete-spacetime version of the non-relativistic mapping: the *non-biased* classical random walk yields, by analytic continuation, the CTQW [34]. At the discrete level, the CTQW as a non-relativistic limit of the DTQW was derived by Strauch in 2006 [124].

At the path-integral level, analytical continuation is used:

1. In the non-relativistic framework, to compute probability amplitudes in quantum

²⁶If the support is not bounded, and this merely a technical point, one tends to the effective speed of light in the limits $x \rightarrow \pm\infty$, where x is the position of the walker.

²⁷For English translations of the original four-part paper, go to http://www.physics.drexel.edu/~bob/Quantum_Papers/Schr_1.pdf, http://www.physics.drexel.edu/~bob/Quantum_Papers/Schr_2.pdf, http://www.physics.drexel.edu/~bob/Quantum_Papers/QAEP3.pdf, and http://www.physics.drexel.edu/~bob/Quantum_Papers/QAEP4.pdf.

²⁸The diffusion equation is satisfied, in particular, by the expectation value of the Wiener process, a result known as the Feynman-Kac formula [118].

²⁹Also called Wick rotation, which maps the (1+3)D Minkowski spacetime to the 4D Euclidean space [122].

³⁰The telegrapher's equation is satisfied, in particular, by the expectation value of a certain kind of Poisson process, studied by Kac et al. [123].

³¹This mapping is recalled in a work of 2013 by Boettcher, Falkner and Portugal [67], on the non-perturbative renormalization of quantum walks. A work of 2016, by Boettcher, Li and Portugal, keeps exploring the direction of non-perturbative renormalization [68]. Portugal has published, in 2013, a book entitled *Quantum walks and search algorithms*.

mechanics, by mapping the Feynman measure to the Wiener measure^{32,33} [125].

2. In the relativistic framework:

- (a) For bosons, to compute either scattering amplitudes in bosonic quantum field theory, in which the on-shell free fields obey the Klein-Gordon equation, or, in the case we already have quantum results, their Wick-rotated equivalents, namely the correlators in bosonic statistical field theory, in which the equilibrium non-interacting field obeys the massive (or screened) Laplace (or sourceless Poisson) equation. Recall that these dynamical or equilibrium equations are obtained by functional optimization of the corresponding path integral.
- (b) For fermions, to achieve the same computational aim as in the bosonic case.

Regarding the on-shell fields, the fermionic case is that which is described in the first paragraph of this subsection³⁴. In a Feynman-checkerboard approach, difficulties arise in spatial dimensions greater than one (the one-dimensional case is solved by Feynman's original checkerboard, as mentioned above). Let us stress that the starting-point problem does not deal with the functional integration, but with the on-shell (or equilibrium) fields: indeed, the association, through analytical continuation, between the Dirac equation and the telegrapher's equations, *is only done in one spatial dimension*; Gaveau and Jacobson [114] underline that, in the higher-dimensional case, "it is not clear how to obtain an underlying stochastic process (related by analytic continuation)". It seems we deal here with a matter of structure of the Dirac equation in more than one dimension, or, in other words, with the spacetime view of *relativistic* quantum mechanics³⁵, that was precisely not clear to Feynman because of this higher-dimensions problem, which is why he did not include his one-dimensional checkerboard model [97] in his "Space-time approach to *non-relativistic* quantum mechanics" [127].

To overcome those difficulties in the higher-dimensional fermionic path integral,

³²It is actually the standard way to give the Feynman measure a definite meaning.

³³Note that the path-integral formulation of quantum mechanics was developed by Feynman during his PhD. A scan of the original PhD dissertation is available at <http://cds.cern.ch/record/101498/files/Thesis-1942-Feynman.pdf?version=1>.

³⁴In the case of bosons, the passage from the Klein-Gordon equation to its non-relativistic limit, which is also the Schrödinger equation, is derived in [126], in the more general case of an additional non-linear term. Is there a stochastic process associated to a solution of the Euclidean version of the Klein-Gordon equation, as provided by the Feynman-Kac formula in a non-relativistic context? I haven't seen such a mapping in the literature. One can define relativistic stochastic processes (RSP) [49], which satisfy an equation that yields, in the non-relativistic limit, a kind of diffusion equation [47], but this equation satisfied by the RSP cannot, in its present form, be mapped to the Klein-Gordon equation by analytic continuation.

³⁵The problem is certainly deeper than a mass-coupling issue in the (1+3)D Dirac equation (the mass couples two Weyl equations in the Weyl representation). The problem might also, at least in the massless case, not be a fermion/boson problem, since in one of his books [108], Feynman notices the presence of superluminal paths in the photonic path integral, as pointed out by W. Ichinose [107], while photons are bosons, not fermions. Massless fermions are, as photons (massless spin-1 bosons), helical particles (the helicity, projection of the spin along the momentum, is a good quantum number); their wavefunctions transform the same way under Lorentz transformations, through the same little group, which is $SE(2) = ISO(2)$ in 1+3 dimensions; actually it is sometimes said that the little group for massless fermions is the double cover of $ISO(2)$ (if we define the little group at the level of the half-integer-spin representation and not the original Lorentz group), but, again, it is not clear to me that the problem comes, in the massless case, from this double cover, because of this note by Feynman. In the Weyl representation of the Clifford algebra, massless fermions are described by two independent (no mass coupling) Weyl equations.

the standard approach is that of Grassman variables³⁶ [128, 30, 129]. It is still an open question whether the Feynman checkerboard can be properly extended to more than one spatial dimension, as an alternative to the Grassman-variables approach – it may actually rather be another view of Grassman’s variables, but which may be very enlightening. An interesting paper by Gaveau and Schulman [130] tighten the link between the checkerboard picture and the Grassman-variables approach, but does not achieve the aim of formulating the “Dirac-particle path integral as a sum over path – possibly constrained – on an *ordinary* manifold” [130]. In Fig. 1 of this paper is given a nice diagram depicting the relations discussed in the present section. I reproduce it in Fig. 1.

Note also that, while the Schrödinger equation³⁷ limits the Dirac equation in the non-relativistic approximation, the diffusion equation limits the telegrapher’s equation at long times³⁸, i.e. in the limit where the propagation speed of the signal goes to infinity³⁹.

³⁶A German-to-English translation of Grassman’s paper on the application of his exterior product (also called wedge product) to mechanics is available at http://neo-classical-physics.info/uploads/3/0/6/5/3065888/grassmann_-_mechanics_and_extensions.pdf. This product is one of the tools of Cartan’s exterior calculus, which is a powerful framework to do differential geometry on fiber bundles, either with flat base manifolds, as in classical electromagnetism, or with curved base manifolds, as in general relativity, or ‘simply’ on, e.g., curved surfaces of materials. Cartan developed the exterior derivative, that acts on the exterior product pretty much like the standard derivative acts on a standard product, but with an additional dimension-dependent antisymmetrical property.

³⁷Plus an additional spin term in the presence of an external magnetic field.

³⁸The propagating signal, having ballistic spread, is ‘attenuated more and more’, i.e. with a diffusion coefficient, and its spread becomes diffusive.

³⁹A good short lecture chapter by G. Randall on (i) the continuum limit of the persistent classical random walk, namely the telegrapher’s equations, and (ii) the propagation (or ballistic) and diffusion limits (or, by Wick rotation, ultrarelativistic and non-relativistic limits) of the latter, can be found at <https://ocw.mit.edu/courses/mathematics/18-366-random-walks-and-diffusion-fall-2006/lecture-notes/lecture10.pdf>.

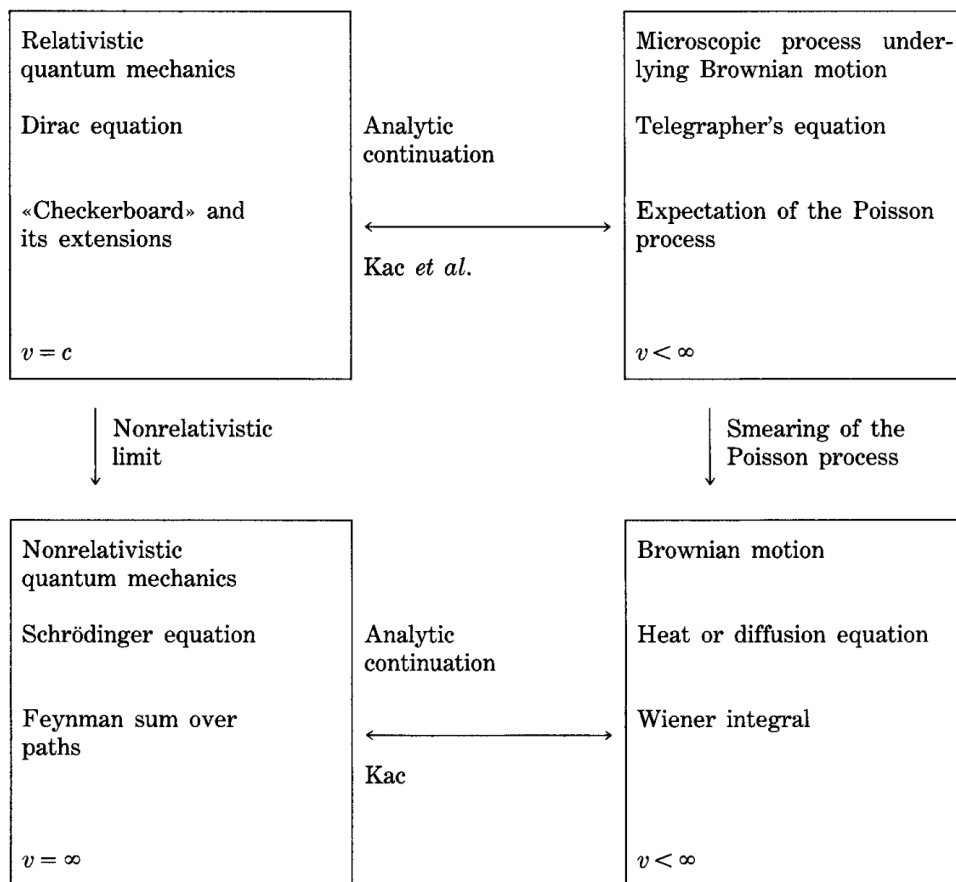


Figure 1: “Interrelations between physical systems”, from [130]. The extensions of the checkerboard to more than one spatial dimension are still unsatisfying currently, see the discussion above.

Two-dimensional DTQWs in electromagnetic fields (Publications [1] and [2])

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1.1 Higher-dimensional (discrete-time) quantum walks

MOTIVATIONS

The aim of this long introduction to Publications [1] and [2] is to give a relatively detailed historical review of important results on (higher-dimensional) quantum walks, quantum information and quantum simulation.

There are several ways to extend DTQWs to higher-dimensional coin and/or node spaces. Historically, the first extensions to higher dimensions that we encounter in the literature under the name of ‘quantum walks’ are those developed by quantum-algorithmics authors, in the early 2000’s, but particular cases of such extensions had actually already appeared before in the community of physics simulation, and more precisely, of cellular automata, in the 90’s, as we will detail below. Let us first come back a bit in time.

1.1.1 From the Turing machine to Meyer’s and then Ambainis’s one-dimensional quantum walks

The principle of modern computers is the Turing machine, proposed by Turing, mathematician and one of the first computer scientists, in his seminal paper of 1936 [70]. Cellular automata (CA) were then introduced by both the mathematician Ulam and the mathematician and physicist Von Neumann [131], to simulate, with computing machines, (classical) physics governed by local rules. Feynman, physicist, added his contribution to the computing era by proposing in 1982 a model to quantize these CA [42], which was formally developed by Deutsch [132]. The term ‘quantum cellular automaton’ (QCA) appeared in a paper by Grössing and Zeilinger [61] in 1988, although their model differs from that of Feynman and Deutsch. Meyer, mathematical physicist, entered quantum computing and quantum simulation with the aforementioned background. The main part of his work is nowadays still at this crossing between quantum simulation and quantum computing. In his seminal paper “From quantum cellular automata to quantum lattice gases” [33], Meyer shows how to obtain what are now called 1D DTQWs as a particular family of 1D reversible (i.e. unitary¹) QCA². In particular, he explains that imposing unitarity to homogeneous 1D QCA, results in a trivial dynamics. That is why [33] (i) Grössing and Zeilinger relax the unitarity constraint in their paper [61], and (ii) Meyer weakens the homogeneity constraint, as follows. First, (ii.a) Meyer weakens the strict homogeneity³ to a one-every-two-cells homogeneity. To preserve unitarity, the only case that can be retained is that of ‘non-interacting’ pairs of cells, i.e. each pair evolves independently from the other pairs, with no quantum

¹Unitarity implies reversibility, and the converse also holds in standard quantum mechanics, see the following discussion, <https://physics.stackexchange.com/questions/150733/unitarity-of-a-transformation-and-reversibility-imply-one-another>. The relaxation of the unitarity constraint is usually explicitly mentioned.

²Again (see above the definition I give for classical cellular automata), and as commonly done, the locality of the evolution rules is implied in what I call QCA.

³This means (I use Meyer’s notations) that at time $t + 1$ and discrete position x on the line, the state $\phi(t + 1, x)$ of the QCA is obtained from the states which are at t on positions $x - 1$, x and $x + 1$, namely $\phi(t, x - 1)$, $\phi(t, x)$ and $\phi(t, x + 1)$, in a manner which is the same for each $\phi(t + 1, x)$ on the space line; to be more precise, $\phi(t + 1, x) = w_{-1}\phi(t, x - 1) + w_0\phi(t, x) + w_{+1}\phi(t, x + 1)$, with w ’s that do not depend on x at $t + 1$ (for any t).

superpositions of pairs. This can be viewed as creating the spin degree of freedom, but each spin is still independent from the others. Second, (ii.b) Meyer adds to the model the alternate evolution (sometimes called partitioning or staggered rule), characteristic of DTQWs, and performed by what we refer to nowadays as the spin-dependent shift, which makes the pairs of cells (i.e. the spins) interact (i.e. superpose) and allow propagation to occur. He thus connects his work to Feynman’s checkerboard, recalling the link with the Dirac equation. Computational work on 1D DTQWs is then continued by computer scientists, the denomination ‘quantum walk’ appearing for the first time in a paper title in the paper “One-dimensional quantum walk” by Ambainis et al. [39], in 2001.

1.1.2 Higher dimensions in, essentially, a quantum-computing perspective: exponential speedup of this research field in the 2000’s?

1.1.2.1 Higher-dimensional coin space in a combinatorial abstract node space

This 1D-DTQW model [39] is then quickly extended to arbitrary d -regular graphs, by Dorit Aharonov, Ambainis, Kempe and Vazirani [133]. In this model, the coin operation acts, at each of the n nodes of the graph, on qudits (generalization of qubits i.e. spins-1/2), belonging to a d -dimensional coin space, and the qudit-dependent shift transports each component of the qudit to one of the d different neighbors. In this work, the vertex (i.e. position) space is abstract, and is not connected to physical dimensions. The authors (i) define the basic tools to study the spreading properties of DTQWs on such graphs, among which the mixing time, and (ii) prove the existence of a disappointing lower bound in this mixing time: DTQWs can *mix* at most ‘only’ (almost) quadratically faster than their classical counterparts, classical random walks (CRWs) (mixing time of $O(n \log n)$ for DTQWs, vs. $O(n^2)$ for CRWs). This ‘bad news’ is then reexamined on the particular case of an hypercube⁴ by Moore and Russell [134], who show that the same bound exists for continuous-time quantum walks (CTQWs). These results are however quickly followed by better news in a paper by Kempe [135]: DTQWs *hit* exponentially faster than CRWs (first evidence of exponential speedup enabled by DTQWs). Previous and similar but somehow weaker results were given for CTQWs by Fahri and Guttman in their seminal paper [34], and then reviewed by Childs and the two previous authors [136]: these authors found an exponentially-smaller ‘local’ (I use this word) hitting time on some particular graphs.

1.1.2.2 Higher-dimensional physical node space

Shortly after the publication of this generalization of DTQWs by computer scientists, a different extension to higher dimensions was proposed by the physicists Mackay, Bartley, Stephenson and Sanders [137].

This extension is explicitly viewed as a way to move a discrete-time quantum walker in higher-dimensional physical spaces. For a D -dimensional physical space, the coin space is built as the tensorial product of D two-dimensional coin spaces, and has thus dimension 2^D . The spin-dependent shift then moves a walker located at some node, not to its $2D$ nearest neighbors in the ‘natural’ D -dimensional hypercubic lattice induced by the D elementary qubit-dependent shifts, but to its 2^D D -th nearest neighbors, and the walker does thus not

⁴The hypercube is widely used in algorithmics, to handle computations on bit strings. It is one of the regular graphs for which the number of nodes satisfies $n = 2^d$. For any d -regular graph with n nodes, the number of edges is $e = nd/2$, but this is still not sufficient to characterise the hypercube.

explore this whole ‘natural’ hypercubic lattice, but only one of the D independent sublattices generated by such a transport (which are generically not hypercubic). For example in two dimensions, the 2- (i.e. next-) nearest neighbors of the node $(0,0)$, are $(1,1)$, $(-1, -1)$, $(1, -1)$ and $(-1,1)$. In $D = 2$, the number of nearest neighbors and of D -th nearest neighbors happen to be equal (to 4) so that, apart from the fact that there is a (unique) useless sublattice, the coin space has a dimension which *is* the minimal one to move a walker on a square lattice, which is the natural hypercubic lattice in $2D$ (square lattice); but this is just a coincidence: the lattice explored, although square, is *not* the original one induced by the $D = 2$ elementary qubit-dependent shifts. This coincidence disappears for $D > 2$. In $D = 3$, for example, the number of nearest neighbors is $2D = 6 < 2^D = 8$, the number of next-next-nearest neighbors. To fully explore a given cubic lattice, one could use the generalization described in the previous subsection, with a coin space having dimension $2D = 6$. The sublattice explored by the present generalization is not cubic, but *body-centered cubic*, and this scheme is natural to explore such a lattice. Note that this body-centered cubic sublattice can only be $d = 2^D$ regular either if it is infinite, i.e., in practice, in the bulk, or if we consider periodic boundary conditions, which makes the D -dimensional lattice a D -dimensional torus.

After recalling the definition of two equally-weighting transformations, namely the discrete Fourier transform (DFT) and the Grover operator (GO), the authors show that the entanglement between the spatial dimensions, produced by these transformations (thanks to their alternate action with the spin-dependent shift), can serve to reduce the rate of spread of the DTQW, with respect to an evolution by the D -tensorized Hadamard gate, a separable transformation which thus produces no entanglement between the spatial dimensions. Since the extensions to higher dimensions are done in a systematic way, the rate of spread always increases with D for a given transformation.

This seminal paper about the spreading properties of DTQWs in higher *physical* dimensions, was followed by another study by Tregenna, Flanagan, Mail and Kendon [138]. In this paper are presented short but conceptually comprehensive and systematic studies of some phenomenal spreading properties of quantum walks on low-degree graphs, from two to four, as well as some comparisons with CTQWs; it is in particular shown how, thanks to the coin degree of freedom, one can better monitor the propagation in DTQWs than in CTQWs.

1.1.2.3 Quantum walks for spatial search and universal computation

The results described in the two previous sections regarding the spreading properties of quantum walks, are bricks with which to elaborate more complex algorithms. Spatial search is one of those.

• Early quantum algorithms, Grover’s search and followings

The recent review of 2016 by Giri and Korepin [139], gives a nice straight-to-the-point introduction to quantum search algorithms derived from Grover’s.

Before getting into the precise subject, the authors present, through some of the early quantum algorithms, some of the essential features of quantum algorithms that may be used to speedup computing power (provided these algorithms run on a quantum computer). First, they describe the very basic Deutsch algorithm, which enables to find, in single query

to the quantum oracle (quantum query), whether some function of a single qubit and taking at most two different values (Boolean function) is constant or balanced, while one needs two queries to a classical oracle (classical query) for such a task to be fulfilled; this illustrates quantum parallelism. Second, they show that this number of quantum queries does not grow with the number k of input qubits⁵ if one uses the Deutsch-Jozsa algorithm⁶, while one needs $2^{k-1} + 1$ classical queries in the worst case. Rather than the classical equivalent to the Deutsch algorithm, it is more efficient to use, to fulfill the proposed task with large inputs on a classical computer, an algorithm which is similar but fulfills the job in only d classical queries; the authors show that the quantum version of this algorithm, variation of the Deutsch-Jozsa algorithm called the Bernstein-Vazirani algorithm, ensures the same performance of a single quantum query. The authors do not discuss Shor's famous quantum algorithm of 1994 [36, 37], which is (i) not a search algorithm, and (ii) widely studied in the literature. Shor's algorithm enables prime-number factorization of an integer n in a time (i.e. number of steps, there is no oracle here) $O((\log n)^3)$; we say that the algorithm is polynomial, with exponent 3, in the physical input size, which is $\log n$. To be precise, the algorithm actually runs in a time $O((\log n)^2(\log \log n)(\log \log \log n))$ (which is better than $O((\log n)^3)$). This is a big improvement with respect to the best known classical algorithm performing such a task, "Gordon's adaptation" [37] of the so-called number field sieve [140], which does the job in a sub-exponential time $O(\exp(c(\log n)^{1/3}(\log \log n)^{2/3}))$.

Giri and Korepin then present in depth many variants of Grover's famous spatial search algorithm of 1996 [38]; there is in particular a distinction between full and partial database search, the latter being achieved by the Grover-Radhakrishnan-Korepin algorithm. The basic important result presented in Grover's seminal paper is the following: instead of the $O(n)$ classical queries that are needed to find a given element in a database of n elements, Grover's quantum-mechanical algorithm only needs $O(\sqrt{n})$ quantum queries, which is a quadratic improvement. It can be shown, and this is an important restrictive result to have in mind, that $O(\sqrt{n})$ is a lower bound for *any* quantum search algorithm [141, 142, 143].

• Spatial search with DTQWs: AA, SKW, AKR, AKR-Tulsi, MNRS

We have seen that Grover's algorithm finds a given item among n in a time $O(\sqrt{n})$, which is a lower bound for any quantum search algorithm, and any DTQWs-based search algorithm will *not* go below this bound. One of the aims of DTQWs-based search algorithms is to search only with local operations, Grover's algorithm being "highly non-local" [144]. The first DTQW-based search algorithm to reach the aforementioned lower bound is the SKW algorithm, suggested by Shenvi, Kempe and Whaley [144] for a search on the hypercube (abstract space). This paper was then followed by the well-known AKR algorithm, by Ambainis, Kempe and Rivosh [40], that manages to adapt the previous algorithm to hypercubic lattices of dimension D (physical space, explored by standard lattices, which *have much lower spreading capacities than the hypercube of dimension $d = \log n$*), containing a number of nodes $n = (\sqrt[D]{n})^D$, the optimal performance of $O(\sqrt{n})$ being reached for $D \geq 3$. In $D = 2$, the running time is $O(\sqrt{n} \log n)$, and the authors show that it is sufficient to have a two-dimensional (instead of a four-dimensional) coin space to reach this lower bound.

⁵More precisely, the input is a series of k bits, namely a k -bit, and this k -bit is treated as a k -qubit by the algorithm, i.e. it is viewed as a basis vector of a 2^k -dimensional Hilbert space.

⁶The function is said balanced if it takes one of the two possible values for exactly half of all the possible inputs, i.e. half of the possible k -bits.

The AKR algorithm combines (i) the monitoring capacities of coins in DTQWs [138, 144], and (ii) the scheme developed by Aaronson and Ambainis [145], in order to surmount the difficulty of implementing Grover’s algorithm on a 2D grid⁷ (they also add to this scheme ‘amplitude amplification’ to increase its probability of success). These results [145, 144, 40] were compiled and phrased in a highly simplified framework by Szegedy [147], as quantum counterparts to classical Markov chains.

Further developments have focused on increasing the probability of success of the search (without increasing the time search). All these developments were used by Magniez, Nayak, Roland and Santha, to construct their MNRS algorithm [148], a simplified version of which is given (i) in Santha’s review of 2008 [149], which deals with many computing problems other than search, and (ii) in an updated version of [148], namely [150]. Some of the latest developments in increasing the probability of success are the 100% chances of success achieved in the SKW algorithm [151], and the time $O(\sqrt{n \log n})$ reached in the AKR algorithm in 2011 [152] (thus disproving Szegedy’s “probably optimal” [147] referring to the $O(\sqrt{n \log n})$); this last result is achieved by managing to get rid of the amplitude amplification included in the original AKR algorithm, which demands an $O(\sqrt{\log n})$ running time, but with no need of any other modification of the original algorithm, as previously done by Tulsi [153] and later by Krovi et al. [154] to reach the same $O(\sqrt{n \log n})$. In the first three paragraphs of his paper [153], Tulsi gives a clear and fast sum-up of the ‘previous episodes’.

• **Parallel and/or joint research with CTQWs: search problem and universal computation, by Childs and others**

Here we report some of the key steps reached by CTQWs in the run ‘between’ continuous- and discrete-time quantum walks in both the quest for the optimization of the search problem and universal quantum computation. Quickly after Kempe’s result on the exponential hitting-time speedup provided by DTQWs, Childs et al. [155] published a paper showing that CTQWs can be exponentially fast in oracle-type problems, in particular, search (Kempe’s result dealt with a non-oracular problem). Two years later, in 2004, Childs and Goldstone [156] show via CTQWs that the lower bound of $O(\sqrt{n})$ can be reached on the hypercube and in the ‘physical’ search problem, for lattices of dimension $D \geq 5$, while in lower dimensions only $O(\sqrt{n} \text{polylog } n)$ is reached, a worse performance than the solution provided one year later by Ambainis et al. with DTQWs [145] and then by the AKR algorithm [40], already discussed above.

While many quantum-computing teams were busy improving the AKR algorithm, from 2005 to 2008, Childs kept working with CTQWs, “perhaps easier to define” [9], and published in 2009 his “Universal computation by quantum walk” [9], showing CTQWs can be used as computational primitives for *any* quantum algorithm, and not only search problems. This paper was followed in 2012 by an extensive generalization to multi-particle quantum walks [10].

In 2006, Strauch precisely connected the continuous- and the discrete-time quantum walks [35], underlying that, “at least in [the] simple case” [35] he treats, the coin degree of freedom is irrelevant to the speedup provided by DTQWs-based algorithms, and that

⁷As he explicitly stated in the abstract of his paper, Benioff [146] considered null the possibility that the implementation of Grover’s algorithm on a 2D grid could outperform classical search on such a grid. As explicitly stated in the abstract of their paper, Aaronson and Ambainis [145] disproved Benioff’s claim.

the speedup is only due to a “simple interference process” [35]. This work was followed by an in-depth generalization to arbitrary graphs by Childs [157]. In 2010, the results of the first paper by Childs on universal quantum computation via CTQW, were recast in the framework of DTQW, by Lovett et al. [158].

• Latest developments in quantum computing

In 2014, a 3-nearest-neighbors CTQW-algorithm has been designed for spatial search on graphene lattices [159, 160]. A recent work by Chakraborty, Novo, Ambainis and Omar [161], show, using CTQWs, that “spatial search by quantum walk is optimal for almost all graphs”, meaning that “the fraction of graphs of n vertices for which this optimality holds tends to one in the asymptotic limit” [161].

A recent paper by Wong [162] proves with CTQWs that the Johnson graph $J(n,3)$ supports fast search (i.e. in a time $O(\sqrt{n})$), thus generalizing the same results obtained previously for (i) $J(n,1)$ with the CTQW version of Grover’s algorithm by Childs and Goldstone [156], and (ii) $J(n,2)$. Note that Johnson graphs were already used as support by Ambainis to develop his “Quantum walk algorithm for element distinctness” [163, 164, 41].

1.1.3 Higher dimensions in the perspective of simulating physical phenomena

1.1.3.1 The community of non-linear physics and gas kinetic theory: FHP, LBE, QBE

• On the history of fluid dynamics, up to the Boltzmann equation

To learn about the history of fluid mechanics “From Newton’s principles to Euler’s equations”, see the paper by Darrigol and Frisch at <https://www-n.oca.eu/etc7/EE250/texts/darrigol-frisch.pdf>. In his *General Principles of the Motion of Fluids*⁸, published in 1757, Euler derives two out of the three equations which are nowadays known as the Euler equations for inviscid (i.e. non-viscous) fluids.

These two equations are (i) the momentum conservation with local pressure and generic external forces, and (ii) the mass conservation. These original equations are the current most general ones for inviscid fluids⁹. In particular, they *are* valid for compressible fluids. The question of the solutions of these equations is a different one. We have (i) five scalar unknowns, namely the three components of the Eulerian speed field, the pressure, and the density, and (ii) four scalar equations: three given by the momentum conservation, and one by the mass conservation (also called continuity equation). This means that even if we manage to make Euler’s seminal system linear (with, for example, some ansatz

⁸A scan of the original manuscript, written in French and published by the Prussian Royal Academy of Sciences and Belles-Lettres, in Berlin, is available on The Euler Archive at <http://eulerarchive.maa.org/docs/originals/E226.pdf>. Ref. [165] is an English translation adapted from Burton’s by Frisch.

⁹This is true in the hypothesis of local thermodynamical equilibrium; otherwise, one can use, in some situations, the more general framework of so-called extended thermodynamics, a branch of non-equilibrium thermodynamics.

for the unknowns), it will be under-determined¹⁰, except for incompressible fluids, whose density is a constant. Euler already mentions, after summing up his 3+1 equations, that a fifth equation should exist¹¹ between pressure, density, and, in Euler’s words “the heat of the fluid particle”, which is nowadays called the internal specific (i.e. per-unit-volume) energy, essentially related to the temperature of the fluid (proportional, for ideal gases). Thermodynamics developed later, in the whole 19th century, and at Euler’s time the distinction between the concepts of ‘heat’ and ‘temperature’ was at least not properly formalized.

The equation between these three quantities (which also involves the Eulerian speed field), is the energy-balance equation. A first relation of this kind enabled Laplace to make the first correct calculation of the sound speed [166]. This condition was later recognized as (i) an adiabatic condition [167], in the context of a developing thermodynamics, and, more precisely, as (ii) an isentropic¹² condition (which is an idealized adiabatic condition), after Clausius introduced the concept of entropy in 1865 [168]: indeed, the equation can simply be stated as the conservation of the entropy of any fluid particle.

To focus on the convective term of the momentum-conservation equation, which is the non-linear term, the pressure term is sometimes dropped, which leads to the (inviscid) Burgers equation. In addition to be physically motivated in some cases, this approximation often simplifies the search for solutions for the speed field.

After deriving the two aforementioned equations, Euler shows that, when the fluid is incompressible, the integral form of the momentum-conservation equation yields Bernoulli’s original theorem, published in 1738, and which was only valid for incompressible fluids, although nowadays one can write down a compressible version. For a pre-Eulerian history of partial differentiation, see the paper by Cajori at http://www.math.harvard.edu/archive/21a_fall_14/exhibits/cajori/cajori.pdf.

In his *Memoir on the Laws of the Motion of Fluids* of 1822, Navier [45] introduced the notion of viscosity, but “he did not developed the concept of shear”¹³. The present form of the Navier-Stokes (momentum-conservation) equation was written by Stokes in 1845¹⁴. The Navier-Stokes equations describe the fluid motion at the so-called mesoscopic scale, which is much greater than the microscopic scale, but still much smaller than the macroscopic scale¹⁵.

The Boltzmann equation, derived in 1872 [169, 170], describes the evolution of an out-of-equilibrium fluid (gas or liquid), which emerges at mesoscopic and macroscopic scales

¹⁰For a general definition of over- and under-determination of a system of PDEs, see https://www.ljll.math.upmc.fr/frey/cours/UdC/ma691/ma691_ch3.pdf. The author of the following notes on the subject, <https://www.researchgate.net/file.PostFileLoader.html?id=56498d8b5cd9e3774f8b4569&assetKey=AS:296325611573251@1447660939976>, feels “we should not attach too much importance to this terminology”. One can put the Euler equations and, more generally, the Navier-Stokes equations, into the form of a quasilinear system.

¹¹I wonder whether such a statement is made by thinking rather ‘physically’ or ‘mathematically’, thinking of the determination of linear systems; probably both. I should investigate on the thermodynamics of Euler’s time.

¹²Note that Kelvin’s circulation theorem holds for isentropic or barotropic fluids.

¹³See Huilier’s note on Navier at http://www.daniel-huilier.fr/Enseignement/Histoire_Sciences/Histoire.pdf.

¹⁴A scan of the original paper [46] can be found at <http://www.chem.mtu.edu/~fmorriso/cm310/StokesLaw1845.pdf>.

¹⁵See http://s2.e-monsite.com/2010/03/16/02/meca_flu.pdf, Chap. 1, for a quick discussion on these three scales.

from the collisional dynamics of the classical microscopic particles it is made of. It is an equation on the (one-point) probability distribution function of the fluid particles. From this Boltzmann equation, one can derive¹⁶ [171, 172, 173] mesoscopic-scale equations (such as the standard Navier-Stokes equation), by taking the so-called hydrodynamical limit¹⁷ [174], which essentially consists in a “patching together of equilibria which are varying slowly in space and time” [56]. A recent paper (2016) by Chow et al. [175] gives an analytical solution for the N -dimensional compressible Euler equations with damping, for a barotropic (pressure only function of the density) fluid, with the pressure as function of the density given by a power law.

• The lattice Boltzmann equation (LBE)

The following few lines on the history of the lattice Boltzmann equation are strongly inspired from Scholarpedia’s sum-up on the subject, see http://www.scholarpedia.org/article/Lattice_Boltzmann_Method. Experts on the discretization of the Boltzmann equation noted that the first *simplified* discretizations of the Boltzmann equation, from the 60’s to the mid 80’s, were rather used to find analytically-tractable solutions of the Boltzmann equation, and not as alternatives to the discretizations of the Navier-Stokes equation in a numerical-computation perspective. The idea of simulating fluid dynamics with lattice-gas models was introduced in 1986 by Frisch, Hasslacher and Pomeau, with their well-known FHP lattice-gas cellular automaton [56]. This model runs, in dimension 2, on a hexagonal lattice, to fulfill an isotropy condition, unsatisfied by the preceding HPP automaton developed by Hardy, de Pazzis and Pomeau [176, 55] in the 70’s; in 3 dimensions, a suitable lattice is given by the projection of a face-centered-hypercube of dimension 4 on one of the coordinate axis [57]. The collision rules at each vertex are inspired by a discrete Boltzmann model [177]. Here is a 1989 review on “Cellular automaton fluids” [178]. Several pitfalls of the FHP automaton lead to the development, in the late 80’s and 90’s, of the so-called lattice Boltzmann methods¹⁸ [179].

• The quantum (lattice) Boltzmann equation (QBE): a DTQW!

In 1992, Succi and Benzi published their “Lattice Boltzmann equation for quantum mechanics” [180], inspired (in part) by the FHP automaton [56]. The central idea of this important paper is that “the non-relativistic Schrödinger equation ensues from the relativistic Dirac equation under the same conditions which govern the passage from the LBE to the Navier Stokes equation” [180]. To accept this statement without further clarifications, recall that the LBE is a *simplified* discrete Boltzmann equation, and this simplification procedure gets rid of some microscopical degrees of freedom of the original Boltzmann equation. Of course, one still has to find a suitable discretization of the Dirac equation, and this is done via an operator-splitting technique. It is straightforward to implement in this scheme a minimal coupling to an external Abelian potential. In 2015, the (1+1)D QBE is explicitly iden-

¹⁶Maxwell first realized this, see the following online scan of his *Scientific papers*, <http://strangebeautiful.com/other-texts/maxwell-scientificpapers-vol-ii-dover.pdf>.

¹⁷See the following notes by, respectively, Golse, <http://www.cmls.polytechnique.fr/perso/golse/Surveys/FGEm04.pdf>, and Villani, http://archive.numdam.org/article/SB-2000-2001__43__365_0.pdf, which presents results obtained by Bardos, Golse, Levermore, Lions, Masmoudi and Saint-Raymond.

¹⁸A short review of the book by Succi [179], written by Yeomans, is available at <http://physicstoday.scitation.org/doi/pdf/10.1063/1.1537916>.

tified with a (1+1)D quantum walk by Succi [18], the a straightforward generalization to (1+3)D, with steps taken alternatively in the 3 spatial directions of the lattice, and not at the same time as in [181], which enables to write these equations sticking to the ‘physical’ low-dimensional coin spaces associated to spinors, as opposed to the ‘algorithmical’ ones, built by tensorial products of qubits [181].

1.1.3.2 From particle physics to cellular automata: Wolfram, ’t Hooft, Bialynicki-Birula, Yepez

After a PhD in particle physics, obtained in 1979 at the age of 20, Wolfram turned into complex systems and cellular automata as a tool to model them. He developed the formal-computation software Mathematica and the search engine Wolfram Alpha. His ideas and findings on cellular automata are summarized in his book *A New Kind of Science* [182]. In the mid 80’s, Wolfram had already developed many ideas on cellular automata, which inspired other theoretical physicists. His seminal paper on “Cellular automata as models of complexity” [183] is cited in the FHP-automaton paper [56].

In 1988, ’t Hooft introduced a cellular automaton to describe quantum systems [184]. In 2014, he wrote a book on the *Cellular Automaton interpretation of Quantum Mechanics* [185]; for an online free version, go to <https://arxiv.org/abs/1405.1548>. In 1994, Bialynicki-Birula wrote the “Weyl, Dirac, and Maxwell equations on a lattice as unitary cellular automata” [186].

1.1.3.3 Note

More authors and works are evoked in the introduction, and discussed more lengthily in the conclusion. The authors include the teams Cirac-Zohar-Reznik, Zoller’s, D’Ariano-Perinotti-Bisio, Arrighi-Facchini-Di Molfetta, Chandrasekhar-Busch, to cite only some of the members of each team. All these works deal with relativistic aspects. A huge amount of works deal with non-relativistic quantum simulation, including, among those working with cold atoms, Zoller’s team, the team Bloch-Cirac, the team Meschede-Alberti, and that of Dalibard. Among the teams working with photons, let us mention the team Silberhorn-Sansonetti and the team Mataloni-Sciarrino, to cite only a few.

1.2 Publications [1] and [2]: DTQWs in electromagnetic fields

ABSTRACT

Both these publications deal with 2D DTQWs interacting with electromagnetic fields. Publication [1] is devoted to relativistic Landau levels in a constant and homogeneous artificial (or synthetic) magnetic field. The study is perturbative in the step of the lattice, around the continuum limit, i.e. the wavepackets are large with respect to the step. We also present, through numerical simulations, some phenomenology demonstrating the confining properties of the magnetic field, beyond the continuum limit and the previous perturbative effects. Publication [2] exhibits an electromagnetic gauge theory on the (1+2)D spacetime lattice for DTQWs, so that these DTQWs interact with *general* 2D electromagnetic fields. Lattice counterparts of Maxwell's equations are suggested, which preserve the charge current conservation on the lattice. For weak electric and magnetic fields, i.e. tiny fractions of 2π , the Brillouin zone, known phenomenology is recovered, such as the $\mathbf{E} \times \mathbf{B}$ drift or Bloch oscillations. For high fields, i.e. sizeable fractions of the Brillouin zone, the spreading properties strongly depend on whether or not the values of the electric and magnetic fields are rational fractions of the Brillouin zone.

I give below a compact presentation of these two publications [1, 2].

Let us first give some background: first, an extended ‘recap’ of the 1D case [93, 90] (Subsection 1.2.1), and second, the expression of the 2D DTQW-operator with electromagnetic coupling (Subsection 1.2.2). This 2D walk operator is the central ingredient of the two publications, whose initial purpose and first achievement is to extend the 1D results to dimension 2.

Recall that the one-step evolution is given by Eq. (2), that is (I make explicit the time-dependence of the walk operator, which is in order in the cases we are going to deal with):

$$|\Psi_{j+1}\rangle = \hat{W}_j |\Psi_j\rangle. \quad (1.1)$$

1.2.1 State-of-the-art ‘recap’ on the 1D electric DTQW

In dimension 1, there can be no magnetic field¹⁹, and the 1D DTQW-operator with electric coupling reads (see Eqs. (41)):

$$W_j^{1D} = e^{i\Delta\alpha_j} U(\Delta\theta, \Delta\xi_j) S, \quad (1.2)$$

where $\Delta\alpha_{j,p}$ is an overall (i.e. spin-independent) local (i.e. time- and position-dependent) phase shift, the spin-dependent shift S is given by Eq. (15), and where I have introduced a

¹⁹Unless one embeds this single dimension into a higher-dimensional space, which is sometimes called ‘effective 1D’, i.e. the motion is constrained to be one-dimensional but the actual physical space has a higher dimension. This is not the case here, the scheme is strictly 1D.

1D²⁰ coin operation with mixing angle $\Delta\theta$ and spin-dependent local phase shift $\pm\Delta\xi_{j,p}$,

$$U(\Delta\theta, \Delta\xi_{j,p}) = C(\Delta\theta) F(\Delta\xi_{j,p}), \quad (1.3)$$

with the standard coin operation $C(\theta)$ and the spin-dependent phase-shift operator $F(\xi)$, given respectively by Eqs. (28) and (42). We write the mixing angle and the phases as (see below why)

$$\Delta\theta = -\epsilon_m m \quad (1.4a)$$

$$\Delta\alpha_{j,p} = \epsilon_A (A_0)_{j,p} \quad (1.4b)$$

$$\Delta\xi_{j,p} = \epsilon_A (A_1)_{j,p}. \quad (1.4c)$$

Note that $\Delta\theta$ could be chosen (j,p) -dependent.

The electric²¹ interpretation of this walk is threefold. The first interpretation is explained in depth in Subsection i.2.2²², the second is introduced in Subsection i.2.3, and the third is a generalization, to an arbitrary electric field, of the interpretation adopted in Refs. [187, 87, 88] in the case of a non-generic constant and uniform electric field²³:

- First, considering $\Psi_{j,p} = \Psi(\epsilon_l j, \epsilon_l p)$, where $\epsilon_l = \epsilon_x = \epsilon_t$ is the spacetime-lattice step (the subscript ‘ l ’ is for ‘lattice’), choosing $\epsilon_m = \epsilon_A = \epsilon_l = \epsilon$ ²⁴, and taking the continuum limit $\epsilon \rightarrow 0$, the one-step evolution equation (1.1) with walk operator (1.2) yields the (1+1)D Dirac equation for a relativistic spin-1/2 fermion of mass m and charge -1 , coupled to an electric potential with covariant time and spatial components A_0 and A_1 , see Eq. (43).
- Second, the walk satisfies the following gauge invariance [90] on the spacetime lattice with nodes labelled by (j,p) (we have recast the results of Subsection i.2.3): Eq. (1.1) with the walk operator (1.2) is invariant under the following substitutions:

$$\Psi \rightarrow \Psi' = \Psi e^{-i\phi} \quad (1.5a)$$

$$A_\mu \rightarrow A'_\mu = A_\mu - d_\mu \phi, \quad (1.5b)$$

where $\phi_{j,p}$ is an arbitrary local phase change, and where we have introduced the following discrete derivatives (finite difference operators):

$$d_0 = (L - \Sigma_1)/\epsilon_A, \quad d_1 = \Delta_1/\epsilon_A, \quad (1.6)$$

²⁰In contrast with coin operations acting on coin spaces greater than 2 and are associated to multidimensional spin-dependent shifts.

²¹There is no magnetic field in this 1D scheme.

²²This first interpretation is only valid in the limit of both (i) wavefunctions whose width is large with respect to the spatial-lattice step, and which vary over time periods which are large with respect to the time step, and (ii) weak variations of the electric potential, i.e. $d_\mu A^\nu \ll \pi$ for $\mu, \nu = 0, 1$.

²³The paper of 2006 by Bañuls et al. [187] shows that this constant and uniform electric field can be obtained through either a spatial or a temporal discrete derivative, but the discrete gauge invariance is not exhibited (which is linked to the fact that the case of an arbitrary electric field is not treated). In the ‘Electric-quantum-walk’ experiment with neutral atoms in a 1D optical lattice, by Genske et al. [87], the electric field is obtained with the (discrete) *spatial* derivative; the paper by Cedzich et al. [88] provides theoretical interpretations of the experimental results, which are far beyond the continuum situation, and deal with revivals of the initial state, due to the periodicity of the system (this periodicity disappears in the continuum limit).

²⁴If these small parameters differ from each other by proportionality factors only, it changes nothing to the equation obtained in the continuum limit except from such proportionality factors in front of either A , m , or the lattice coordinates. However, one of these small parameters can be, for instance, a power of another small parameter, possibly non-integer, which makes the continuum limit change; see Subsection i.1.4.

where, for any (j,p) -dependent quantity Q ,

$$(LQ)_{j,p} = Q_{j+1,p} \quad (1.7a)$$

$$(\Sigma_1 Q)_{j,p} = \frac{Q_{j,p+1} + Q_{j,p-1}}{2} \quad (1.7b)$$

$$(\Delta_1 Q)_{j,p} = \frac{Q_{j,p+1} - Q_{j,p-1}}{2} . \quad (1.7c)$$

Note that d_1 is a standard finite difference in the spatial direction (defined over two sites), while d_0 can be viewed as the mean between two standard finite-differentiated convective derivatives (with Eulerian speed equal to 1), one going forward, and the other backwards²⁵:

$$(d_0 Q)_{j,p} = \frac{1}{2\epsilon_A} \left[\{ (Q_{j+1,p} - Q_{j,p}) + (Q_{j,p} - Q_{j,p-1}) \} + \{ (Q_{j+1,p} - Q_{j,p}) + (Q_{j,p} - Q_{j,p+1}) \} \right]. \quad (1.8)$$

In the continuum limit, the finite-difference operators d_0 and d_1 yield the standard partial derivatives ∂_0 and ∂_1 , and the lattice gauge invariance (1.5) yields the standard gauge invariance of the Dirac equation in (1+1)D continuous spacetime.

Eventually, one can define the following lattice equivalent of the electric²⁶ tensor in 1+1 dimensions,

$$(F_{\mu\nu})_{j,p} = (d_\mu A_\nu)_{j,p} - (d_\nu A_\mu)_{j,p} , \quad (1.9)$$

where $(\mu, \nu) \in \{0, 1\}$. This quantity is (i) antisymmetric by construction, (ii) invariant under (1.5), and (iii) its continuum limit yields the usual electric tensor. Moreover, we can check the following conservation equation on the lattice:

$$d_0 J^0 + d_1 J^1 = 0 , \quad (1.10)$$

where J^μ is invariant under (1.5) and has the same expression as the Dirac current in (1+1)D continuous spacetime (but is defined on the lattice).

- Third, the walk operator (1.2) can be obtained from the standard walk having only an angle $\Delta\theta \neq 0$, i.e. with $\Delta\alpha_{j,p} = \Delta\xi_{j,p} = 0$, by implementing a ‘Bloch phase’ $e^{i(\Delta\alpha_{j,p} \pm \Delta\xi_{j,p})}$ ²⁷, which reminds of that acquired by tight-binding electrons driven, in dimension 1, by a superimposed arbitrary electric field, where the $+$ is for the electron tunneling in one direction, and the $-$ for the other direction. To be precise on the tight-binding procedure in the presence of electromagnetic fields: one mathematically *adds* the *scalar* potential $\sim \Delta\alpha_{j,p}$ to the tight-binding Hamiltonian, and performs, to account for the presence of the *vector* potential, a Peierls substitution on the hopping (off-diagonal) matrix elements, namely $t \rightarrow t e^{\pm \Delta\xi_{j,p}}$, see Eq. (12) in [188]. In the case of a constant and uniform electric field, this condensed-matter system yields the well-known Bloch oscillations of the electrons, with period inversely proportional to the electric field. Despite the phenomenal similarities between such a DTQW-scheme and the 1D tight-binding Hamiltonian with superimposed electric field, there are two *fundamental* differences. First: in the DTQW, the particle, which has a spin (or pseudo-spin), undergoes a spin-dependent transport, while in the tight-binding

²⁵This was pointed out to me by D. Meschede.

²⁶It contains no magnetic field.

²⁷I use the same denomination as in [87]: the so-called Bloch phase is that which implements the electric potential, namely, with contravariant components, $\sim (\Delta\alpha_{j,p}, \Delta\xi_{j,p})$.

Hamiltonian, the left-right jump has *nothing* to do with spin, it is due to *tunneling*²⁸. Second, here (i) the Peierls flux exponential is implemented, not on the Hamiltonian, as standardly done with tight-binding Hamiltonians, but on the (one-step) evolution operator, and (ii) the implementation of the scalar potential is not equivalent either, although there is a closer matching²⁹, because of the generic non-commutativity of the one-step evolution operators. Eventually, there is a third difference whose ‘importance’ (to define) I haven’t completely evaluated yet: in the DTQW-scheme, time is discrete, while it is continuous in tight-binding Hamiltonians.

1.2.2 Walk operator for the 2D DTQW with electromagnetic (i.e. Abelian) coupling

Now the walker $|\Psi_j\rangle$ lives, in real space, on a 2D lattice with nodes $(p_1, p_2) \in \mathbb{Z}^2$.

We build the 2D DTQW operator by doing a 1D walk in the first spatial direction, with spin-dependent phase shift $\Delta\xi_{j,p_1,p_2}^{(1)}$, followed by another 1D walk but in the other spatial direction, with spin-dependent phase shift $\Delta\xi_{j,p_1,p_2}^{(2)}$ ³⁰:

$$W_j^{2D} = e^{i\Delta\alpha_j} \left[U\left(f^-(\Delta\theta), \Delta\xi_j^{(2)}\right) S^{(2)} \right] \left[U\left(f^+(\Delta\theta), \Delta\xi_j^{(1)}\right) S^{(1)} \right], \quad (1.11)$$

where the mixing angle $\Delta\theta$ is encoded through

$$f^\pm(\Delta\theta) = \pm \frac{\pi}{4} + \frac{\Delta\theta}{2}. \quad (1.12)$$

²⁸The DTQW-scheme is intrinsically chiral, and this has nothing to do with the presence or absence of a magnetic field. In the case of tight-binding Hamiltonians, one can include spin-orbit corrections [189, 190] when a magnetic field is applied, but again the left/right jump has *nothing* to do with that, it is due to tunneling. (Note that the probabilities of going left or right by tunneling can be modified by a superimposed magnetic field *only* if the latter breaks the translational symmetry of the system; this might be a way of simulating a biased coin operation with such a condensed-matter system, or, rather, a simulation of this condensed-matter system.)

²⁹To the exponential implemented on the DTQW one-step evolution operator, $e^{i\Delta\alpha_{j,p}}$, corresponds a scalar potential $\sim \Delta\alpha_{j,p}$, which is precisely that *added* (no multiplication like for the Peierls substitution) to the tight-binding Hamiltonian.

³⁰Similar constructions can be found, in a quantum-computing perspective (if we are to categorize), in the AKR paper (2005) [40] and in the paper by Di Franco et al. (2011) [191], and, in the perspective of simulating quantum physics with cellular automata, in the papers by Succi et al. (1993) [180], Bialinicki-Birula (1994) [186], Yepez (2002) [192], Strauch (2006) [124], and, more recently, Arrighi et al. (2015, 2016) [74, 193] and Succi et al. (2015) [18]. Note the following papers by Yepez: these two rather old ones (2002) [194, 195], and this recent proceeding of 2016 [58].

1.2.3 Publication [1]: Landau levels for discrete-time quantum walks in artificial magnetic fields

ABSTRACT

In this publication, we present a new family of 2D DTQWs which coincides, in the continuum limit, with the Dirac dynamics of a relativistic spin-1/2 fermion coupled to a constant and uniform magnetic field. This allows us to extend standard relativistic Landau levels from the continuum Dirac dynamics to the lattice situation, where the walker is indeed ‘sensitive’ to the non-vanishing step of the spacetime lattice. Such Landau levels for DTQWs are built perturbatively in the step, around the continuum situation. We eventually demonstrate, through numerical simulations, that the parameter interpreted as the magnetic field in the continuum limit, has, beyond both (i) the continuum limit and (ii) perturbative effects of the step, qualitatively the same confining properties as a standard magnetic field. The possibility of quantum simulation of condensed-matter systems by DTQWs is also discussed.

1.2.3.1 Short but detailed review and comments

In Section 2 of the paper, we introduce the above walk, Eq. (1.11), but *only* in the particular case

$$\Delta\alpha_{j,p_1,p_2} = 0, \quad \Delta\xi_{j,p_1,p_2}^{(1)} = 0, \quad \Delta\xi_{j,p_1,p_2}^{(1)} = Bp_1\epsilon, \quad (1.13)$$

where $B \in \mathbb{R}$ is the parameter that is interpreted as a constant and uniform magnetic field in the continuum limit³¹, derived in Section 3 of the paper.

Note this technical formal point: the two coin matrices introduced in the paper do *not* correspond to the two U ’s of the above equation, (1.11), but after expanding the matrix products in the paper, one can recast the equations exactly as (1.11). This is so simply because the correspondence between the DTQW-equations and the two matrices chosen to write these equations in a compact form is not one to one, but one to many³².

Section 4 is devoted to a study of how the non-vanishing step of the spacetime lattice modifies the eigenstates of the continuum-limit Hamiltonian, which are the well-known relativistic Landau levels. The study is perturbative in the step ϵ , the zeroth order being the continuum situation. The zeroth-order eigen-energies are well-known; they vary as the square root of the level³³. There are two usual choices for the eigenstate basis of the Landau levels. We choose the so-called Hermite basis, for which the momentum along y is a good

³¹Outside the continuum limit, the confinement properties of B , exhibited in Section 5 of the paper, also endow B with a phenomenal *qualitative* magnetic interpretation.

³²When writing this paper we had not figured out the suitable compact form of Eq. (1.11) because we had not figured out the minimal possible gauge invariance on the lattice. That compact form is given in our next paper [2]; it enables, in particular, a straightforward correspondence between the lattice gauge fields and those in the continuum.

³³Have in mind that this square-root dependence is that expected for relativistic Dirac fermions or gapped graphene-like quasiparticles (which behave effectively exactly as the former), in contrast with the linear dependence expected for non-relativistic particles.

quantum number³⁴ (this is possible in the chosen Landau gauge); this choice is natural because translations are symmetries of the mesh on which the walker lives, and the walker ‘sees’ this mesh at higher orders. In Appendix B of the paper, we compute analytically the first-order corrections to (i) the eigen-energies (which vanish) and to (ii) the Hermite eigenvectors, and we numerically check in the body of the paper that these corrections are correct³⁵ (see Figs. 4 and 5 of the paper). We also provide, in Fig. 3, a typical (relative) change induced by the corrections on the probabilities of presence of the five first Landau levels. These plots may be useful for, e.g., a comparison with future experimental data.

Section 5 aims at giving a flavor of the phenomenology of our scheme well beyond the continuum limit (the perturbative computation can intrinsically only go, a priori, slightly beyond). We show that the parameter B has the same qualitative confinement properties as a standard magnetic field in continuous spacetime.

In the conclusion (Section 6), we stress that, if we view the DTQW as a way to discretize the Dirac equation, (i) this discretization is a naive symmetric one, and suffers from fermion doubling, which happens at the boundaries of the Brillouin zone, but that (ii) this does not preclude the use of this discretization around the Dirac cone, located at the center of the Brillouin zone, i.e. for small wavevectors (in comparison with the size of the Brillouin zone), which is the only limiting case where the Dirac-fermion interpretation, i.e. the continuum limit, makes sense.

³⁴The other eigenvector basis is the Laguerre basis, for which the good quantum number is a certain gauge-invariant angular momentum, see [196] and Appendix I for an expression of the gauge-invariant generator of an arbitrary symmetry of the electromagnetic field.

³⁵I have checked that, for the Laguerre basis at zeroth order, the DTQW-scheme converges when the lattice step goes to zero, but the convergence is not improved when I add the first-order corrections to the eigenvectors, maybe because these corrections only make sense if the rotational symmetry of space is not broken for a non-vanishing step, while this is *not* the case in our scheme, which uses a square lattice.



Landau levels for discrete-time quantum walks in artificial magnetic fields



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HIGHLIGHTS

- Explicit construction of discrete-time quantum walks (DTQWs) whose continuous limit coincides with the dynamics of a Dirac fermion coupled to a magnetic field.
- Construction of Landau levels for these DTQWs.
- Results show that DTQWs can be used as quantum simulators of magnetic effects in condensed matter.

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ABSTRACT

A new family of 2D discrete-time quantum walks (DTQWs) is presented and shown to coincide, in the continuous limit, with the Dirac dynamics of a spin 1/2 fermion coupled to a constant and uniform magnetic field. Landau levels are constructed, not only in the continuous limit, but also for the DTQWs *i.e.* for finite non-vanishing values of the time- and position-step, by a perturbative approach in the step. Numerical simulations support the above results and suggest that the magnetic interpretation is valid beyond the scope of the continuous limit. The possibility of quantum simulation of condensed-matter systems by DTQWs is also discussed.

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1. Introduction

Quantum walks (QWs) were introduced in the literature by Y. Aharonov [1] and D.A. Meyer [2]. They are models of coherent quantum transport in discrete space. This article focuses on Discrete-Time Quantum Walks (DTQWs), which are quantum formal analogues to Classical Random Walks (CRWs). A typical 1D quantum walker carries a two-state internal degree of freedom or spin. At each time-step of a DTQW, the spin of the walker is rotated deterministically through a so-called coin operator and the walker then undergoes a spin-dependent position shift to the left or to the right. This evolution naturally entangles the spin and the position of the walker. The basic construction just outlined has been generalized to higher spatial dimensions and/or coin spaces of dimension higher than two [3,4]. Two standard reviews on (DT)QWs are [5,6].

DTQWs have been realized experimentally with a wide range of physical objects and setups [7–13]. They are important in a large variety of contexts, ranging from fundamental quantum physics [8,14] to quantum algorithmics [15–20], solid state physics [21–24] and biophysics [25,26].

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Contrary to CRWs, DTQWs are actually deterministic. Indeed, while CRWs describe diffusion, DTQWs describe wave propagation at finite velocity. DTQWs are therefore linked with Lorentz geometry [27] and in particular with the Dirac equation.¹

It has been shown recently [29–31] that several families of 1D DTQWs could be interpreted as discrete models of spin 1/2 Dirac fermions coupled to electric and relativistic gravitational fields. The aim of this article is to extend these results to magnetic fields. We thus introduce a new family of 2D DTQWs and show that the formal continuous limit of this family coincides with the Dirac dynamics of a spin 1/2 fermion coupled to a constant and homogeneous magnetic field orthogonal to the 2D space in which the walk propagates.

The eigenvalues of the Hamiltonian generating this continuous dynamics are well-known and are called the relativistic Landau levels. We show by a perturbative computation that Landau levels also exist for the discrete dynamics of the DTQWs and discuss how the corresponding eigenstates and probability densities are influenced by the finite non-vanishing time- and position-step. All results are finally supported by numerical simulations.

The results presented in this article strongly support that DTQWs can be used for quantum simulation of condensed-matter systems and spintronics. Indeed, much of the recent research on condensed-matter physics involves the 2D interaction of electrons with magnetic fields. Landau levels play a prominent role in this field and are for example one of the key ingredients of the quantum Hall effect [32], which has current important applications in metrology [33], and could also be used in quantum computation [34–36]. Thus, the existence of Landau levels for the DTQWs make DTQWs natural promising candidates for quantum simulation of many interesting phenomena, including the quantum Hall effect.

2. Fundamentals

Consider the DTQW defined by the following set of discrete evolution equations:

$$\begin{pmatrix} \psi_{j+1/2,p,q}^L \\ \psi_{j+1/2,p,q}^R \end{pmatrix} = \mathbf{U}(\alpha_p(\nu, B), \theta^+(\nu, m)) \begin{pmatrix} \psi_{j,p+1,q}^L \\ \psi_{j,p-1,q}^R \end{pmatrix} \\ \begin{pmatrix} \psi_{j+1,p,q}^L \\ \psi_{j+1,p,q}^R \end{pmatrix} = \mathbf{V}(\alpha_p(\nu, B), \theta^-(\nu, m)) \begin{pmatrix} \psi_{j+1/2,p,q+1}^L \\ \psi_{j+1/2,p,q-1}^R \end{pmatrix}, \quad (1)$$

where

$$\mathbf{U}(\alpha, \theta) = \begin{bmatrix} e^{i\alpha} \cos \theta & ie^{i\alpha} \sin \theta \\ ie^{-i\alpha} \sin \theta & e^{-i\alpha} \cos \theta \end{bmatrix}, \quad \mathbf{V}(\alpha, \theta) = \begin{bmatrix} e^{i\alpha} \cos \theta & ie^{-i\alpha} \sin \theta \\ ie^{i\alpha} \sin \theta & e^{-i\alpha} \cos \theta \end{bmatrix}, \quad (2)$$

$$\alpha_p(\nu, B) = \nu^2 \frac{Bp}{2}, \quad (3)$$

$$\theta^\pm(\nu, m) = \pm \frac{\pi}{4} - \nu \frac{m}{2}, \quad (4)$$

and ν, B, m are arbitrary parameters. The indices j and p, q are integers which label discrete time and positions in 2D discrete space, respectively. The wave function Ψ lives in a two-dimensional Hilbert space and is thus represented by a ‘spinor’ Ψ with components (ψ^L, ψ^R) in a certain (j, p, q) -independent basis (b_L, b_R) of this Hilbert space, i.e. $\Psi = \psi^L b_L + \psi^R b_R$.

To make notations less cumbersome, we write $\mathbf{U}^+(\nu) = \mathbf{U}(\alpha_p(\nu, B), \theta^+(\nu, m))$ and $\mathbf{V}^-(\nu) = \mathbf{V}(\alpha_p(\nu, B), \theta^-(\nu, m))$. Of the three angles entering the definitions of $\mathbf{U}^+(\nu)$ and $\mathbf{V}^-(\nu)$, only one depends on the point at which the transport is computed, and only through the first space-coordinate p . The parameters B and m will eventually be interpreted as a magnetic field and as a mass. The interpretation of the parameter ν will be discussed below.

The evolution from ‘time’ j to time $j + 1$ proceeds in two steps. In the first step, the DTQW is transported by operator $\mathbf{U}^+(\nu)$ from time j to time $j + 1/2$ along the first space direction (p -direction). In the second step, the DTQW is transported by operator $\mathbf{V}^-(\nu)$ from time $j + 1/2$ to time $j + 1$ along the other space direction (q -direction). Note however that the values of Ψ at times $j + 1/2, j \in \mathbb{N}$ are not taken into account in the DTQW i.e. the DTQW is the succession of the values taken by Ψ at all integer times j . The values of Ψ at half-integer times are thus merely a tool to advance the DTQW in ‘time’. Equations relating directly ψ_{j+1} to ψ_j can be deduced from (1) and read:

$$\begin{aligned} \psi_{j+1,p,q}^L &= e^{2i\alpha_p} \cos \theta^+ [\cos \theta^+ \psi_{j,p+1,q+1}^L + i \sin \theta^+ \psi_{j,p-1,q+1}^R] \\ &\quad + ie^{-2i\alpha_p} \sin \theta^+ [i \sin \theta^+ \psi_{j,p+1,q-1}^L + \cos \theta^+ \psi_{j,p-1,q-1}^R], \\ \psi_{j+1,p,q}^R &= ie^{2i\alpha_p} \sin \theta^- [\cos \theta^+ \psi_{j,p+1,q+1}^L + i \sin \theta^+ \psi_{j,p-1,q+1}^R] \\ &\quad + e^{-2i\alpha_p} \cos \theta^- [i \sin \theta^+ \psi_{j,p+1,q-1}^L + \cos \theta^+ \psi_{j,p-1,q-1}^R]. \end{aligned} \quad (5)$$

¹ Indeed, Feynman [28] developed in 1965 a QW-like path discretization for Dirac fermions.

3. Continuous limit

To determine the formal continuous limit of this DTQW, we proceed as in Refs. [31,29,30,37]. We first introduce (dimensionless) time and space steps ΔT , ΔX , ΔY and interpret $\psi_{j,p,q}$ and α_p as the value $\Psi(M)$ and $\alpha(M)$ taken by certain functions Ψ and α at point M with (dimensionless) space–time coordinates $T_j = j \Delta T$, $X_p = p \Delta X$, $Y_q = q \Delta Y$. Since DTQWs are essentially discrete waves, it makes sense to choose $\Delta T = \Delta X = \Delta Y$ (cubic lattice in space–time) [30,31] and denote by ϵ the common value of all three space–time steps. Eqs. (5) then transcribe into:

$$\begin{aligned}\psi^L(T_j + \epsilon, X_p, Y_q) &= e^{2i\alpha(X_p)} \cos \theta^- [\cos \theta^+ \psi^L(T_j, X_p + \epsilon, Y_q + \epsilon) + i \sin \theta^+ \psi^R(T_j, X_p - \epsilon, Y_q + \epsilon)] \\ &\quad + i e^{-2i\alpha(X_p)} \sin \theta^- [i \sin \theta^+ \psi^L(T_j, X_p + \epsilon, Y_q - \epsilon) + \cos \theta^+ \psi^R(T_j, X_p - \epsilon, Y_q - \epsilon)], \\ \psi^R(T_j + \epsilon, X_p, Y_q) &= i e^{2i\alpha(X_p)} \sin \theta^- [\cos \theta^+ \psi^L(T_j, X_p + \epsilon, Y_q + \epsilon) + i \sin \theta^+ \psi^R(T_j, X_p - \epsilon, Y_q + \epsilon)] \\ &\quad + e^{-2i\alpha(X_p)} \cos \theta^- [i \sin \theta^+ \psi^L(T_j, X_p + \epsilon, Y_q - \epsilon) + \cos \theta^+ \psi^R(T_j, X_p - \epsilon, Y_q - \epsilon)].\end{aligned}\quad (6)$$

We then let ϵ tend to zero. The differential equations fixing the dynamics of the formal continuous limit are determined by expanding (6) around $\epsilon = 0$ and balancing the zeroth- and first-order terms in ϵ . The zeroth-order terms only balance if $\mathbf{V}^-(\nu)\mathbf{U}^+(\nu) \rightarrow 1$ when $\epsilon \rightarrow 0$. This condition implies that ν has to tend to zero with ϵ . The most interesting scaling turns out to be $\nu = \epsilon$ and the first-order terms then deliver the following differential equations for (ψ^L, ψ^R) :

$$\begin{aligned}(-iBX - \partial_Y - m)\psi^L + i(\partial_T + \partial_X)\psi^R &= 0 \\ i(\partial_T - \partial_X)\psi^L + (iBX + \partial_Y - m)\psi^R &= 0.\end{aligned}\quad (7)$$

This system can be written in the simple so-called manifestly covariant form:

$$(i\gamma^\mu D_\mu - m)\Psi = 0, \quad (8)$$

where the matrices

$$[(\gamma^0)_b^a] = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad [(\gamma^1)_b^a] = i\sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad [(\gamma^2)_b^a] = i\sigma_3 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad (9)$$

$(a, b) \in \{L, R\}^2$, obey the $(2 + 1)$ dimensional flat space–time Clifford algebra relations $\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\eta^{\mu\nu}$ (with $\eta_{\mu\nu} = \text{diag}(1, -1, -1)$), and the covariant derivative D is defined by $D_\mu = \partial_\mu - iA_\mu$, with

$$A_0 = A_1 = 0, \quad A_2 = -BX. \quad (10)$$

The vector potential A generates a uniform magnetic field B orthogonal to the (X, Y) plane and Eq. (8) is the Dirac equation describing the dynamics of a spin 1/2 fermion of mass m and charge -1 coupled to this magnetic field in $(2 + 1)$ -dimensional space–time [32,38–41]. To consider a particle of generic charge q , perform the substitution $B \rightarrow -qB$. The characteristic propagation speed of the Dirac equation (8) is 1 (remember that the time and space variables T and X are dimensionless). In practice, the Dirac equation is used to describe (i) ‘actual’ spin 1/2 particles at high energy [42], in which case the characteristic speed is the speed of light c , and (ii) low-energy excitations of graphene-like materials (also called Dirac materials), whose dispersion relation can be linearized at low energy around the so-called Dirac points [32], in which case the characteristic speed v is the so-called Fermi velocity of the material (in the case of graphene, $v \simeq c/300$). We stress that, in condensed matter, the Dirac equation is thus only an effective description of long wavelength/small wave number excitations and that the Dirac equation certainly becomes invalid at wave numbers comparable to the size of the Brillouin zone.

4. Landau levels

4.1. Hamiltonian of the DTQW

The eigenvalues of the Hamiltonian generating the continuous limit dynamics (8) are the well-known relativistic or Dirac Landau levels. We will now determine the eigenvalues and the eigenstates of the original DTQW for small but finite values of the time- and space-step ϵ .

To be definite, we suppose that space is infinite in both directions and introduce a discrete Fourier transform in the q - (i.e. Y -) direction. We thus write, for all functions f defined on space–time:

$$\hat{f}(T_j, X_p, K) = \sum_{q \in \mathbb{Z}} f(T_j, X_p, Y_q) \exp(-iKY_q), \quad (11)$$

and the inversion relation reads

$$f(T_j, X_p, Y_q) = \frac{1}{2\pi} \int_{-\pi/\epsilon}^{\pi/\epsilon} \hat{f}(T_j, X_p, K) \exp(iKY_q) dK. \quad (12)$$

We recall that $Y_q = q\epsilon$, $q \in \mathbb{Z}$ and the associated wave-vector K is thus a continuous real variable which takes all values in the interval $[-\pi/\epsilon, \pi/\epsilon]$. As ϵ tends to zero, the discrete transform goes into the standard continuous Fourier transform.

Assuming analyticity and considering directly the scaling $\nu = \epsilon$, the exact discrete dynamics of the DTQW reads in Fourier space:

$$\begin{aligned}\hat{\Psi}(T_j + \epsilon, X_p, K) &= \mathbf{W}(\epsilon, B, \theta^+(\epsilon, m), \theta^-(\epsilon, m), X_p - \chi(K, B)) \left(\mathbf{D}(\epsilon) \hat{\Psi} \right)_{(T_j, X_p, K)} \\ &= \left(\mathbf{Q}(\epsilon, B, m) \hat{\Psi} \right)_{(T_j, X_p, K)},\end{aligned}\quad (13)$$

where

$$\chi(K, B) = -\frac{K}{B}, \quad (14)$$

$$\begin{aligned}[\mathbf{W}_b^a(\epsilon, B, \theta^+, \theta^-, X)] &= \begin{bmatrix} e^{i\epsilon BX} \cos \theta^- \cos \theta^+ - e^{-i\epsilon BX} \sin \theta^- \sin \theta^+ & i [e^{i\epsilon BX} \cos \theta^- \sin \theta^+ + e^{-i\epsilon BX} \sin \theta^- \cos \theta^+] \\ i [e^{i\epsilon BX} \sin \theta^- \cos \theta^+ + e^{-i\epsilon BX} \cos \theta^- \sin \theta^+] & -e^{i\epsilon BX} \sin \theta^- \sin \theta^+ + e^{-i\epsilon BX} \cos \theta^- \cos \theta^+ \end{bmatrix},\end{aligned}\quad (15)$$

and

$$[\mathbf{D}_b^a(\epsilon)] = \begin{bmatrix} \exp(\epsilon \partial_X) & 0 \\ 0 & \exp(-\epsilon \partial_X) \end{bmatrix}, \quad (16)$$

with $(a, b) \in \{L, R\}^2$. Eq. (13) defines the operator $\mathbf{Q}(\epsilon, B, m)$.

If a Hamiltonian $\mathbf{H}(\epsilon, B, m)$ generates the dynamics (13), then

$$\hat{\Psi}(T_j + \epsilon, X_p, K) = \left(\exp(-i\epsilon \mathbf{H}(\epsilon, B, m)) \hat{\Psi} \right)_{(T_j, X_p, K)}. \quad (17)$$

The existence of the formal continuous limit presented in the preceding section is traced by the fact that, for all values of B and m , the operator $\mathbf{Q}(\epsilon, B, m)$ tends to unity as ϵ tends to zero. Thus, the logarithm of $\mathbf{Q}(\epsilon, B, m)$ is defined, at least for small enough values of ϵ . A solution to (17) is therefore

$$\mathbf{H}(\epsilon, B, m) = \frac{i}{\epsilon} \ln \mathbf{Q}(\epsilon, B, m), \quad (18)$$

with

$$\ln \mathbf{Q} = \sum_{n=1}^{+\infty} \frac{(-1)^{n-1}}{n} (\mathbf{Q} - 1)^n = \sum_{n=1}^{+\infty} \sum_{k=0}^n \frac{(-1)^{k+1}}{n} \binom{n}{k} \mathbf{Q}^k. \quad (19)$$

Let $\mathbf{H}(\epsilon, B, m) = \sum_{k=0}^{+\infty} \epsilon^k \mathcal{H}^{(k)}(B, m)$ be the expansion of $\mathbf{H}(\epsilon, B, m)$ in powers of ϵ . The expression of some $\mathcal{H}^{(k)}(B, m)$ can be obtained by extracting all the terms of order ϵ^k in (19). It turns out (see Appendix A) to be convenient to represent the Hamiltonian, not in the original basis (b_L, b_R) chosen in spin state, but in the new basis (b_-, b_+) defined by

$$b_- = \frac{1}{\sqrt{2}}(b_L + b_R), \quad b_+ = \frac{1}{\sqrt{2}}(-b_L + b_R). \quad (20)$$

In this new basis, we find

$$[(\mathcal{H}^{(0)})_v^u(B, m)]_{(X, K)} = \begin{bmatrix} m & -i(\partial_X + B(X - \chi(K, B))) \\ i(-\partial_X + B(X - \chi(K, B))) & -m \end{bmatrix} \quad (21)$$

and

$$[(\mathcal{H}^{(1)})_v^u(B, m)]_{(X, K)} = \begin{bmatrix} iB[1/2 + (X - \chi(K, B))\partial_X] & -m\partial_X \\ m\partial_X & -iB[1/2 + (X - \chi(K, B))\partial_X] \end{bmatrix}, \quad (22)$$

where $(u, v) \in \{-, +\}^2$.

The Landau levels of the DTQWs are, by definition, the eigenvalues of the Hamiltonian $\mathbf{H}(\epsilon, B, m)$. These levels are related to the so-called eigenvalues of the DTQW, which are by definition [43,44] the eigenvalues of the operator $\exp(-i\epsilon \mathbf{H}(\epsilon, B, m))$. Thus, if E_l is a Landau level, the corresponding eigenvalue of the DTQW is $\mu_l = \exp(-i\epsilon E_l)$.

4.2. Energy-eigenstates

4.2.1. Zeroth-order energy-eigenstates: relativistic Landau levels

The zeroth-order Hamiltonian $\mathcal{H}^{(0)}(B, m)$ is the Hamiltonian of the Dirac equation (8). Its eigenvalues are the so-called relativistic Landau levels $E_l^{(0)}$ [32,45]. The ground state is labelled by $l = n = 0$, and the excited states by $l = (\lambda, n)$, where $\lambda = \pm$ and $n \in \mathbb{N}^*$. The associated energies are:

$$E_l^{(0)} = \begin{cases} -\text{sgn}(B)m & l = n = 0 \quad \text{ground state} \\ \lambda\sqrt{m^2 + 2|B|n} & l = (\lambda, n) \quad \text{excited states.} \end{cases} \quad (23)$$

The ground-state energy is proportional to the mass of the fermion, as expected for relativistic ‘particles’. This energy has the same sign as $(-1 \times B)$, or qB for a generic charge q . The sign λ of the excited-states energies can be positive or negative, which is expected for Dirac fermions. In the context of high-energy particle physics, the states of negative energy are interpreted as fermions of opposite charge with positive energy. In the context of condensed-matter systems, the states of negative energy correspond to ‘holes’ in the valence band, and the mass corresponds to a ‘gap’ between the valence and conduction bands,² which translates into insulating properties of the material (in the case of graphene, this gap vanishes). The energies of the relativistic Landau levels have a square-root dependence in $|B|n$ (see Fig. 1), in contrast with the linear dependence of the non-relativistic Landau levels.

Let us now discuss the eigenstates of $\mathcal{H}^{(0)}(B, m)$. To each energy level corresponds an eigenspace of infinite dimension. There are two usual choices of basis in these eigenspaces. The first basis is made of vectors which are not only eigenvectors of $\mathcal{H}^{(0)}(B, m)$, but also of the Y component \mathcal{P}_Y of the momentum operator. Note that this operator generates translations in the Y direction and that the mesh on which the DTQW is defined is invariant by such translations. This basis is the one used in the present article. It is best determined by working in the representation introduced in Section 4.1 above and by searching for the eigenvectors of the matrix appearing in (21).

The full computation of the vectors constituting this basis is given in Appendix A. The two spin-components $(\phi^\pm)_l^{(0)}(X, K)$ of these vectors are, as a function of X , two consecutive eigenfunctions of an effective 1D harmonic oscillator (HO) centred at point $\chi(B, K) = -K/B$. The fact that $|\chi(B, K)|$ decreases with $|B|$ reflects the confining properties of B . The HO has pulsation $\omega = 2|B|$, which is linear in $|B|$ as the classical cyclotron pulsation. The HO-eigenfunctions have a characteristic length $a = 1/\sqrt{|B|}$, which again traces the confining properties of B . Regarding the n -dependence of the HO-eigenfunctions, their spatial extension scales as \sqrt{n} . Since the n th eigenfunction has n nodes which can roughly be considered equally spaced [46], these nodes are typically separated by a distance $\sqrt{n}/n = 1/\sqrt{n}$. Fig. 2 displays, for $K = 0$, the probability densities $P_l^{(0)}(X, K) = |(\phi^-)_l^{(0)}(X, K)|^2 + |(\phi^+)_l^{(0)}(X, K)|^2$ associated to the first eigenvectors.

The second usual choice is to use basis vectors which are eigenstates of both $\mathcal{H}^{(0)}(B, m)$ and of a certain gauge-invariant angular momentum [47]. This choice of basis is not natural in the context of this article, because the angular momentum generates rotations, which are not symmetries of the mesh on which the DTQW is defined.

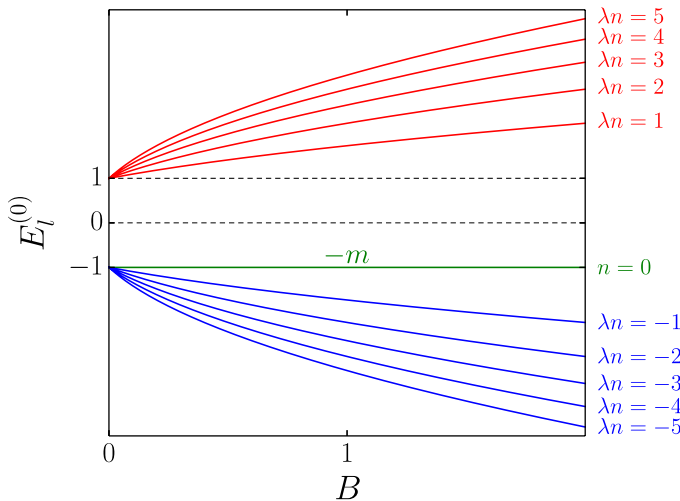


Fig. 1. Relativistic Landau levels $E_l^{(0)}$ as functions of the magnetic field B , for a Dirac fermion of mass $m = 1$ and charge $q = -1$. The ground state is labelled by $l = n = 0$ and the excited states by $l = (\lambda, n)$, with $\lambda = \pm$ and $n \in \mathbb{N}^*$.

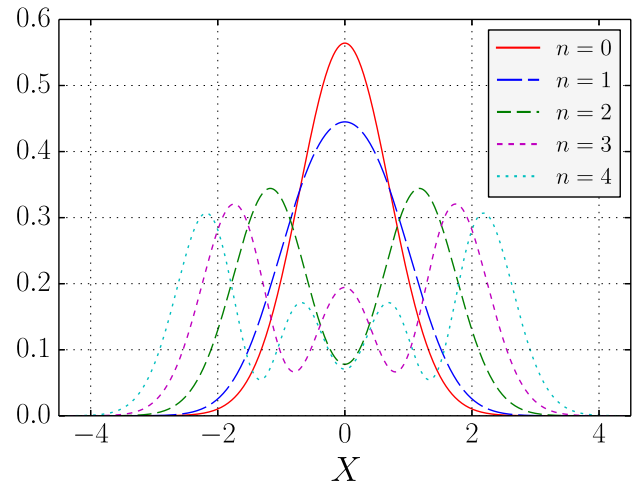


Fig. 2. Probability densities of the Hermite eigenvectors associated to the relativistic Landau levels, as functions of X , for mode $K = 0$, magnetic field $B = 1$, mass $m = 1$ and charge $q = -1$. We have plotted the states $l = n = 0$ and $l = (+, n)$ for $n = 1, 4$.

² The concepts of ‘holes’ and ‘mass gap’ are general to condensed-matter systems, and not specific to Dirac materials.

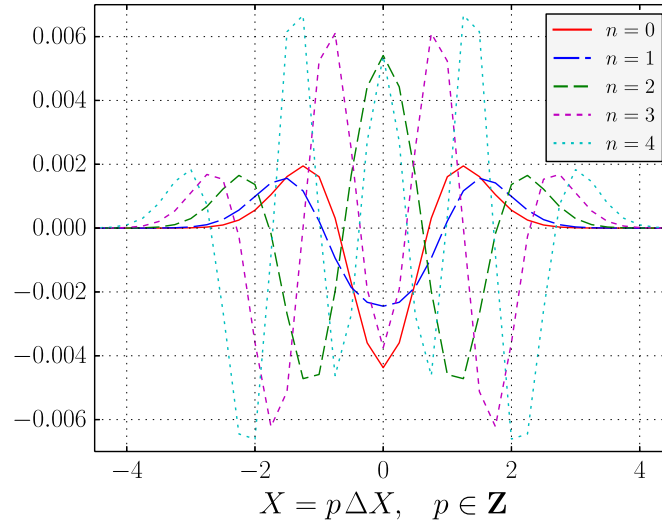


Fig. 3. Differences between the probability densities associated to the Landau levels of the DTQW, computed analytically at first order in the time- and position-step (see Appendix B), and those associated to the standard relativistic Landau levels. All curves correspond to $\Delta X = 0.25$, $K = 0$, $\lambda_n = +$, $B = 1$, $m = 1$, and n labels the energy state.

4.2.2. First-order energy-eigenstates

As discussed in the Introduction, Landau levels play a crucial role in many condensed matter phenomena, for example the quantum Hall effect. If one hopes to simulate these phenomena with DTQWs, it is thus important to check that Landau levels exist, not only for the continuous limit, but also for the discrete walks themselves. The purpose of this section is to provide a perturbative construction of the Landau levels for the DTQWs at first order in the finite time- and position-step ϵ .

The eigenvalues and eigenstates of the full Hamiltonian $\mathbf{H}(\epsilon, B, m)$ can be obtained from those of $\mathcal{H}^{(0)}(B, m)$ by using perturbation theory. Appendix B presents the computation at first order in ϵ . It is found that the first-order corrections to the energy levels identically vanish. However, the first-order corrections to the eigenfunctions do not vanish. The probability density of the energy eigenstates of the DTQW is thus different from the probability density of the relativistic Landau levels corresponding to the continuous Dirac dynamics. Typical results are presented in Fig. 3.

All displayed profiles correspond to the Fourier mode $K = 0$ and are thus symmetric with respect to $X = 0$. Giving ϵ a finite value increases (resp. decreases) the central density for levels corresponding to even (resp. uneven) values of n , the only exception being the fundamental $n = 0$, for which the central density decreases. An n -dependent number of maxima and minima also occur on either side of $X = 0$.

The validity of the analytical perturbative computation of the Landau levels for the DTQW can be supported by numerical simulations. *A priori*, the Hamiltonian $\mathbf{H}^{(r)}(\epsilon, B, m) = \sum_{k=0}^r \epsilon^k \mathcal{H}^{(k)}(B, m)$ describes the dynamics of the DTQW, not at order r , but at order $r + 1$ in ϵ . This is so because the Dirac equation (8) and the corresponding Hamiltonian (21) are obtained from the exact equations defining the DTQW by a Taylor expansion at first order in ϵ , and thus describe the dynamics of the DTQW, not at zeroth order, but at first order in ϵ (at zeroth order in ϵ , the DTQW leaves the state unchanged, see above Section 3). Let now $E_l^{(r)}$ and $\Phi_l^{(r)}(X, K)$ be the l th eigenvalue and the corresponding eigenstate of $\mathbf{H}^{(r)}(\epsilon, B, m)$, both computed at order r in ϵ . If the perturbative computation is correct, the time-evolution of $\Phi_l^{(r)}(X, K)$ by the DTQW should be entirely controlled, at order $r + 1$ in ϵ , by $E_l^{(r)}$. In particular, after one time-step of the exact DTQW, $\Phi_l^{(r)}(X, K)$ should evolve into a state $W_l^{(r)}(X, K)$ which can be approximated, at order $r + 1$ in ϵ , by $\tilde{W}_l^{(r)}(X, K) = e^{-iE_l^{(r)} \times \Delta T} \Phi_l^{(r)}(X, K)$. For each K , the distance between the two functions of X , $W_l^{(r)}(X, K)$ and $\tilde{W}_l^{(r)}(X, K)$, can be evaluated by

$$\delta_l^{(r)}(K) \equiv \frac{\|W_l^{(r)}(\cdot, K) - \tilde{W}_l^{(r)}(\cdot, K)\|}{\|\tilde{W}_l^{(r)}(\cdot, K)\|}, \quad (24)$$

where $\|\cdot\|$ stands for the L^2 norm of a position (X -)dependent function Ψ defined on the lattice:

$$\|\Psi\| = \left[\sum_{p=-p_{\max}(\epsilon)}^{p_{\max}(\epsilon)} (|\psi^L(X_p = p\epsilon)|^2 + |\psi^R(X_p = p\epsilon)|^2) \epsilon \right]^{\frac{1}{2}}, \quad (25)$$

where $p_{\max}(\epsilon)$ scales as $1/\epsilon$.

Figs. 4 and 5 display how $\delta_l^{(r=0)}(K = 0)$ and $\delta_l^{(r=1)}(K = 0)$ scale with ϵ for various values of $l = (+, n)$ and for various values of B . These figures clearly confirm that $\delta_l^{(r=0)}(K = 0)$ scales as ϵ^2 and $\delta_l^{(r=1)}(K = 0)$ scales as ϵ^3 for a large range of ϵ -values which extends well above 10^{-1} . This numerical result thus supports the literal perturbative construction of the Landau levels for the DTQW.

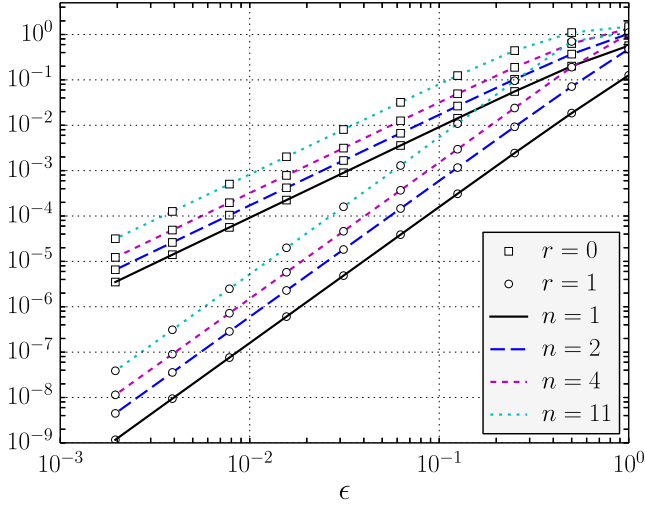


Fig. 4. Distances $\delta_l^{(r=0)}(K=0)$ and $\delta_l^{(r=1)}(K=0)$ as functions of ϵ for various values of $l = (+, n)$, with $B = 1$ and $m = 1$.

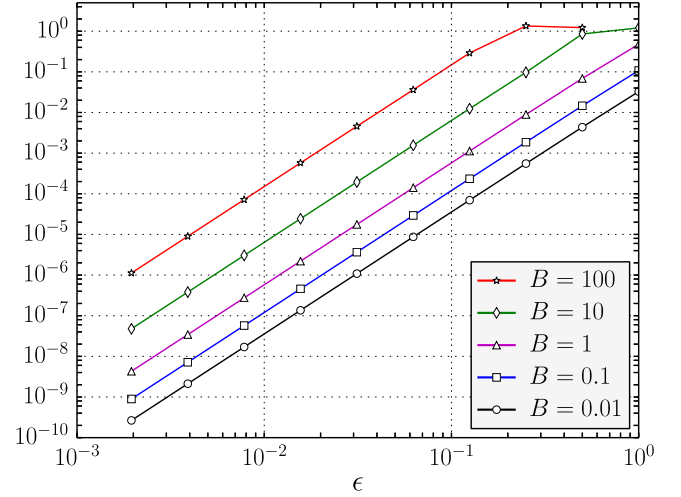


Fig. 5. Distance $\delta_l^{(r=1)}(K=0)$ as a function of ϵ for various values of B , with $l = 0$ and $m = 1$.

5. Non stationary density profiles of the DTQW

Let us now look at some interesting non-stationary density profiles generated by the DTQW dynamics. We will consider simple localized initial states and the corresponding trajectories. These are clearly outside the scope of the continuous limit and provide an outlook of the phenomenology one might expect from an experimental realization of the 2D DTQWs under consideration. These simulations support the interpretation of the parameter B as a magnetic field even outside the continuous limit. In what follows, the time- and space-step ϵ is set to unity so that the instants have coordinates $T_j = j\epsilon = j$ and the vertices of the mesh have coordinates $X_p = p\epsilon = p$ and $Y_q = q\epsilon = q$ with $(j, p, q) \in \mathbb{N} \times \mathbb{Z}^2$. The probability ‘density’ of the walker at time j and point (p, q) is defined by $P(j, p, q) = |\psi^L(j, p, q)|^2 + |\psi^R(j, p, q)|^2$.

We consider initial states of Gaussian probability density

$$G_w(p, q) = \frac{1}{\mathcal{N}_w} N_w(p, q) = \frac{1}{\mathcal{N}_w} \frac{e^{-\frac{p^2+q^2}{2w^2}}}{(\sqrt{2\pi}w)^2}, \quad (26)$$

where w is a strictly positive real number and \mathcal{N}_w is the normalization constant on the 2D-lattice:

$$\mathcal{N}_w = \sum_{p=-p_{\max}}^{p_{\max}} \sum_{q=-q_{\max}}^{q_{\max}} N_w(p, q). \quad (27)$$

By convention, G_0 is the Dirac mass at the origin of coordinates:

$$G_{w=0}(p, q) = \begin{cases} 1 & \text{if } (p, q) = 0 \\ 0 & \text{elsewhere.} \end{cases} \quad (28)$$

Of course, choosing an initial density does not fully specify the initial wave functions $\psi^{L/R}(j=0, p, q)$. We choose the following initial condition, for which the left component of the walker is a real number and carries all the probability density:

$$\begin{aligned} \psi_w^L(j=0, p, q) &= \sqrt{G_w(p, q)} \\ \psi_w^R(j=0, p, q) &= 0. \end{aligned} \quad (29)$$

The p -spread of the distribution at time j is defined by:

$$\sigma_w^p(j) = \left[\sum_{p=-p_{\max}}^{p_{\max}} \sum_{q=-q_{\max}}^{q_{\max}} p^2 P_w(j, p, q) \right]^{\frac{1}{2}} \quad (30)$$

where P_w is the probability density generated by the initial condition (29). The q -spread is defined in a similar manner.

Fig. 6 displays the time evolution of the p -spread for $m = 1$ and different values of B . For all values of B considered in this figure, the q -spread is equal to the p -spread up to the precision of the numerical computation (data not shown). This figure shows that the walk with $B = 0$ propagates ballistically. For non vanishing B , the dynamics is at first ballistic and

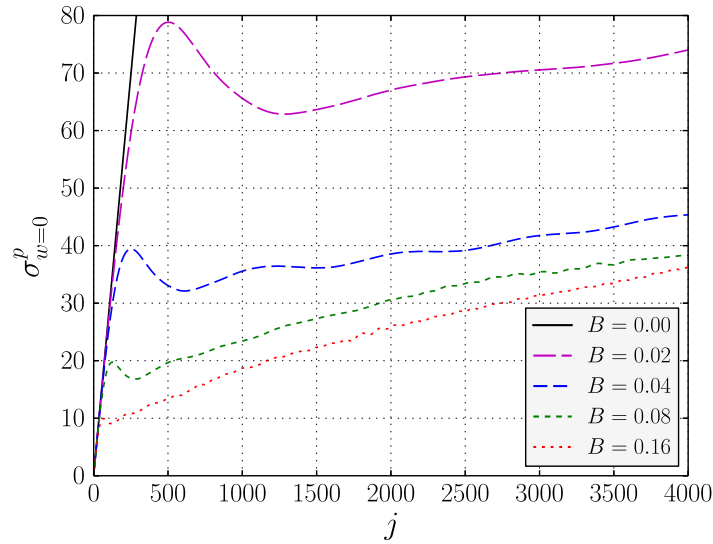


Fig. 6. Time evolution of the p -spread of a Dirac-delta initial condition evolved through our 2D DTQW with $m = 1$, for different values of B .

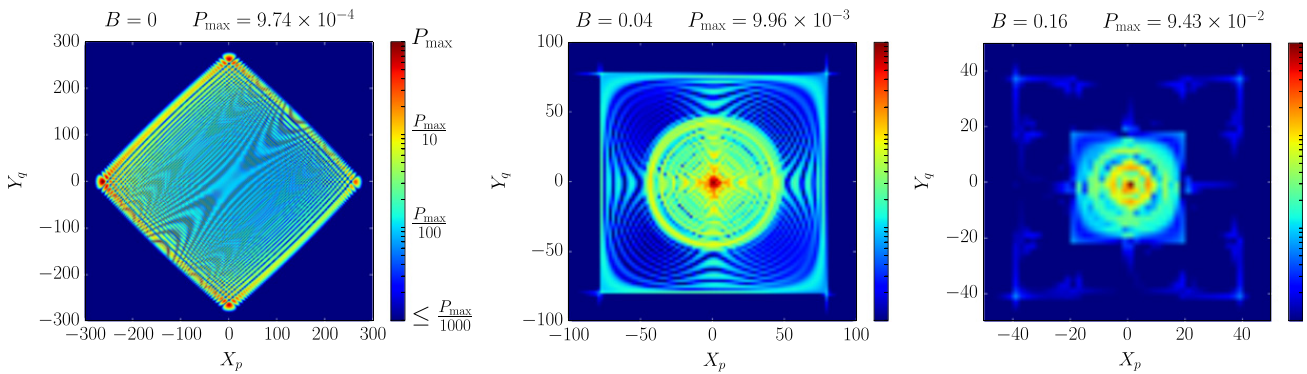


Fig. 7. Probability density of Dirac-delta initial condition evolved through our 2D DTQW with $m = 1$, for different values of B , at time $j = 500$. We show this probability density over 3 decades, from its maximum value P_{\max} down to $P_{\max}/1000$. The initial state having a Dirac-delta probability density carried by a single spin component, the probability density vanishes every 2 steps in both X and Y directions; to have a better visualization of the patterns, we have only plotted the non-vanishing values and (cubically) interpolated them.

then followed by a quasi-confined regime whose radius is, at a given time, a decreasing function of B . Note also that the time during which the DTQW behaves ballistically decreases as B increases.

Fig. 7 shows, for $m = 1$ and different values of B , the probability density contours at time $j = 500$. The zero- B plot (left) shows a maximum located on the left front, which is about 3 times bigger than the right-front local maximum (3.08×10^{-4}), while the top- and down-front local maxima are almost equal (6×10^{-4}). Increasing B localizes the walker in a roughly circularly-symmetric profile within a radius which is (again) a decreasing function of B . Taken together, Figs. 6 and 7 show that the parameter B has on the DTQW the same qualitative effects as those induced by a standard magnetic field on a Dirac fermion moving in continuous space-time. Note that both figures display results which fall well outside the scope of the continuous limit.

Fig. 8 displays contours of the probability density P_w for different values of w . The time is $j = 500$, the mass is equal to unity and the magnetic field vanishes. As w increases, the interference patterns get more and more circular, and the presence of the underlying lattice becomes less and less noticeable.

6. Discussion

We have constructed a family of 2D DTQWs which admits as continuous limit the standard Dirac dynamics of a relativistic spin 1/2 fermion coupled to a constant and uniform magnetic field. We have then shown perturbatively that Landau levels exist for this family, not only in the continuous limit, but also for finite non-vanishing values of the time- and position-step. We have finally presented numerical simulations which (i) support the existence of Landau levels for the DTQWs (ii) suggest that the magnetic interpretation of the discrete dynamics is still valid even outside the continuous limit.

Let us now discuss the results presented in this article. The family of 2D DTQWs considered in this work lives in a two-dimensional Hilbert space *i.e.* the wave function of the walk has two components. This is consistent with standard spinor theory, because irreducible representations of the Clifford algebra in $(2 + 1)$ dimensional space-times are indeed

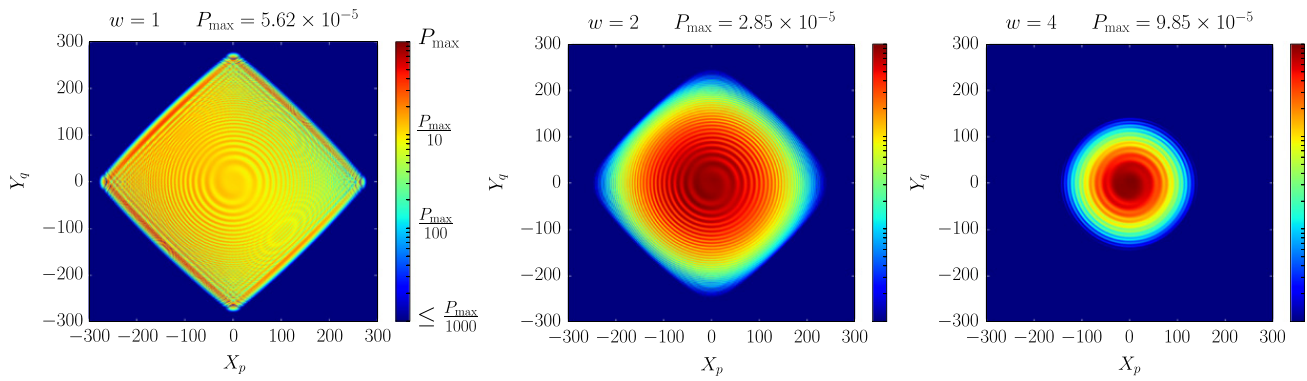


Fig. 8. Probability density, at time $j = 500$, of initial states of increasing width w from left to right, evolved through our 2D DTQW with $m = 1$ and $B = 0$.

two-component spinors. To explore the full 2D lattice, each walk in the family alternates between time-steps in which it propagates in the X -direction and time-steps in which it propagates in the Y -direction. A general walk exploring the 2D lattice in this way is defined by two 2×2 matrices belonging to $SU(2)$ and a phase. Each of the two matrices is characterized by three Euler angles. Thus, a general 2D DTQW with two components is defined by seven real parameters (angles), which generally depend on time and space. For the record, a general 1D DTQW with two components is defined by an arbitrary time- and space-dependent matrix in $SU(2)$ and a phase *i.e.* by four time- and space-dependent parameters (angles). Previous investigations of 1D DTQWs coupled to artificial electric fields teach that the mass of the walk is encoded in the ' θ ' Euler angle and that electric fields are encoded in the phase parameter and in one of the remaining two Euler angles. This experience has been used in constructing the DTQWs studied in this article.

Building the family (1) of DTQWs also required a choice of gauge. We have chosen to work in a gauge where the vector potential depends only on one Cartesian coordinate (X), because this makes it possible to use Fourier transforms with respect to the other Cartesian coordinate (Y), which facilitates the computation of Landau levels. All numerical computations have been carried out in (X, K) -space, where K is the wave number associated to Y . In particular, no Fourier transform with respect to X has been used.

Generally speaking, all results pertaining to the continuous limits of DTQWs can be envisaged from two different points of view. The first one consists in viewing the DTQWs as discrete schemes approximating partial differential equations. The second one consists in viewing the DTQWs as physical systems in their own right, and to consider their continuous limits as tools allowing a greater insight into a fundamentally discrete dynamics. This second point of view appears especially natural in the context of quantum algorithmics, and it has been strengthened by the existence of recent laboratory experiments on DTQWs. This is the point of view we have adopted in the present article. Let us nevertheless discuss rapidly our results from the first point of view.

The Dirac equation is notoriously difficult to discretize [48,49]. Naive symmetric discretizations suffer from the so-called fermion-doubling phenomenon [50]. Other methods are based on the Wilson [51] or staggered [52,53,51] fermion discretizations, but they break chiral symmetry and they also exhibit instabilities and spurious diffusive behaviour. A particularly efficient method has been proposed in Refs. [48,54]. The DTQWs defined by (5) are symmetric discretization. As such, they do exhibit fermion doubling, and this can be checked for example by a direct examination of the dispersion relation associated to (5). Thus, DTQWs are not the best tool to compute accurately numerical solutions of the Dirac equation. This however does not invalidate the use of DTQWs as quantum simulators of condensed-matter physics. Indeed, as already discussed in Section 3, the Dirac equation is used in condensed matter only as an effective description of small wave number excitations and the description of excitations in terms of Dirac fermions moving in continuous space certainly becomes invalid at wave numbers comparable to the size of the Brillouin zone of the material, where the excitations 'see' the size of the underlying lattice. For small wave numbers, the DTQWs do reproduce the Dirac equation. Because of fermion doubling, the DTQWs do *not* reproduce the Dirac equation for wave numbers comparable to the size of the Brillouin zone but for these wave numbers, the Dirac equation is not physically realistic anyway. Thus, fermion doubling does not preclude the use of DTQWs as quantum simulators of small wave number excitation transport in condensed matter. Moreover, since DTQWs are based on a lattice, they are probably the best tool to model, in graphene-like materials, the transport of excitations with wave numbers comparable to the size of the Brillouin zone, which 'see' the underlying lattice [55,56]. Let us finally refer to Ref. [57] for an in-depth presentation of the links existing between QWs, the Dirac equation and the quantum lattice Boltzmann model.

A final, rather technical remark is in order. Obtaining the Dirac equation (8) as the continuous limit of the DTQW considered in this article requires two very different ingredients. The first one is the identification of the indices j , p and q with integers labelling points on a regular Cartesian lattice in space-time. The second ingredient is the choice of the same step ϵ for all three space-time directions. Both ingredients are non trivial and changing them could prove useful in certain contexts. For example, choosing the integers j , p and q as labels of arbitrary, not necessarily Cartesian coordinates could be useful to study DTQWs on manifolds. And having different steps for the different coordinates could help studying solutions of the DTQWs with different variation scales in the time and/or in the two spatial directions.

The conclusions presented in this article are an extension of previous results which show that several families of 1D DTQWs can be interpreted as Dirac spin 1/2 fermions coupled to arbitrary non-constant and non-homogeneous electric and gravitational fields. Preliminary computations show that the family considered in this article can be extended into a larger family where the 2D quantum walker can be coupled to arbitrary electromagnetic fields as well as general relativistic gravitational fields. This extension will be presented elsewhere. Even larger extensions which include other gauge fields should be investigated too. Note that 1D and 2D DTQWs based on four-component wave functions have also been proposed [56]. The connection of these alternate walks to relativistic fermions coupled to electromagnetic fields certainly deserves exploring.

Finally, the above results strongly suggest that DTQWs can be used for spintronics and for quantum simulation of condensed-matter systems under magnetic fields, including possible simulations of the quantum Hall effect.

Appendix A. Relativistic Landau levels

A.1. Normalized eigenfunctions of the squared zeroth-order Hamiltonian

The first step in searching for the relativistic Landau levels is to search for the eigenvalues and eigenvectors of $(\mathcal{H}^{(0)}(B, m))^2$ in basis (b_-, b_+) , because this operator is diagonal in that basis. From (21), one is thus led to solving the system

$$\mathcal{E}^\pm \phi^\pm = \left(-\frac{\partial^2}{\partial X^2} + \frac{1}{2} M \omega^2 (X - \chi(K, B))^2 \right) \phi^\pm, \quad (\text{A.1})$$

where (ϕ^-, ϕ^+) are the two components of some eigenfunction of $(\mathcal{H}^{(0)}(B, m))^2_{(X, K)}$ in basis (b_-, b_+) , E^2 is the corresponding eigenvalue of $(\mathcal{H}^{(0)}(B, m))^2$ and

$$M = 1/2, \quad \omega = 2|B|, \quad \mathcal{E}^\pm = E^2 - m^2 \pm B. \quad (\text{A.2})$$

Suppose first that both ϕ^- and ϕ^+ do not vanish identically. Eq. (A.1) then imply

$$E^2 = \left(n^\pm + \frac{1}{2} \right) \times 2|B| + m^2 \mp B, \quad (\text{A.3})$$

$$\phi^\pm(X, K) = \phi_{n^\pm}^{HO}(X - \chi(K, B)), \quad (\text{A.4})$$

where $n^\pm \in \mathbb{N}$ and ϕ_n^{HO} is the normalized n th 1D harmonic oscillator energy eigenstate, which reads

$$\phi_n^{HO}(X) = \frac{e^{-\frac{X^2}{2a^2}}}{\pi^{1/4} \sqrt{2^n n!} \sqrt{a}} H_n(X/a), \quad \text{with } H_n(X) = (-1)^n e^{X^2} \partial_X^n e^{-X^2}, \quad a = \frac{1}{\sqrt{|B|}}. \quad (\text{A.5})$$

Eqs. (A.3) lead to $(n^+ - n^-) = \text{sgn}(B)$. The eigenvectors of $(\mathcal{H}^{(0)}(B, m))^2$ are thus of the form

$$B > 0 : [(\Pi_n^{B>0})^u(X, K)] = \begin{pmatrix} \alpha \phi_{n-1}^{HO}(X - \chi(K, B)) \\ \beta \phi_n^{HO}(X - \chi(K, B)) \end{pmatrix} \quad (\text{A.6})$$

$$B < 0 : [(\Pi_n^{B<0})^u(X, K)] = \begin{pmatrix} \beta \phi_n^{HO}(X - \chi(K, B)) \\ \alpha \phi_{n-1}^{HO}(X - \chi(K, B)) \end{pmatrix}, \quad (\text{A.7})$$

where $u \in \{-, +\}$, $n \in \mathbb{N}^*$ and α, β are two complex numbers obeying $|\alpha|^2 + |\beta|^2 = 1$ (normalized eigenvectors).

The squared Hamiltonian $(\mathcal{H}^{(0)}(B, m))^2$ also admits eigenvectors with one identically vanishing spin component in basis (b_-, b_+) . For these eigenvectors, Eq. (A.1) degenerate into a single equation. The non-vanishing spin component, say ϕ^- (resp. ϕ^+) is then identical to an arbitrary eigenfunction ϕ_n^{HO} of the harmonic oscillator Hamiltonian and the corresponding eigenvalue of $(\mathcal{H}^{(0)}(B, m))^2$ is $\mathcal{E}_n^2 = (n + \frac{1}{2}) \times 2|B| + m^2 + B$ (resp. $\mathcal{E}_n^2 = (n + \frac{1}{2}) \times 2|B| + m^2 - B$).

A.2. Normalized eigenfunctions of the zeroth-order Hamiltonian

Any normalized eigenfunction of the Hamiltonian $\mathcal{H}^{(0)}(B, m)$ is also a normalized eigenfunction of its square and is thus one of the functions determined above. The discrimination between the functions that are actual eigenfunctions of

$\mathcal{H}^{(0)}(B, m)$ and those which are not is best made by computing directly the action of the Hamiltonian $\mathcal{H}^{(0)}(B, m)$ on all eigenfunctions of $(\mathcal{H}^{(0)}(B, m))^2$.

One thus finds the ground-state energy $E_0^{(0)} = -\text{sgn}(B)m$ and the corresponding normalized eigenfunction $\Phi_0^{(0)}(X, K) = \phi_0^{HO}(X - \chi(K, B)) b_{\text{sgn}(B)}$, which has an identically vanishing spin component. The other eigenstates are labelled by an integer $n \in \mathbb{N}^*$ and a sign $\lambda = \pm 1$. The eigenvalues are $E_{\lambda,n}^{(0)} = \lambda\sqrt{m^2 + 2|B|n}$ and the normalized eigenstates, that we note $\Phi_{\lambda,n}^{(0)}(X, K)$, are of the form (A.6), (A.7) with

$$\alpha_{\lambda,n} = -i\sqrt{\frac{2|B|n}{(E_{\lambda,n} - \text{sgn}(B)m)^2 + 2|B|n}}, \quad \beta_{\lambda,n} = \frac{E_{\lambda,n} - \text{sgn}(B)m}{\sqrt{(E_{\lambda,n} - \text{sgn}(B)m)^2 + 2|B|n}}. \quad (\text{A.8})$$

Appendix B. First-order corrections to the eigenvalues and eigenstates of the zeroth-order Hamiltonian

As seen in Appendix A, the eigen-elements of $\mathcal{H}^{(0)}(B, m)$ are labelled by $l = 0$ or (λ, n) , with $\lambda = \pm$ and $n \in \mathbb{N}^*$.³ We now apply perturbation theory for the Hamiltonian $\mathbf{H}^{(1)}(\epsilon, B, m) = \mathcal{H}^{(0)}(B, m) + \epsilon \mathcal{H}^{(1)}(B, m)$. To lighten notations, we define

$$\langle l' | \mathcal{H}^{(1)} | l \rangle \equiv \int_{-\infty}^{+\infty} dX \sum_{\substack{u=\pm \\ v=\pm}} \left((\Phi_l^{(0)}(X, K))^u \right)^* (\mathcal{H}^{(1)}(B, m))^u_{v|(X,K)} (\Phi_{l'}^{(0)}(X, K))^v. \quad (\text{B.1})$$

At first order in ϵ , the eigenstates of $\mathbf{H}^{(1)}(\epsilon, B, m)$ can be written $\Phi_l^{(1)} = \Phi_l^{(0)} + \epsilon \Delta_l^{(1)}$, with:

$$\Delta_0^{(1)} = \sum_{\lambda'=\pm 1} \sum_{\substack{n' \neq 0 \\ n' \neq n}} \frac{\langle \lambda', n' | \mathcal{H}^{(1)} | 0 \rangle}{E_0^{(0)} - E_{\lambda',n'}^{(0)}} \Phi_{\lambda',n'}^{(0)}, \quad (\text{B.2})$$

$$\Delta_{\lambda,n}^{(1)} = \sum_{\lambda'=\pm 1} \sum_{\substack{n' \neq 0 \\ n' \neq n}} \frac{\langle \lambda', n' | \mathcal{H}^{(1)} | \lambda, n \rangle}{E_{\lambda,n}^{(0)} - E_{\lambda',n'}^{(0)}} \Phi_{\lambda',n'}^{(0)} + \frac{\langle -\lambda, n | \mathcal{H}^{(1)} | \lambda, n \rangle}{E_{\lambda,n}^{(0)} - E_{-\lambda,n}^{(0)}} \Phi_{-\lambda,n}^{(0)} + \frac{\langle 0 | \mathcal{H}^{(1)} | \lambda, n \rangle}{E_{\lambda,n}^{(0)} - E_0^{(0)}} \Phi_0^{(0)}, \quad (\text{B.3})$$

having made the standard phase choice that $\Delta_l^{(1)}(\cdot, K)$ is orthogonal to $\Phi_l^{(0)}(\cdot, K)$.

The Hamiltonian matrix elements can be written, for $(n, n') \in (\mathbb{N}^*)^2$,

$$\begin{aligned} \langle \lambda', n' | \mathcal{H}^{(1)} | \lambda, n \rangle &= \frac{iB}{2} (\alpha_{\lambda',n'}^* \alpha_{\lambda,n} - \beta_{\lambda',n'}^* \beta_{\lambda,n}) \delta_{n',n} + iB (\alpha_{\lambda',n'}^* \alpha_{\lambda,n} I_{n'-1,n-1} - \beta_{\lambda',n'}^* \beta_{\lambda,n} I_{n',n}) \\ &\quad + m (\beta_{\lambda',n'}^* \alpha_{\lambda,n} J_{n',n-1} - \alpha_{\lambda',n'}^* \beta_{\lambda,n} J_{n'-1,n}), \end{aligned} \quad (\text{B.4})$$

where $\delta_{n',n}$ is the Kronecker symbol and where, for $(n, n') \in \mathbb{N}^2$,

$$I_{n',n} = \int_{-\infty}^{+\infty} dX X \phi_{n'}^{HO}(X) \partial_X [\phi_n^{HO}(X)], \quad (\text{B.5})$$

$$J_{n',n} = \int_{-\infty}^{+\infty} dX \phi_{n'}^{HO}(X) \partial_X [\phi_n^{HO}(X)]. \quad (\text{B.6})$$

Expression (B.4) can be extended to $l = 0$ and $l' = 0$, having preliminarily defined

$$\alpha_0 = 0, \quad \beta_0 = 1. \quad (\text{B.7})$$

Thanks to the following recurrence relations:

$$a\sqrt{2} \partial_X [\phi_n^{HO}(X)] = \sqrt{n} \phi_{n-1}^{HO}(X) - \sqrt{n+1} \phi_{n+1}^{HO}(X), \quad (\text{B.8})$$

$$2XH_n(X) = 2n H_{n-1}(X) + H_{n+1}(X), \quad (\text{B.9})$$

³ In this labelling, we forget about the quantum number K , which can be considered as a parameter in our problem. Indeed, this quantum number K corresponds to an essential degeneracy of the full Hamiltonian of the DTQW, namely $\mathbf{H}^{(1)}(\epsilon, B, m)$; this degeneracy will hence not be removed by our perturbative computation.

we can compute integrals (B.5) and (B.6), and finally find the following expressions for the Hamiltonian matrix elements:

$$\langle \lambda', n' | \mathcal{H}^{(1)} | \lambda, n \rangle = \begin{cases} \operatorname{sgn}(B) \sqrt{n-1} \left[\frac{iB}{2} (\alpha_{\lambda',n'}^* \alpha_{\lambda,n} \sqrt{n'} - \beta_{\lambda',n'}^* \beta_{\lambda,n} \sqrt{n}) + \frac{m}{a\sqrt{2}} \beta_{\lambda',n'}^* \alpha_{\lambda,n} \right] & \text{for } n' = n-2 \\ -\operatorname{sgn}(B) \frac{m\sqrt{n}}{a\sqrt{2}} (\alpha_{\lambda',n}^* \beta_{\lambda,n} + \beta_{\lambda',n}^* \alpha_{\lambda,n}) & \text{for } n' = n \\ \operatorname{sgn}(B) \sqrt{n+1} \left[\frac{iB}{2} (-\alpha_{\lambda',n'}^* \alpha_{\lambda,n} \sqrt{n} + \beta_{\lambda',n'}^* \beta_{\lambda,n} \sqrt{n'}) + \frac{m}{a\sqrt{2}} \alpha_{\lambda',n'}^* \beta_{\lambda,n} \right] & \text{for } n' = n+2 \\ 0 & \text{otherwise,} \end{cases} \quad (\text{B.10})$$

which again can be extended to $l = 0$ and $l' = 0$. Hence, the sums in Eqs. (B.2) and (B.3) reduce to sums over $n' = n \pm 2$, and, because of the relation between α_l and β_l (Eqs. (A.8) and (B.7)), the first-order corrections to the energies vanish, i.e. $\langle l | \mathcal{H}^{(1)} | l \rangle = 0$.

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1.2.4 Publication [2]: Quantum walks and discrete gauge theories

— ABSTRACT —

In this publication, we present a new family of 2D DTQWs which coincides, in the continuum limit, with the Dirac dynamics of a relativistic spin-1/2 fermion coupled to a generic electromagnetic field in dimension 2. We extend the electromagnetic interpretation beyond the continuum limit, by showing the existence of (i) a lattice gauge invariance, (ii) a lattice invariant quantity, and (iii) conserved currents on the lattice. This allows us to suggest lattice equivalents to Maxwell's equations. Summing-up, we build a DTQW-based Abelian U(1) lattice gauge theory, in (1+2)D. We recover, through numerical simulations, known phenomenology, both a standard one, associated to standard electromagnetic fields, and a less standard one, associated to periodically-driven system, which, in particular, matches qualitatively with recent results on DTQWs, both in one and two dimensions.

1.2.4.1 Short but detailed review and comments

This is the paper where, in Section II, we give the proper compact form of the 2D DTQW-operator with generic electromagnetic coupling, Eq. (1.11). The continuum electromagnetic interpretation is given in Section II: the continuum limit of the scheme is that of a spin-1/2 Dirac fermion, with mass m and charge -1 , coupled to an electromagnetic potential with contravariant components $A_0 \sim \Delta\alpha$, $A_1 \sim -\Delta\xi^{(1)}$ and $A_2 \sim -\Delta\xi^{(2)}$, where, as for the 1D case, the symbol ' \sim ' means that between the A_μ 's and the phase shifts, there is a factor ϵ_A (see Eqs. (1.4b) and (1.4c)) which is taken equal to the spacetime-lattice step ϵ_t and goes to zero in the continuum, where the discrete coordinate p_1 (p in the paper) becomes the continuous one x (X in the paper), and p_2 (q in the paper) becomes y (Y in the paper). In addition to this formal continuum limit, shown on the evolution equation for the quantum particle, we show numerically that the limit is correct, as follows: we run the MQTD scheme with an initial condition whose time evolution through the Dirac equation (for constant and uniform crossed electric and magnetic fields) can be computed in closed form, and we compare this explicit continuum time evolution to the MQTD time evolution for decreasing spacetime-lattice steps, see Figs. 1 and 2 of the paper.

After a generalization, in Section III, of the 1D results on the lattice gauge invariance (Eq. (8) of the paper generalizes Eq. (1.5)), and gauge invariants (Eq. (11) of the paper generalizes Eq. (1.9)), we present, in Section 4, a lattice version of (the inhomogeneous³⁶) Maxwell's equations (Eq. (20) of the paper), which ensure the current conservation on the lattice (Eq. (17) of the paper). These lattice Maxwell equations yield the standard ones in the continuum limit. This means we can theoretically quantum simulate, in the continuum limit, a first-quantized Abelian gauge theory: the spin-1 bosons³⁷ evolve through Maxwell's equations, and the fermions through the Dirac equation.

Section 5 is devoted to the phenomenal properties of the 2D electromagnetic DTQW beyond the continuum limit. A detailed discussion of the two different 'small parameters'

³⁶The homogeneous ones are satisfied *by construction* on the lattice.

³⁷The spin-1 boson is, in this (1+2)D case, (A_0, A_1, A_2) , and thus has three internal states.

is now in order. The first small parameter, ϵ_t , is the spacetime-lattice step. The second small parameter, ϵ_A , is that associated to the lattice gauge field. The continuum limit requires that both ϵ_t and ϵ_A tend to zero. But one can envisage taking only one of the two parameters as actually small, either (i) large wavefunctions, i.e. $\epsilon_t \simeq 0$, or (ii) weak gauge-field variations, i.e. a gauge field which varies on temporal and spatial scales much larger than ϵ_t , i.e. $\epsilon_A \simeq 0$ ^{38,39}:

1. If we are in situation (ii), we recover known phenomenology. First, we recover the classical $\mathbf{E} \times \mathbf{B}$ drift [82], even if (i) is not satisfied – i.e. even if the walker ‘sees’ the edge of the Brillouin zone –, which is a priori non-obvious; see Figs. 4 (bottom propagating front) and 5 of the paper. Second, we recover tight-binding phenomenology [197, 198, 84]: Bloch oscillations for a vanishing magnetic field in Fig. 3, and top propagating front for a non-vanishing magnetic field in Fig. 4. In contrast with the classical $\mathbf{E} \times \mathbf{B}$ drift, this tight-binding phenomenology *demands* that (i) be unsatisfied at some point in the dynamics, i.e. that the walker ‘see’ the edge of the Brillouin zone⁴⁰. This tight-binding phenomenology is qualitatively not that unexpected (see the third item in Subsection 1.2.1).
2. If (ii) is not satisfied, i.e. if the gauge-field variations ‘see’ the edge of the Brillouin zone, i.e. reaches a sizeable fraction of 2π , then the dynamics is strongly dependent on whether the electric and magnetic field are *exact* rational fractions of 2π , see Figs. 6 and 7 of the paper. This phenomenology has already been studied in depth in dimension 1, for a sole electric field, by Cedzich et al. (2013) [88], and has been studied more recently in dimension 2 for a sole magnetic field by Yalçınkaya et al. (2015) [89], and, for a sole electric field, by Bru et al. (2016) [79].

³⁸More formally, what is ‘weak’ is the discrete temporal or spatial derivative of the gauge field; in the Abelian case, these discrete derivatives correspond essentially to the electric and magnetic synthetic fields defined on the lattice.

³⁹One can obviously refine this picture by ‘dezooming’ only on either the temporal or the spatial lattice. Such a distinction is necessary for a mapping to CTQWs.

⁴⁰The $\mathbf{E} \times \mathbf{B}$ drift is ‘blind’ to (i), while the tight-binding phenomenology demands non-(i).

Quantum walks and discrete gauge theories

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A particular example is produced to prove that quantum walks can be used to simulate full-fledged discrete gauge theories. A family of two-dimensional walks is introduced and its continuous limit is shown to coincide with the dynamics of a Dirac fermion coupled to arbitrary electromagnetic fields. The electromagnetic interpretation is extended beyond the continuous limit by proving that these discrete-time quantum walks (DTQWs) exhibit an exact discrete local $U(1)$ gauge invariance and possess a discrete gauge-invariant conserved current. A discrete gauge-invariant electromagnetic field is also constructed and that field is coupled to the conserved current by a discrete generalization of Maxwell equations. The dynamics of the DTQWs under crossed electric and magnetic fields is finally explored outside the continuous limit by numerical simulations. Bloch oscillations and the so-called $\mathbf{E} \times \mathbf{B}$ drift are recovered in the weak-field limit. Localization is observed for some values of the gauge fields.

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I. INTRODUCTION

Discrete-time quantum walks (DTQWs) are formal generalizations of classical random walks. They were first studied in a systematic fashion by Meyer [1], whereas similar but different quantum discrete dynamics was first considered in Refs. [2–4]. DTQWs have been realized experimentally with a wide range of physical objects and setups [5–11] and are studied in a large variety of contexts, ranging from fundamental quantum physics [11,12] to quantum algorithmics [13,14], solid-state physics [15–18], and biophysics [19,20].

Particular quantum cellular automata [21,22], among which DTQWs [23] are defined on various regular lattices [24], are known to reproduce, in the continuous limit, the dynamics of free Dirac fermions in one, two, or three spatial dimensions. Recently, such connections have been extensively extended to Dirac fermions coupled to gauge fields [25–32]. More precisely, one-dimensional (1D) DTQWs have been proposed which reproduce the dynamics of Dirac fermions coupled to arbitrary electric [25–27] and/or gravitational [28–31] fields, and a two-dimensional (2D) DTQW simulating the coupling of a Dirac fermion to a constant uniform magnetic field was proposed in Ref. [32].

For all existing DTQWs, the gauge fields are encoded in the time and space dependence of the operator advancing the fermion in discrete space-time. They act on the fermion but the dynamics of the fermion has no effect on the gauge fields. In other words, the gauge fields play the roles of imposed external fields. In particular, they are not advanced by their own discrete dynamical equations, as is for example the case in lattice gauge theories (LGTs). The main purpose of this article is to remedy this problem and introduce a complete self-consistent model based on DTQWs where both the fermions and the fields are advanced by compatible discrete dynamical equations.

The first brick in such a self-consistent model is a family of DTQWs which exhibit an exact discrete gauge invariance associated to a certain group G and which describes the

coupling of Dirac fermions to arbitrary G -gauge fields. The existing literature contains only one such family. The associated gauge group is $U(1)$ and the DTQWs describe the coupling of 1D Dirac fermions to arbitrary electric fields. Electromagnetism is, however, degenerate in one dimension. There is no magnetic field and Maxwell equations reduce to the Maxwell-Gauss equation, which contains no time derivative. We therefore switch to two dimensions and introduce a family of DTQWs whose continuous limit coincides with the dynamics of a Dirac fermion coupled to 2D arbitrary electromagnetic fields. We then show that these DTQWs admit (i) an exact discrete $U(1)$ gauge invariance, (ii) a gauge-invariant discrete electromagnetic tensor (i.e., gauge-invariant electric and magnetic fields defined on the discrete lattice of the DTQWs), and (iii) a discrete conserved current. We finally combine the discrete electromagnetic tensor and the discrete conserved current into discrete gauge-invariant Maxwell equations which imply current conservation. This literal material is complemented by numerical computations which explore how the DTQWs which serve as a basis for the whole construct behave outside the continuous limit. Even outside this limit, the DTQWs display in the weak-field regime several well-known features usually associated to standard continuous motions in electromagnetic fields, including Bloch oscillations and the so-called $\mathbf{E} \times \mathbf{B}$ drift. In the regime of strong fields, the discrete dynamics depends crucially on whether the fields are rational or not, as expected from previous work on other DTQWs [26,27,33]. We finally discuss possible applications of our results to quantum simulation and quantum algorithmics and highlight how the discrete gauge theory based on DTQWs differs from standard LGTs.

II. ELECTROMAGNETIC DTQWS

A. The walks and their formal continuous limit

We consider DTQWs with two-component wave functions (2D coin or spin space) defined on a discrete $(1+2)$ -dimensional space-time where instants are labeled by the index $j \in \mathbb{N}$ and space points on the 2D square lattice are labeled by the indices $(p, q) \in \mathbb{Z}^2$. The evolution equation for the wave

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function reads

$$\Psi_{j+1,p,q} = \mathbf{U}(\theta^-(\epsilon_m, m), \epsilon_A A_{j,p,q}^2, \epsilon_A A_{j,p,q}^0) \mathbf{T}_2 \\ \times \mathbf{U}(\theta^+(\epsilon_m, m), \epsilon_A A_{j,p,q}^1, 0) \mathbf{T}_1 \Psi_{j,p,q}, \quad (1)$$

where the action of the shift operators \mathbf{T}_1 and \mathbf{T}_2 on the 2D wave function $\Psi_{j,p,q} = (\psi_{j,p,q}^-, \psi_{j,p,q}^+)^T$ (the superscript T denotes the transposition) is

$$\mathbf{T}_1 \Psi_{j,p,q} = (\psi_{j,p+1,q}^-, \psi_{j,p-1,q}^+)^T, \quad (2) \\ \mathbf{T}_2 \Psi_{j,p,q} = (\psi_{j,p,q+1}^-, \psi_{j,p,q-1}^+)^T.$$

The coin operator $\mathbf{U}(\theta, \xi, \alpha) \in \mathbf{U}(2)$ is the product of three simpler operators:

$$\mathbf{U}(\theta, \xi, \alpha) = e^{i\alpha} \mathbf{1} \times \mathbf{C}(\theta) \times \mathbf{S}(\xi) \\ = \begin{bmatrix} e^{i\alpha} & 0 \\ 0 & e^{i\alpha} \end{bmatrix} \begin{bmatrix} \cos \theta & i \sin \theta \\ i \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} e^{i\xi} & 0 \\ 0 & e^{-i\xi} \end{bmatrix}. \quad (3)$$

The first operator $\mathbf{S}(\xi)$ is a spin-dependent phase shift parametrized by the angle ξ , the second operator $\mathbf{C}(\theta)$ is a standard coin operator with angle θ , and the third operator performs a global multiplication by the phase α .

In the continuous limit, the parameter m , which enters the definition of the constant angles $\theta^\pm(\epsilon_m, m) = \pm \frac{\pi}{4} - \epsilon_m \frac{m}{2}$, is interpreted as the mass of the walk and the three angles A^0 , A^1 , and A^2 , which may depend on (j, p, q) , are interpreted as the components of an electromagnetic potential. The positive parameters ϵ_m and ϵ_A are introduced to trace the importance of m and A and tend to zero in the continuous limit. All the parameters and angles are dimensionless.

The formal continuous limit of the DTQWs, Eq. (1), can be determined by the method used in Refs. [28,29,32,34–36]: we first introduce a (dimensionless) spacetime-lattice step ϵ_l and interpret any (j, p, q) -dependent quantity $Q_{j,p,q}$ as the value taken by a function $Q(X^0, X^1, X^2)$ at time $X_j^0 = j\epsilon_l$ and spatial position $(X_p^1 = p\epsilon_l, X_q^2 = q\epsilon_l)$. We then consider the scaling $\epsilon_m = \epsilon_A = \epsilon_l = \epsilon$ and let ϵ tend to zero. We expand Eq. (1) at first order in ϵ around the generic space-time point (X_j^0, X_p^1, X_q^2) . For the continuous limit to exist, the zero-order terms of the expansion must balance each other; this constraint is automatically verified by the DTQWs defined by Eq. (1).

The first-order terms of the expansion in ϵ deliver the differential equation which determines the dynamics of the walker in the continuous limit. This equation reads

$$(i\gamma^\mu \mathcal{D}_\mu - m)\Psi = 0. \quad (4)$$

Here, the γ matrices are defined by $\gamma^0 = \sigma_1$, $\gamma^1 = i\sigma_2$, and $\gamma^2 = i\sigma_3$, where the Pauli matrices are

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (5)$$

and $\mathcal{D}_\mu = \partial_\mu - iA_\mu$ is the covariant derivative associated to Maxwell electromagnetism, with $A_0 = A^0$, $A_1 = -A^1$, and $A_2 = -A^2$. The γ matrices satisfy the (1+2)-dimensional flat-space-time Clifford algebra $\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\eta^{\mu\nu} \mathbf{1}$, where $[\eta^{\mu\nu}] = \text{diag}(1, -1, -1)$ is the Minkowskian metric. Equation (4) is the Dirac equation describing the dynamics of a spin-1/2 fermion of mass m and charge -1 coupled to the electromagnetic potential A . To consider a

generic charge g , just perform the substitution $A \rightarrow -gA$. In Eq. (4), the characteristic speed is 1 because we have chosen the same value ϵ_l for the dimensionless time and space steps.

B. Rate of convergence towards the continuous limit

Since the formal continuous limit is obtained from the DTQW dynamics by keeping terms that are first order in ϵ , one expects the discrepancy between a solution of the DTQW and the corresponding solution of the Dirac equation to scale as ϵ^2 . This can be tested numerically by computing the distance between an exact time-independent solution of the Dirac equation and the time evolution of this solution by the DTQW. For simplicity we choose $A_0 = -EX^1$, $A_1 = 0$, and $A_2 = -BX^1$, which do not depend on X^2 and generate crossed, constant, and uniform electric and magnetic fields. The Hamiltonian and the momentum in the X^2 direction can then be diagonalized simultaneously. For $E = 0$, the eigenstates are called relativistic Landau levels [32]. For $0 < \beta = E/B < 1$, the eigenstates can be obtained from the relativistic Landau levels by a boost of velocity β . The resulting eigenstates $\phi_{l,K}(X^1, X^2) = \Phi_l(X^1, K) \exp(iKX^2)$ and eigenenergies $\mathcal{E}_{l,K}$ are labeled by a couple (l, K) where $l = 0$ or $l = (\pm, n)$ with $n \in \mathbb{N}^*$ and K is the eigenmomentum in the X^2 direction. In one time step ϵ , the DTQW evolves $\Phi_l(X^1, K)$ into a certain function $W_l(X^1, K)$ which should be approximated, at first order in ϵ , by $\tilde{W}_l(X^1, K) = \exp(-i\mathcal{E}_{l,K} \times \epsilon) \Phi_l(X^1, K)$. For each K , the distance between the two functions $W_l(\cdot, K)$ and $\tilde{W}_l(\cdot, K)$ can be evaluated by

$$\delta_l(K) \equiv \frac{\|W_l(\cdot, K) - \tilde{W}_l(\cdot, K)\|}{\|\tilde{W}_l(\cdot, K)\|}, \quad (6)$$

where $\|\cdot\|$ stands for the L^2 norm of a position-dependent (i.e., X^1 -dependent) function Ψ defined on the lattice:

$$\|\Psi\| = \left[\sum_{p=-p_{\max}(\epsilon)}^{p_{\max}(\epsilon)} (|\psi^-(X_p^1)|^2 + |\psi^+(X_p^1)|^2) \epsilon \right]^{\frac{1}{2}}, \quad (7)$$

where $p_{\max}(\epsilon)$ scales as $1/\epsilon$. Figures 1 and 2 display how $\delta_l(K=0)$ scales with ϵ for various values of $l = (+, n)$ and for various values of β , having fixed $B = 1$ and $m = 1$. These figures clearly confirm that $\delta_l(K=0)$ scales as ϵ^2 for a large range of ϵ values.

III. DISCRETE GAUGE INVARIANCE AND ELECTROMAGNETIC FIELDS

The discrete equations (1) are invariant, not only under a global phase change of the spinor Ψ , but also under the more general, local gauge transformation

$$\Psi_{j,p,q} \rightarrow \Psi'_{j,p,q} = e^{-i\phi_{j,p,q}} \Psi_{j,p,q}, \quad (8)$$

$$(A_\mu)_{j,p,q} \rightarrow (A'_\mu)_{j,p,q} = (A_\mu)_{j,p,q} - (d_\mu \phi)_{j,p,q},$$

where the three “discrete-derivative” (finite-difference) operators d_μ are defined by

$$d_0 = (L - \Sigma_2 \Sigma_1)/\epsilon_A, \quad d_1 = \Delta_1/\epsilon_A, \quad d_2 = \Delta_2 \Sigma_1/\epsilon_A, \quad (9)$$

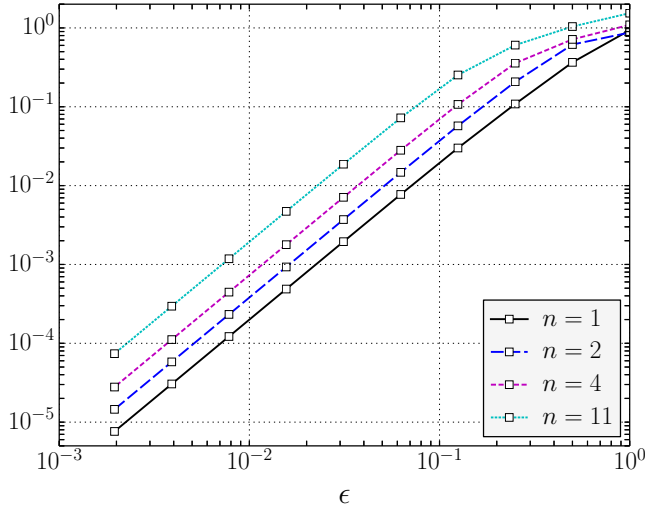


FIG. 1. Distance $\delta_l(K=0)$ as a function of ϵ for various values of $l = (+, n)$.

with

$$\begin{aligned} (LQ)_{j,p,q} &= Q_{j+1,p,q}, \\ (\Sigma_1 Q)_{j,p,q} &= (Q_{j,p+1,q} + Q_{j,p-1,q})/2, \\ (\Sigma_2 Q)_{j,p,q} &= (Q_{j,p,q+1} + Q_{j,p,q-1})/2, \\ (\Delta_1 Q)_{j,p,q} &= (Q_{j,p+1,q} - Q_{j,p-1,q})/2, \\ (\Delta_2 Q)_{j,p,q} &= (Q_{j,p,q+1} - Q_{j,p,q-1})/2. \end{aligned} \quad (10)$$

This local gauge invariance is a discrete version of the standard continuous $U(1)$ local gauge invariance associated to electromagnetism and displayed by the Dirac equation (4). A straightforward computation now shows that the three quantities F_{01} , F_{02} , and F_{12} defined by

$$(F_{\mu\nu})_{j,p,q} = (d_\mu A_\nu)_{j,p,q} - (d_\nu A_\mu)_{j,p,q} \quad (11)$$

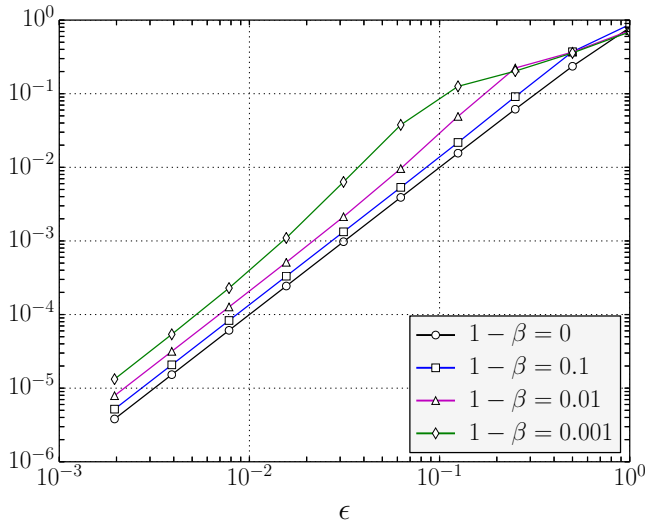


FIG. 2. Distance $\delta_l(K=0)$ as a function of ϵ for various values of β .

are gauge invariant. These are clearly discrete versions of the usual electromagnetic tensor components $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. In particular, F_{01} and F_{02} represent respectively the two components E_1 and E_2 of a 2D discrete electric field [parallel to the plan of the (p, q) grid] and the component F_{12} represents a discrete magnetic field B_3 perpendicular to the plan of the (p, q) grid.

IV. GAUGE-INVARIANT CONSERVED CURRENT AND DISCRETE MAXWELL EQUATIONS

Let

$$\tilde{\Psi}_{j,p,q} = U(\theta^+(\epsilon_m, m), \epsilon_A A_{j,p,q}^1, 0) T_1 \Psi_{j,p,q} \quad (12)$$

be the state of the walker after the shift along the p direction and the first coin operation. The spatial density associated to $\tilde{\Psi}_{j,p,q}$ is

$$\tilde{\Psi}_{j,p,q}^\dagger \tilde{\Psi}_{j,p,q} = |\Psi_{j,p+1,q}^-|^2 + |\Psi_{j,p-1,q}^+|^2. \quad (13)$$

Introducing notations $\rho = |\Psi^-|^2 + |\Psi^+|^2$ and $\mathcal{J} = |\Psi^+|^2 - |\Psi^-|^2$, we can rewrite the previous equation as

$$\tilde{\rho}_{j,p,q} = (\Sigma_1 \rho)_{j,p,q} - (\Delta_1 \mathcal{J})_{j,p,q}. \quad (14)$$

The same computation carried out for $\Psi_{j+1,p,q} = U(\theta^-(\epsilon_m, m), \epsilon_A A_{j,p,q}^2, \epsilon_A A_{j,p,q}^0) T_2 \tilde{\Psi}_{j,p,q}$ results in

$$(L\rho)_{j,p,q} = (\Sigma_2 \tilde{\rho})_{j,p,q} - (\Delta_2 \tilde{\mathcal{J}})_{j,p,q}. \quad (15)$$

Inserting Eq. (14) into Eq. (15) gives the discrete conservation equation

$$(L\rho)_{j,p,q} = (\Sigma_2 \Sigma_1 \rho)_{j,p,q} - (\Sigma_2 \Delta_1 \mathcal{J})_{j,p,q} - (\Delta_2 \tilde{\mathcal{J}})_{j,p,q}. \quad (16)$$

All operators defined in Eqs. (10) commute with each other; in particular, $\Sigma_2 \Delta_1 = \Delta_1 \Sigma_2$, so that the conservation equation can be written

$$(D_\mu J^\mu)_{j,p,q} = 0, \quad (17)$$

where the new finite-difference operators D_μ read

$$D_0 = d_0, \quad D_1 = d_1 \Sigma_2, \quad D_2 = \Delta_2 / \epsilon_A, \quad (18)$$

and the probability current on the square lattice is given by

$$\begin{aligned} J_{j,p,q}^0 &= \rho_{j,p,q} = |\psi_{j,p,q}^+|^2 + |\psi_{j,p,q}^-|^2, \\ J_{j,p,q}^1 &= \mathcal{J}_{j,p,q} = |\psi_{j,p,q}^+|^2 - |\psi_{j,p,q}^-|^2, \\ J_{j,p,q}^2 &= \tilde{\mathcal{J}}_{j,p,q} = |\tilde{\psi}_{j,p,q}^+|^2 - |\tilde{\psi}_{j,p,q}^-|^2. \end{aligned} \quad (19)$$

In the continuous limit, the discrete conservation equation (17) becomes the standard conservation equation $\partial_\mu j^\mu = 0$ of the 2D Dirac current $j^\mu = \bar{\Psi} \gamma^\mu \Psi$, with $\bar{\Psi} = \Psi^\dagger \gamma^0$.

Having identified the discrete current J^μ and the finite-difference operators involved in the discrete continuity equation (17) makes it possible to write the following simple discrete equivalent to Maxwell equations:

$$(D_\mu F^{\mu\nu})_{j,p,q} = (J^\nu)_{j,p,q}, \quad (20)$$

which connects the discrete electromagnetic tensor $(F_{\mu\nu})_{j,p,q}$ to the discrete current $(J^\mu)_{j,p,q}$. Indeed, Eq. (20) has the standard Maxwell equations as a continuous limit and ensures the conservation of the discrete current $(J^\mu)_{j,p,q}$ because

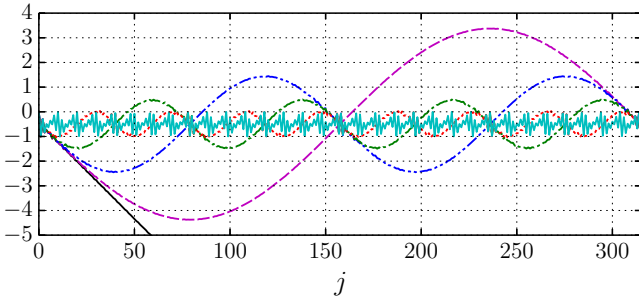


FIG. 3. Time evolution of the p mean for E walks with $\epsilon_A E = 0$ (black, solid), 0.02 (magenta, dashed), 0.04 (blue, dot-dot-dashed), 0.08 (green, dot-dashed), 0.16 (red, dotted), and 0.64 (cyan, solid). The oscillating period is $T_{\text{Bloch}} = 2\pi/(\epsilon_A E)$ with an error of less than one lattice site.

it implies $(D_\nu J^\nu)_{j,p,q} = (D_\nu D_\mu F^{\mu\nu})_{j,p,q}$, which vanishes identically because operators D_μ commute with each other and because $(F^{\mu\nu})_{j,p,q}$ is antisymmetric.

V. SIMULATIONS OUTSIDE THE CONTINUOUS LIMIT

We now focus on constant and uniform discrete electric and magnetic fields, for example, $\mathbf{E} = E\mathbf{u}_1$ and $\mathbf{B} = B\mathbf{u}_3$ where \mathbf{u}_1 and \mathbf{u}_3 are two unitary vectors respectively along the p (or X^1) axis of the grid and perpendicular to the plane of the grid. A potential generating these fields is $(A_0)_{j,p,q} = -Ep\epsilon_l$, $(A_1)_{j,p,q} = 0$, $(A_2)_{j,p,q} = -Bp\epsilon_l$. Walks with $B = 0$ ($E = 0$) are referred to as E walks (B walks). Walks with $E \neq 0$ and $B \neq 0$ are referred to as EB walks.

Quantities of particular interest are the probability of presence of the walker $P_{j,p,q} = |\psi_{j,p,q}^-|^2 + |\psi_{j,p,q}^+|^2$ and, for $l = p$ or q , its time-dependent l mean (l spread), defined as the time-dependent average (square-rooted average) value of l (l^2) computed with P as time-dependent probability law on (p, q) .

All computations are carried out with $\epsilon_m m = 1$, $\epsilon_l = 1$ and the same simple initial condition: $\psi^-(j=0, p, q) = 1$ if $(p, q) = (0, 0)$ and 0 elsewhere; $\psi^+(j=0, p, q) = 0$ for all (p, q) . The only remaining free parameters are $\epsilon_A E$ and $\epsilon_A B$. As now discussed, DTQWs for which both $\epsilon_A E$ and $\epsilon_A B$ are much smaller than unity exhibit regimes which resemble continuous physics. DTQWs with larger values of $\epsilon_A E$ and $\epsilon_A B$ behave very differently, and can even localize.

Figure 3 shows the time evolution of the p mean for several E walks. For $\epsilon_A E = 0$, the p mean varies linearly with time. This ballistic transport is typical of homogeneous DTQWs, i.e., DTQWs whose coin operators do not depend on the space-time point. Moreover, transport occurs towards negative values of p only because the initial state has a vanishing ψ^+ . For $\epsilon_A E \neq 0$, the p mean oscillates in time around the value $X^1 = -0.5$ [37] with a period which coincides with the so-called Bloch period $T_{\text{Bloch}} = 2\pi/(\epsilon_A E)$ with an error smaller than one time step. Bloch oscillations were first predicted by Bloch [38] and Zener [39] for electrons moving in solids. They have been observed in 2D photonic lattices [40] and 1D electric DTQWs [26,41]. As $\epsilon_A E$ reaches a sizable fraction of 2π , T_{Bloch} becomes of the order of a few time steps.

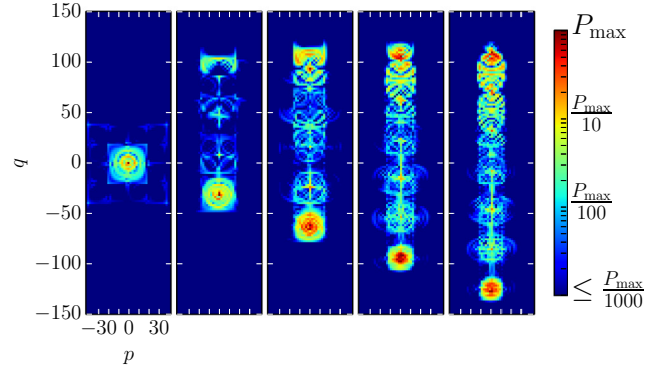


FIG. 4. Probability density, at time $j = 500$, for EB walks with $\epsilon_A B = 0.16$. From left to right, $\epsilon_A E = 0, 0.01, 0.02, 0.03, 0.04$, and $P_{\text{max}} = 0.0943, 0.0578, 0.0209, 0.0181, 0.0178$. The bottom front corresponds essentially to the classical $\mathbf{E} \times \mathbf{B}$ drift.

Another oscillating mode with period of the order of one time step then appears and dominates the dynamics.

Figure 4 displays the probability densities at time $j = 500$ for several EB walks with $\epsilon_A B = 0.16$. For $\epsilon_A E = 0$ (left), the walker is quasicontained around the origin, with a typical radius which slowly increases with the time j and is, at each j , a decreasing function of $\epsilon_A B$ (data not shown; see Ref. [32] for details). When $\epsilon_A E \neq 0$, the walker spreads in the q direction, up and down. The bottom front propagates with a speed which coincides with E/B , as supported by Fig. 5. This corresponds to the classical so-called $\mathbf{E} \times \mathbf{B}$ drift of a charged particle under crossed constant and uniform electric and magnetic fields (see, e.g., Ref. [42]). The roughly circularly symmetric “Landau profile” obtained for $\epsilon_A E = 0$ seems to be transported at the drift velocity. The behavior of the top front is counterintuitive from the classical perspective. The top front spreads with a speed which seems independent of $\epsilon_A E$. A very similar behavior has already been pointed out in Ref. [43] for quantum particles moving under the influence of superimposed electric and magnetic fields in a 2D periodic potential with tight binding.

Previous work on DTQWs coupled to electric or magnetic fields [26,27,33] has shown that walks with field values which are rational multiples of 2π (“rational fields”) follow very peculiar dynamics. Figure 6 displays the q spread of EB walks

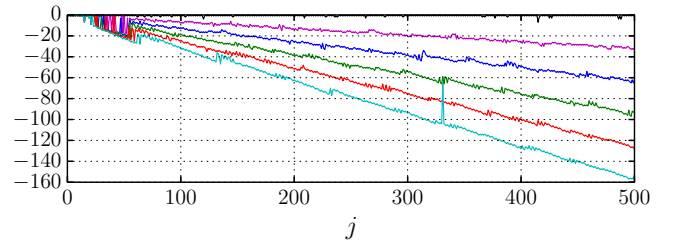


FIG. 5. Time evolution of the q coordinate of the bottom-front local maximum of the probability density, for EB walks with $B = 0.16$. From top to bottom, $E = 0$ (black), 0.01 (magenta), 0.02 (blue), 0.03 (green), 0.04 (red), and 0.05 (cyan). This maximum propagates in the direction of $\mathbf{E} \times \mathbf{B}$ (up to small oscillations in the p direction) and with speed E/B up to a 1% precision.

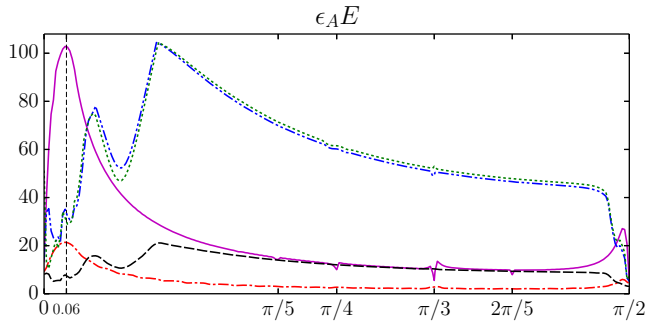


FIG. 6. Evolution of the q spread as a function of $\epsilon_A E$ for EB walks with magnetic field $\epsilon_A B = 0.16$ at times $j = 100$ (red, dot-dashed) and $j = 500$ (magenta, solid), $\epsilon_A B = 1$ at times $j = 100$ (black, dashed) and $j = 500$ (blue, dot-dot-dashed), and $B = \pi/3 \simeq 1.047$ (green, dotted) at time $j = 500$.

as a function of $\epsilon_A E$ at two times and different values of $\epsilon_A B$. For $\epsilon_A B = 0.16$, which is not a rational multiple of 2π , there is a weak E -field regime (from $\epsilon_A E = 0$ to $\epsilon_A E \simeq 0.06$) in which the q spread increases essentially linearly with $\epsilon_A E$. This is the regime of Figs. 4 and 5. For $\epsilon_A E > 0.06$, the q spread decreases considerably. This weak E -field regime breaks down partially for $\epsilon_A B = 1$ and completely for $\epsilon_A B = \pi/3$, while the q spreading is essentially enhanced for strong values of $\epsilon_A E$. For $\epsilon_A E = \pi/2$ and values of $\epsilon_A B$ which are not rational multiples of 2π , the walk seems to be almost localized in q (this is also the case in the p direction; data not shown). Figure 7 focuses on this apparent localization. In the long-time limit, the walker spreads ballistically for values of $\epsilon_A B$ which are rational multiples of 2π . This ballistic spreading is considerably reduced (quasilocization) for $\epsilon_A B = \pi/4 + \varepsilon$ and $\pi/3 + \varepsilon$, and the walk seems to really localize for $\epsilon_A B = \pi/2 + \varepsilon$. The p spread displays the same qualitative behaviors (data not shown).

VI. CONCLUSION AND DISCUSSION

We have introduced a family of 2D DTQWs which coincides, in the continuous limit, with the dynamics of a Dirac fermion coupled to arbitrary electromagnetic fields. The wave function of these DTQWs has two components and the DTQWs explore the 2D square lattice by advancing alternately in each of the orthogonal directions. Similar, albeit simpler, 2D DTQWs have been discussed, for example, in Refs. [36,44]. We have shown that the DTQWs introduced in this article possess an exact discrete local $U(1)$ gauge invariance, a discrete gauge-invariant conserved current, and a discrete gauge-invariant electromagnetic field, and that field and current can be coupled by discrete generalizations of Maxwell equations. We have also explored the behavior of the DTQWs outside the continuous limit, under weak and strong

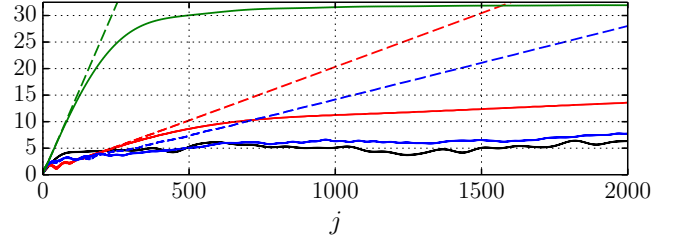


FIG. 7. Time evolution of the q spread for EB walks with $\epsilon_A E = \pi/2$ and $\epsilon_A B = 0.16$ (black, solid), $\pi/4$ (red, dashed), $\pi/4 + \varepsilon$ (red, solid), $\pi/3$ (blue, dashed), $\pi/3 + \varepsilon$ (blue, solid), $\pi/2$ (green, dashed), and $\pi/2 + \varepsilon$ (green, solid), with $\varepsilon = 0.04$.

fields. For weak fields, we have observed discrete versions of the Bloch oscillations and of the so-called $\mathbf{E} \times \mathbf{B}$ drift. We have also observed localization for some higher values of the fields.

The results of this article prove that DTQWs can be used to build full-fledged discrete gauge theories and that laboratory experiments based on quantum walks can, at least in principle, simulate these theories (see, for example, Ref. [26] for a discussion of a quantum-walk experiment already carried out which simulates Dirac fermions coupled to 1D electric fields). On the technical side, the construction we have presented should naturally be extended, not only to Maxwell electromagnetism in four-dimensional space-time, but also to other Yang-Mills gauge theories. Developing second-quantized versions of these discrete theories should also prove interesting.

A full comparison of possible discrete gauge theories based on DTQWs with the usual LGTs [45,46] is beyond the scope of this article. Let us simply mention two differences. First, unlike the “U” parallel transporters in LGTs, gauge fields do not have to be added by hand to the DTQW dynamics, as the connection is already part of the basic definition of DTQWs and most DTQWs are by definition locally gauge invariant [29]. Second, the difference operators (discrete derivatives) which arise in conjunction with the local gauge invariance of DTQWs are more complicated than the usual finite-difference operators used in lattice gauge theories. The mathematical properties of discrete gauge theories based on DTQWs are thus probably very different from the mathematical properties of LGTs.

Finally, DTQWs are useful in a much wider context than high-energy or condensed-matter physics. DTQWs are in particular universal building blocks of quantum algorithms [47] and our results therefore have implications for quantum information. For example, the exploration of graphs by DTQWs could be influenced by creating discrete gauge fields on these graphs. Indeed, not only do gauge fields influence the transport of single DTQWs, but gauge theories provide a novel manner to implement interaction between DTQWs.

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One-dimensional DTQWs in non-Abelian Yang-Mills fields (Publication [3])

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2.1 On non-Abelian Yang-Mills gauge theories

MOTIVATIONS

The aim of this long introduction to Publication [3] is to give a review on the history of Yang-Mills gauge theories, from the discovery of the electric and magnetic forces to standard lattice gauge theories.

Originally introduced in 1954 by Yang and Mills [199] to describe the attractive force that holds protons and neutrons together in the atomic nucleus¹, non-Abelian Yang-Mills gauge theories soon appeared to be a suitable framework to describe the weak force and the strong force between quarks^{2,3}, see Subsection 2.1.1. Non-Abelian Yang-Mills gauge theories have also found applications in condensed-matter physics [203].

2.1.1 Fundamental forces and particle physics

2.1.1.1 The electromagnetic force, a long-range force

• Pre field-notion works

¹For some notes on the (nuclear) isospin degree of freedom and its history, see Appendix J.

²Nucleons are made of quarks, hold together by strong interactions. The electromagnetic force is described by an *Abelian* Yang-Mills gauge theory. A gauge theory is a theory in which the state of the system is invariant under some group of spatiotemporally-dependent (i.e. local) transformations of some of its degrees of freedom. A given such transformation relates two different possible *gauges* to describe the same state of the system. Gravity can also be viewed as a gauge theory, but the attempts to formulate it as a Yang-Mills-type gauge theory remain inconclusive.

³Yang-Mills theories historically arose in a quantum framework. They can however be developed non-quantumly, see Ref. [200]. In second-quantized physics, they have to be renormalized, i.e. they only make sense if the ‘physical’, i.e. measured coupling constant of the interaction, is considered as a function of the energy scale of the physical phenomenon. This energy scale is simply the input total energy of the system if one can consider this system isolated during the phenomenon; in the case of a particle-physics experiment, this total energy is the total kinetic energy given to the particles by accelerating them, before we make them collide. The proof that non-Abelian Yang-Mills theories of the electroweak type are renormalizable was given in 1971 by ’t Hooft, first in the massless [201] and then in the massive [202] gauge-field case.

★ *Electrostatics and Coulomb's force law between electric charges*

In 1785, Coulomb stated, in his *First Memoir on Electricity and Magnetism*⁴, the law which was then to be named after him: the force exerted by a macroscopic or mesoscopic point-like sample of matter of total charge q_1 , on another one of total charge q_2 located at distance r from the first sample, is given by⁵

$$\mathbf{F}_{\text{Coulomb}} = k_e \frac{q_1 q_2}{r^2} \mathbf{u}, \quad (2.1)$$

where \mathbf{u} is the unit vector from the first to the second point-like sample, and k_e is Coulomb's constant, which was later recognized to be

$$k_e = \frac{1}{4\pi\epsilon_0}, \quad (2.2)$$

where ϵ_0 is the vacuum permittivity. The experiment made to prove such a law used a torsion balance. The $1/r^2$ dependence had already been suggested in 1762 by Cavendish, but his experiment was not fully conclusive.

★ *Magnetostatics and Ampère's force law between electric currents*

In 1820, Ørsted made the famous discovery that a magnetic needle is acted on by an electric current⁶. Soon after, the same year, the experimental and theoretical work of Biot and Savart⁷, and then Ampère⁸, lead to the expression of the force exerted by a current element on another one, now called Ampère's force law, and which is the magnetic analogue of Coulomb's force law.

• **Faraday's induction law and concept of (magnetic) field**

The following notes were essentially produced after reading a short paper on the history of the concept of field, by Assis, Ribeiro and Vannucci⁹ [ARV], which contains interesting quotes by Faraday and Maxwell.

In 1831, Faraday presented orally, to the English Royal Society of London, his exper-

⁴See the following scan of the original document, written in French, https://books.google.fr/books?id=by5EAAAACAAJ&pg=PA569&redir_esc=y#v=onepage&q&f=false.

⁵Strictly speaking, a sufficient condition for this law to hold is the spherical symmetry of the charge distribution of each sample. This is what, strictly speaking, 'point-like' means.

⁶Both the original Latin version and the English translation of his 1820 paper "Experiments on the effect of a current of electricity on the magnetic needle", can be found in the 1981 book by Franksen, *H. C. Ørsted – a man of the two cultures*.

⁷See Biot's speech to the French Academy of science, reproduced in the following scan of the second volume of a collection of memoirs of physics published by the French Society of physics in 1885, page 80 and followings, <http://www.ampere.cnrs.fr/bibliographies/pdf/1885-P286.pdf>. See in particular the footnote page 80 for historical details on Biot and Savart's scientific notes. The formula giving the magnetic field (this notion appeared later, in the work of Faraday) created by a current distribution was later (and is currently) named after Biot and Savart. By generating such a magnetic field, this current distribution acts on a charge distribution through the (magnetic part of the) Lorentz force.

⁸See the reproduced speech that follows that of Biot in the aforementioned collection. This work gave its name, in particular, to this Maxwell equation which involves the dynamics (i.e. the time derivative) of the electric field.

⁹See [http://www.ifi.unicamp.br/~assis/The-field-concepts-of-Faraday-and-Maxwell\(2009\).pdf](http://www.ifi.unicamp.br/~assis/The-field-concepts-of-Faraday-and-Maxwell(2009).pdf).

iments showing magnetic induction¹⁰, i.e., roughly speaking, that moving some magnetic material near charges causes their displacement around the material. In this work, he introduces the notion of ‘magnetic curves’ or ‘lines of magnetic force’, but a “clear definition” only appeared, according to [ARV], in a 1852 paper. In 1846, he officially used the word ‘(magnetic) field’, but again, a “clear definition” only appeared, according to [ARV], in a 1850 paper. Faraday “does not seem to have utilized the expression electric field in his works” [ARV].

According to Faraday, the magnetic field was “any portion of space traversed by magnetic power” [ARV], and “he would probably understand” [ARV] the electric field the same way.

• Maxwell’s equations: a dynamics for the electromagnetic field

In 1864, Maxwell gave a presentation to the English Royal Society of London, on “A dynamical theory of the electromagnetic field” [204]. In this work, he presented what are nowadays called Maxwell’s equations, under the form of 20 equations with 20 unknowns, using quaternions¹¹, and showed that, in the absence of charges, one can combine these equations to obtain the same wave propagation equation for both the electric and the magnetic field, whose characteristic speed parameter coincides numerically with the speed of light¹². In his *Treatise on Electricity and Magnetism* of 1873, Maxwell rewrites the equations under the form of 8 equations. The equations were later given their modern form¹³ by Heaviside in 1884, see *The Maxwellians*, by Hunt.

These equations are the result of a synthesis, into local equations, of the work of Ampère, Gauss, Helmholtz, Thomson and Faraday, among others, and was made possible by the introduction of a lacking piece in Ampère’s theorem (see below), the *displacement current*, which corresponds to the time derivative of the electric field \mathbf{E} , up to a constant multiplicative factor¹⁴.

The 4 Maxwell equations are the local forms of 4 corresponding integral theorems derived by Maxwell’s aforementioned predecessors:

¹⁰See a scan of his *Experimental researches in electricity*, published in 1844, at https://docs.lib.noaa.gov/rescue/Rarebook_treasures/QC503F211839_PDF/QC503F211839v2.pdf, or at <https://archive.org/details/experimentalrese00faraiala>. I haven’t seen a single literal equation in these notes.

¹¹Maxwell had already published, in 1861, his “molecular-vortices” – in his own words – to model magnetism, which can simply be viewed as a fluid model of electromagnetism. This work is both a graphical development and a mathematization of the ideas of Faraday on magnetic lines of forces. For the original paper, see https://upload.wikimedia.org/wikipedia/commons/b/b8/On_Physical_Lines_of_Force.pdf. One can actually already extract from this work the modern form of Maxwell’s equations, which use vectorial analysis operators, namely the divergence and the curl. In this paper, Maxwell also suggested that light is an electromagnetic phenomenon. For reviews on Maxwell’s fluid model of magnetism, see, e.g., the paper by Brady and Anderson <https://arxiv.org/pdf/1502.05926.pdf>, and the following presentation <https://www.pprime.fr/sites/default/files/pictures/pages-individuelles/D2/germain/Cargese2004.pdf>.

¹²The first conclusive measure of the speed of light, which determines its correct order of magnitude, is that of Rømer and Huygens in 1675. The value was later more accurately measured by Bradley in 1729, Fizeau in 1849, and Foucault in 1862, two years before Maxwell’s speech.

¹³4 vectorial equations with 2 vectorial unknowns, 1 pseudo-vectorial unknown, and 1 scalar unknown.

¹⁴The displacement current is the time derivative of the *displacement field* \mathbf{D} , which is indeed proportional to the electric field only in the case of (i) vacuum (down to the smaller experimentally testable scales, i.e. even below atomic scales) or of (ii) linear, homogeneous and isotropic materials (above some mesoscopic scale). The proportionality relation reads $\mathbf{D} = \varepsilon \mathbf{E}$, where the proportionality factor ε is the permittivity of the considered material, or simply ε_0 in the case of vacuum. The permittivity of some material needs to be measured experimentally, and can sometimes be theoretically derived, by suitable mesoscopic averages, as a function of the permittivity of vacuum and microscopical data regarding the molecular composition of the material.

1. Gauss's flux theorem (1813), which states that the flux of the electric field across a closed surface is proportional¹⁵ to the total charge contained *within* that closed surface. The local equivalent is that the divergence of the electric field is proportional to the charge density.
2. Gauss's flux theorem for magnetism¹⁶, which states that the flux of the magnetic field around a closed surface always vanishes, which is equivalent to the non-existence of magnetic monopoles, i.e., in analogy with electric phenomena, of magnetic charges¹⁷. The local equivalent is that the divergence of the magnetic field is always zero¹⁸.
3. Faraday's induction law, already mentioned above, which states, roughly speaking, that the time variation of the magnetic flux across a surface induces the surrounding electric charges to move around the magnetic material, about the direction of the average magnetic field generated by the material. The local equivalent is that the time derivative of a magnetic field corresponds to the curl of the electric field. The problems pointed out by Einstein¹⁹ in 1905, regarding the change of point of view²⁰ in such an induction experiment [205], lead him to formulate special relativity, i.e., following earlier work by Poincaré, to realise, with *Gedankenexperiments*, that time is not absolute but depends on the observer, so that Galilean transformations must be substituted by Lorentz transformations²¹.
4. Ampère's circulation theorem, which states that the flux of some current density across a surface determines, through the magnetic permeability²², the circulation of the magnetic field along the edge of this surface. With the additional displacement current introduced by Maxwell, the local version of this theorem becomes the Maxwell-Ampère equation, which states that the magnetic field 'rotates' about the direction

¹⁵The proportionality factor is $1/\varepsilon$.

¹⁶The law already appeared in the work of Lagrange, in 1773.

¹⁷Here are some lines from Wikipedia's web page on Gauss's flux theorem for magnetism: "This idea, of the nonexistence of magnetic monopoles, originated in 1269 by Petrus Peregrinus de Maricourt. His work heavily influenced William Gilbert, whose 1600 work *De Magnete* spread the idea further. In the early 1800s Michael Faraday reintroduced this law, and it subsequently made it into James Clerk Maxwell's electromagnetic field equations."

¹⁸In French teaching, this local equation is sometimes called Maxwell-Thomson equation, because of later work carried out by Thomson: in a problem, Thomson had to add a term to the vector potential he had derived for the divergence of the magnetic field to be zero, because he wanted Maxwell equations to hold. Fitzgerald gave physical interpretations for the addition of such a term. See the book *Cambridge and the rise of mathematical physics*, which cites Buchwald's writings, <http://www.hss.caltech.edu/content/jed-z-buchwald>, http://www.persee.fr/doc/rhs_0151-4105_1998_num_51_1_1308.

¹⁹For the complete work of Einstein, translated in English, one may go to Princeton's dedicated website, <http://einsteinpapers.press.princeton.edu>.

²⁰With Galilean frame changes, which consider time is absolute i.e. does not depend on the observer.

²¹These transformations had already been introduced by Lorentz, as transformations that led Maxwell's equations invariant, and then Poincaré before Einstein already gave some physical interpretations for the different times involved in the transformations. The key idea of Einstein's work, is to realize that what had to be modified were not Maxwell's equations, but Newton's dynamical law, up to then sacralized, and this fundamentally needed a replacement of the Galilean transformations relating inertial frames by these Lorentz transformations that leave Maxwell's equations unchanged. To give a rough picture, this idea came naturally with a previous first key idea, namely to abolish the notion of ether, so that the problem could not come from Maxwell's equations since we had *nothing* to know about a hypothetical medium in which electromagnetic waves would propagate, and whose misunderstanding would give us wrong equations.

²²On can define the magnetic induction $\mathbf{H} = \mathbf{B}/\mu$, where the magnetic permeability μ is a scalar in the case of (i) vacuum, $\mu = \mu_0$, or (ii) a linear, homogeneous and isotropic material, as for the relation between the displacement field and the electric field.

specified by the vectorial sum of currents and displacement currents (i.e. temporal variations of the electric field).

• Quantum electrodynamics

With the advent of quantum mechanics, (non-relativistic) quantum electrodynamics developed, with early contributions by Pauli. This enabled to account for emission and absorption spectra of several atoms, and was one of the great successes of quantum mechanics. Also, the theory was formulated as a consequence of Weyl's gauge principle applied to the global phase invariance of quantum mechanics.

To overcome the problems of the Klein-Gordon equation, straightforwardly derivable with the help of the correspondence principle, Dirac managed to write down a relativistic quantum-mechanical equation for fermions, in which one could implement minimal coupling, and this equation successfully addressed the deviations from experiments that were obtained by deriving the spectrum of the hydrogen atom from the Schrödinger equation.

On pre-QFT relativistic quantum electrodynamics (QED), one may consult Bjorken and Drell's book. For 'the' history of second quantization and relativistic quantum electrodynamics, one may refer to Schwinger's book, *QED and the men who made it*. Landau and Lifshitz's book may also be consulted.

2.1.1.2 The weak force, a short-range force much weaker than the electromagnetic force

• Radioactivity, beta decay, and Fermi's theory of beta decay

In 1896, Becquerel, who was working on phosphorescence, noticed that some of his uranium samples emitted radiations, even the non-phosphorescent ones²³. Becquerel understood these radiations were not the X-rays he was expecting, and he called them 'uranic radiations'. The term 'radioactivity' was introduced by Marie Curie in her scientific reports²⁴. She and Pierre Curie discovered two other radioactive elements, the radium and the polonium. In 1899, Rutherford distinguished three types of radioactive decays, namely alpha, beta and gamma, according to their penetrating power. In 1901 [206, 207], Rutherford and his pupil Soddy understood, analyzing thorium decays, that decays go with a transmutation of the radioactive element, and in 1903, the well-known exponential-decay law for radioactive

²³He wondered whether the radiations emitted by phosphorescent bodies previously exposed to light were X-rays, which had been discovered ('by chance') one year earlier, by Röntgen. To Becquerel, the light emitted by phosphorescent bodies was similar to that emitted by cathodic tubes previously exposed to X-rays, and might thus have been of the same nature. The experiment was the following: Becquerel put his samples on a photographic plate, protected by paper, and wanted to see whether the samples would imprint the plate. Some of the samples had been exposed to light previously, others not. The only samples that imprinted the plaque were the uranium samples, regardless of their previous exposition to light. The plate, called "étiquette bleue", was a successful dry photographic plate commercialized by the Lumière brothers. Here are many details on the experiment and the context, in French, by Basdevant, https://www.bibnum.education.fr/sites/default/files/BECQUEREL_SUR_LES_RADIATIONS_EMISES_BASDEVANT.pdf.

²⁴Here is a very complete website of the American Institute of Physics on Marie Curie, <http://history.aip.org/exhibits/curie/>.

samples was published²⁵ [208]. Evidence for a loss of energy during the beta decay accumulated between 1911 and 1927, and in 1934 [209, 210], Fermi published his famous theory of beta decay (now called beta-minus decay), for the change of a neutron into a proton by emission of an electron (the beta-minus radiation), in which a hypothetical particle, which now corresponds to the antineutrino, is emitted²⁶; in Fermi's picture, the interaction was a contact interaction with no range, but this interaction is now described, as any weak interaction, by a non-contact interaction with short range. This four-fermion interaction was the first version of a weak interaction.

• **Parity violation, chiral vector-minus-axial ($V - A$) theory and CP violation**

★ *Parity violation and the chiral $V - A$ theory with its charged weak bosons W^\pm*

In 1956 Lee and Yang [211] suggested that Fermi's weak interaction might break parity²⁷, and the experimental proof was given one year later, by Wu et al. [212].

Together with the development of perturbative renormalization theory²⁸, this parity violation lead, the same year, Marshak and Sudarshan²⁹ [213, 214], and then Feynman and Gell-Mann [215], to introduce chirality^{30,31} and develop the chiral $V - A$ theory, which introduces two massive and charged mediators for the weak force, namely W^\pm . This is the first unified theory of what is now called the weak interaction.

See the following notes by Lessov on the history of the weak interaction from Fermi's beta decay to the chiral $V - A$ theory, <https://arxiv.org/pdf/0911.0058.pdf>.

★ *CP violation*

²⁵For the original paper, see <http://www.bibnum.education.fr/sites/default/files/rutherford-texte-partie1.pdf>. Some short notes on the 2 men by the American Physical Society, <https://www.aps.org/programs/outreach/history/historicsites/rutherfordsoddy.cfm>, extended historical notes on the context of the discovery, by Bonolis, <http://www.mediathèque.lindau-nobel.org/research-profile/laureate-soddy#page=1>, and a detailed review of the paper by Radyanyi, <https://www.bibnum.education.fr/sites/default/files/Rutherford-analyse-english.pdf>.

²⁶On the intertwined history of neutrinos and neutrons, with Pauli's 1930 contribution and Chadwick's 1932 discovery of the neutron, see the following historical paper, <http://physicstoday.scitation.org/doi/pdf/10.1063/1.2995181>.

²⁷Parity is the transformation that flips all spatial coordinates. It transforms a vector into its opposite, and is in this sense viewed as a 'mirror' transformation. The idea of parity-symmetric physical processes was formalized by Wigner in 1927, see http://www.digizeitschriften.de/download/PPN252457811_1927/PPN252457811_1927___log30.pdf for the original German paper, and http://link.springer.com/chapter/10.1007%2F978-3-662-02781-3_7 for the collected works of Wigner. Parity is a symmetry of classical gravitational laws, electromagnetic laws, was a symmetry of the laws involving the nuclear and strong forces at the time, and is still.

²⁸For some general ideas on perturbative renormalization theory, see Appendix N.

²⁹Some short notes by Sudarshan on the history of the discovery, at <http://quest.ph.utexas.edu/Reviews/VA/VA.pdf>.

³⁰For massless particles, chirality and helicity, the projection of the spin on the momentum, coincide, and 'replace' the spin, since the latter is not a good quantum number for such free particles (their little group is $ISO(2)$ and not $SO(3)$). For massive particles, chirality is not fixed, so that one often uses the Dirac representation, which is not irreducible, and combines left and right chiralities, which are interchanged in some weak interactions.

³¹Only left chirality was introduced, the right chirality being linked to the neutral Z^0 boson, see below.

Landau [216] pointed out that CP, the composition of parity, P, and charge conjugation (i.e. substituting particles by their antiparticles), C, was preserved by the $V - A$ theory of the weak interaction, and this seemed to solve the problem raised by the parity violation: the ‘good transformation’, i.e. the ‘symmetry’ of nature, was CP and not P³². In 1964, however, Christenson, Cronin, Fitch and Turlay [217], showed experimentally that the CP symmetry was broken in the kaon decay (these kaons rarely decay into two pions).

• Glashow’s electroweak unification and its neutral weak boson Z^0

One needs a consistent framework to describe situations where the weak and the electromagnetic forces are involved in interactions involving comparable energy exchanges.

Schwinger suggested the idea of the electroweak unification through a third weak (massive) *neutral* boson, but he gave the task of developing this idea to his PhD student, Glashow, and a paper presenting such a unification through a Z^0 gauge boson was eventually published in 1961³³ [218].

• Spontaneous symmetry breaking, Higgs mechanism and electroweak Standard Model

For historical (and technical) details on the concept of spontaneous symmetry breaking, see the following presentation by Jona-Lasinio, <http://www.gakushuin.ac.jp/univ/sci/phys/notice/JonaLasinioNov09.pdf>. The historical steps by which this phenomenon acquired its maximal recognition and was named that way begin with Heisenberg’s 1959 suggestion that the concept might be relevant in particle physics, and then Nambu’s [219] discovery of such a mechanism in BCS³⁴ superconductivity. With Jona-Lasinio [220], Nambu brought the concept to particle physics, after which Goldstone [221] developed it, which ended up in the formulation of Goldstone’s theorem, with Salam and Weinberg [222]. The theorem is the following. Consider a system in an excited state, which has a degenerate energy groundstate. To minimize its energy, the system goes to one of these groundstates. Goldstone’s theorem states that this is necessarily accompanied by the apparition of an additional scalar mode in the spectrum of the system, for each generator of the broken symmetry, called a Goldstone boson. The theorem states that such a mode should be *massless*.

Anderson first proposed a way to give a mass to Goldstone modes in a non-relativistic framework, and figured out some consequences in particle physics [223]. One year later, the relativistic version, needed for particle physics, was developed by three independent groups, Brout-Englert [224], Higgs [225], and Guralnik-Hagen-Kibble [226]. In 1967, Weinberg [227] and Salam³⁵ [228, 229] included the Higgs mechanism into Glashow’s electroweak unification. The following historical and technical notes by Kibble are very interesting,

³²See this article of the CERN Courier on the “CP violation’s early days”, at <http://cerncourier.com/cws/article/cern/57856>. In the paper by Lee and Yang [211] questioning the conservation of parity in weak interactions, there is a remark about the CP symmetry.

³³For his 1979 Nobel prize lecture, see http://www.nobelprize.org/nobel_prizes/physics/laureates/1979/glashow-lecture.pdf, and here follow interesting historical details compiled by Brooks, <http://www.quantum-field-theory.net/electroweak-unification/>.

³⁴After Bardeen, Cooper and Schrieffer.

³⁵In the following notes, Salam’s contribution is discussed: <https://arxiv.org/pdf/1109.1972.pdf>.

<https://arxiv.org/pdf/1502.06276.pdf>. The unified picture can formally be very briefly summed up as follows:

1. At high energy, one has the so-called electroweak interactions between particles, which are described by a non-Abelian $U_Y(1) \times SU(2)$ Yang-Mills gauge theory^{36,37}. ‘The’ generator of the gauge group $U_Y(1)$ is called *weak hypercharge*, denoted \hat{Y} , and is associated to the B gauge boson. The gauge group $SU(2)$ has three generators \hat{I}_i , $i = 1, 2, 3$, and is associated to the weak-isospin d.o.f., which belongs to a 2D Hilbert space; each generator is associated to a gauge boson W^i . All gauge fields are real-valued 4-vector fields.
2. At low energy, the electroweak internal gauge symmetry $U_Y(1) \times SU(2)$ is spontaneously broken: B and W^3 couple through the Weinberg, or weak angle θ_W , accounting for the photon (field) γ and the neutral weak boson Z^0 , as

$$\begin{pmatrix} \gamma \\ Z^0 \end{pmatrix} = \begin{bmatrix} \cos \theta_W & \sin \theta_W \\ -\sin \theta_W & \cos \theta_W \end{bmatrix} \begin{pmatrix} B \\ W^3 \end{pmatrix}. \quad (2.3)$$

The photon field γ is the spin-1 bosonic field also known as electromagnetic potential, i.e. the gauge field associated to the electromagnetic gauge group $U_{\text{em}}(1)$, whose generator is the electric charge operator, given by $\hat{Q} = \hat{I}_3 + \hat{Y}/2$. The remaining electroweak bosons W^1 and W^2 mix to account for the charged weak bosons, W^\pm :

$$W^\pm = \frac{W^1 \mp i W^2}{\sqrt{2}}. \quad (2.4)$$

The masses of the weak bosons, provided by the Higgs mechanism, are related by

$$M_Z = \frac{M_W}{\cos \theta_W}. \quad (2.5)$$

The theory was validated in two steps: (i) in 1973, the neutral currents caused by the exchange of Z^0 bosons were discovered in the Gargamelle bubble chamber, so that the Glashow-Weinberg-Salam Standard model of electroweak interaction became widely accepted³⁸, and (ii) in 1983, the three weak bosons were detected at CERN, by an experiment led on the LEP.

2.1.1.3 The strong force, a short-range force much stronger than the electromagnetic force

• Atomic model, atomic nucleus and the strong nuclear force

The concept of atom, as well as the word, is usually traced back to Democritus, philosopher, 5th century before Christ, who suggested that matter is composed of small indivisible

³⁶In this notation, the $U_Y(1)$ and $SU(2)$ groups are, as usually said, the *abstract* versions of the matrix groups $U(1)$ and $SU(2)$, and \times denotes the standard ‘cartesian product’, or, rather, ‘group product’, since the denomination ‘cartesian’ is associated to vector spaces, while there is a huge branch of group theory which has nothing to do with vector spaces. If, by $U_Y(1)$ and $SU(2)$, one wants to refer to the representations of the abstract groups in terms of linear automorphisms, one would denote the electroweak symmetry group as $U_Y(1) \otimes SU(2)$.

³⁷Note that $U(1) \times SU(2)$ contains, but is not equal to $U(2)$, see Appendix F. In mathematical group-theory terminology, we say that $U(N)$ is, not the direct, but the semidirect product of $SU(N)$ by $U(1)$.

³⁸Glashow, Weinberg and Salam won the Nobel prize in 1979.

particles. A century later, Aristotle, philosopher, stated instead that any piece of matter is a continuum that can be divided ad infinitum. Because of the huge influence of Aristotle in occidental thinking, this continuum vision prevailed up to the 19th century.

In the second half of the 18th century, the chemist Lavoisier stated the principle of matter conservation in chemical reactions, and in 1808, Dalton suggested a chemistry-grounded atomic model of matter.

In 1897, Thomson concluded from its experiments on cathod rays that negatively charged particles, later called ‘electrons’, can be detached from atoms. He suggested in 1904 the plum pudding model of atom [230], in which the paste is positively charged, and the dried grapes inside are the electrons. The model “purposely”³⁹ avoids the problem of energy loss through Larmor radiation [232], by suggesting the atom should contain a number of electrons one thousand times greater than the numerical value, in grams per mole, of the mass of the atom, which he realized to be impossible in 1906.

In 1911 [233], Rutherford deduced from its 1909 experiments on the deviation of alpha particles by a one-atom-thick layer of gold⁴⁰, that the positive charges in the gold foil are concentrated in volumes much smaller than that of the atom. He thus suggested what is now called Rutherford’s atomic model: the atom is made of a positively charged tiny nucleus, around which the electrons move. In his 1911 paper, Rutherford mentions the necessity to determine experimentally whether the center is actually positive or negative⁴¹.

In 1913 [231, 234], Bohr proposed a model of the atom grounded on Planck’s quanta, first suggested in 1900 to account for the black body radiation⁴², and then used and conceptually developed by Einstein to explain the photoelectric effect, in 1905⁴³. Bohr’s suggestion is, in a semi-classical picture, that only some specific orbits are allowed for the electron in motion around the nucleus, and thus the electron’s energy belongs to a discrete set of possible values, i.e., must be ‘quantized’. This model avoids the radiation problem, and accounts for several atomic emission spectra. These historical landmarks sign the rise of quantum physics.

In 1932, Chadwick discovered the neutron. Within months after this discovery, Heisenberg and Ivanenko proposed neutron-proton models for the atomic nucleus, which included the idea of the (nuclear) isospin, see Appendix J.

In 1935, Yukawa⁴⁴ [235] suggested an analytical form for the nuclear two-body potential, now so-called Yukawa potential, which is a Coulomb potential screened by a decreasing exponential, which makes the range of the nuclear force ‘infinitely’ smaller than that of the

³⁹This is Bohr’s word [231].

⁴⁰See the following short videoclip, <https://youtu.be/VLU4dntonhE>.

⁴¹Rutherford mentions Nagaoka’s theoretically-grounded planetary or Saturnian model, suggested in 1904, in part by the formal correspondence between the Coulomb and the gravitational forces. Nagaoka tried to fix, in his model, the well-known problem of radiating electrons. In 1908, however, he eventually abandoned his model after (i) the failure in reconciling the model with radioactivity and atomic emission rays and (ii) Thomson pointed out unstable oscillations of the electrons orthogonally to the plane of the orbit (see http://link.springer.com/chapter/10.1007%2F978-3-540-70626-7_10). Hope for non-radiating orbits was brought by Ehrenfest’s 1910 paper, but this idea was abandoned during the rise of quantum mechanics.

⁴²See the following two historical reviews on Planck’s seminal work in quantum physics, <https://arxiv.org/pdf/physics/0402064.pdf> and <http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.613.4262&rep=rep1&type=pdf>.

⁴³For an English translation of the original paper, go to http://www.esfm2005.ipn.mx/ESFM_Images/paper1.pdf.

⁴⁴The original paper was reprinted in 1955 [235], see <https://academic.oup.com/ptps/article-lookup/doi/10.1143/PTPS.1.1>.

electromagnetic or gravitational forces⁴⁵. The nuclear force was conceived as transmitted by particles called mesons, which were discovered in 1947. In essence, the modern picture of the nuclear force is the same, but this nuclear force is viewed as a residual force of the underlying so-called strong force between quarks, elementary particles which manifest themselves only⁴⁶ through so-called hadronic bound states; the particles sensitive to the nuclear, and, more generally, the underlying strong force, are called hadrons. Quarks are viewed as the elementary hadrons, and these hadrons divide into two families of bound states: baryons, made of one or several triplets of quarks, such as protons and neutrons, and mesons, made of one or several quark-antiquark pairs.

- Strong (or color) force

- ★ *Six quarks to account for the variety of hadrons*

With the development of particle accelerators and colliders after World War II, many particles were discovered. In 1953, Nakano and Nishijima [236] were able to extract, out of the experimental data, a formula relating the charge, the nuclear isospin, and the baryonic number of particles, in which one had to add a new quantum number, which was then conceptually developed up to 1955 by Nishijima [237], and eventually called *strangeness*. In 1956, Gell-Mann⁴⁷ also suggested the same formula, independently, and the formula is currently known as the Gell-Mann–Nishijima formula. The same year, Sakata [238] suggested the so-called triplet model of hadrons, in which all known hadrons were made out of a combination of particles from the triplet (p, n, Λ) .

The Eightfold Way report, written in 1961 by Gell-Mann [239], is an attempt to describe the strong interaction to which were sensitive the eight spin-1/2 baryons that were known when he wrote the paper. In Gell-Mann’s words, “the most attractive feature of the scheme is that it permits the description of eight vector mesons by a unified theory of the Yang-Mills type (with mass term)”. In the abstract of his paper publicising the Eightfold Way and formally presenting its mathematics [240], Gell-Mann cites Ne’eman, which developed essentially the same 8-vector-mesons picture, independently [241]. The baryons were organized in an octuplet according to charge and strangeness. The model was an alternative to Sakata’s triplet.

One year later, the spin-3/2 baryons were viewed as organized in a decuplet, but this required the existence of a still unobserved baryon, which Gell-Mann called Ω^- . In 1964, the Ω^- was observed [242], and Gell-Mann showed that assuming the hadrons were made of three *flavors* of *quarks*, having fractional charges, would greatly simplify the picture⁴⁸ [243];

⁴⁵If the *range* is defined through the characteristic scale of variation of the exponential, then the electromagnetic and gravitational forces have infinite range.

⁴⁶We shall come back to this fact further down, in Paragraph 2.1.1.3.

⁴⁷An extensive selection of Gell-Mann’s papers is available at <http://longstreet.typepad.com/thesciencebookstore/2013/06/important-papers-of-murray-gell-mann-as-they-appear-in-murray-gell-mann-selected-papers-and-published-by-world-scie.html>.

⁴⁸The three flavors of quarks were *up*, *down*, and *strange*. The word ‘flavor’ came later. In his paper [243], Gell-Mann explicitly states that this triplet is formally highly reminiscent from Sakata’s triplet, and that the quark-picture flavored Lagrangian can be built by analogy with Sakata’s-triplet Lagrangian.

this was also realised independently by Zweig^{49,50}. The power of the quark picture can be illustrated by the following two equalities, as Gell-Mann and Zweig found out:

1. An equality for lowest-flavor-order (i.e. spin-0) mesons:

$$\mathbf{3}_F \otimes \bar{\mathbf{3}}_F = \mathbf{8}_F \oplus \mathbf{1}_F, \quad (2.6)$$

which states that hadronic bound states made of quark-antiquark pairs⁵¹, i.e. spin-0 mesons⁵², belong to a spin-0 meson representation Hilbert space of dimension $8 + 1$, i.e. there are $8 + 1$ basis states, which are the $8 + 1$ spin-0 mesons, which had already been detected in 1964. The subscript F is for ‘flavor’.

2. An equality for lowest-flavor-order (i.e. spin-1/2 and spin-3/2) baryons:

$$\mathbf{3}_F \otimes \mathbf{3}_F \otimes \mathbf{3}_F = \mathbf{10}_F \oplus \mathbf{8}_F \oplus \mathbf{8}_F \oplus \mathbf{1}_F, \quad (2.7)$$

which states that the lowest-order baryons, made of three quarks (each belonging to a flavor representation, noted $\mathbf{3}_F$), organize into a singlet, two octets and a decuplet. The link with the spin-1/2 baryonic octet and the spin-3/2 baryonic decuplet needs however a more in-depth analysis. We refer the reader to first Wikipedia’s article on the quark model and then, e.g., Kosmann-Schwarzbach’s 2010 book on *Groups and symmetries, from finite groups to Lie groups* [244].

The modifications brought to Sakata’s model [245] managed to maintain it as a concurrent of the quark model⁵³, although it was largely abandoned after the experimental evidence, in 1974 at the SLAC, for the J/Ψ meson, viewed as a new, so-called *charmed*, quark-antiquark pair.

In 1973, Kobayashi and Maskawa [247] showed that the CP violation, by some weak interactions, made inconsistent Maki and Ohnuki’s [245] quartet baryon scheme, which had been introduced to overcome the difficulty of the “strangeness changing neutral current” [247] in Sakata’s triplet scheme. This can be translated as a need for a third generation of baryons. Note that the quark picture is neither adopted nor mentioned in their paper, a possible sign that this picture was not fully established yet⁵⁴.

Indirect experimental evidence for the bottom and top quark was found in 1977 and 1995, respectively, at Fermilab.

★ *Eight vector bosons mediating the interactions between quarks: the gluons*

When Gell-Mann published his quark picture to simplify the classification of hadrons, hadronic interactions were still viewed as mediated by mesons, but the quark picture soon

⁴⁹See his two relevant CERN reports, at <http://cds.cern.ch/record/352337/files/CERN-TH-401.pdf>, and <http://library.lanl.gov/cgi-bin/getfile?00323548.pdf>.

⁵⁰Zweig orally presented, in a 1980 conference at Caltech, a highly detailed historical picture of the development of the quark model prior to 1964; his conference notes are available at http://authors.library.caltech.edu/18969/1/Origins_of_the_Quark_Model_Final_Zweig%5B1%5D.pdf.

⁵¹Quarks belong to the three-dimensional flavor representation Hilbert space noted $\mathbf{3}_F$, and the antiquarks to its adjoint, noted $\bar{\mathbf{3}}_F$.

⁵²Mesons made of more than one quark-antiquark pair have a higher-dimensional spin.

⁵³Note that Sakata used the simplifying quark picture in several papers [246].

⁵⁴I wonder whether this paper is one of the last milestone papers on hadronic physics which does not adopt the quark picture.

gave hints about the pitfalls of such a description: interpreting, through the quark picture, the experimental data on the spin-3/2 baryon Δ^{++} , led, in 1965, Greenberg [248] and, independently, Han and Nambu [249], to suggest that quarks may possess an additional degree of freedom, later called *color*, that should be associated to their interaction through a *color charge*, as the electromagnetic interaction is associated to the electric charge.

The color degree of freedom belongs to a three-dimensional Hilbert space, and each vector of an arbitrary reference basis is associated a given color. Now, the force carriers are not directly represented by the generators of naive transformations that would preserve the color norm and which would belong to the symmetry group $U(3)$ of the color representation space, that we note $\mathbf{3}_C$, where C is for ‘color’. Instead, and this is due to the flavor quantum number, the force carriers are represented by *color-anticolor pairs*, in a quantum-mechanical way, i.e. any (normalized) linear combination of such pairs is allowed, provided we built a basis of an appropriated symmetry group with these states. This is the first basic complexity of the so-called (*quantum*) *chromodynamics*, i.e. the study of the strong interaction through the color-charge picture, which is currently the standard framework. The force carriers are called *gluons*. As in the flavor quark picture for hadrons, see Eqs. (2.6) and (2.7), the color picture for gluons holds in the following equality:

$$\mathbf{3}_C \otimes \bar{\mathbf{3}}_C = \mathbf{8}_C \oplus \mathbf{1}_C. \quad (2.8)$$

Now, from experimental data, it was deduced that only the octet, namely $\mathbf{8}_C$, was involved in strong interactions, i.e., in modern words, that the strong interaction should be described by the gauge group $SU(3)$ rather than $U(3)$ ⁵⁵. The “Advantages of the color octet gluon picture”, rather than the color singlet gluon picture previously considered, were described by Fritzsch, Gell-Mann, and Leutwyler in 1973 [250]. These findings are related to the suggestion of considering color as independent from flavor, while Han and Nambu’s early model [249] intertwined both quantum numbers.

• Chromodynamics and its difficulties

The aforementioned group-theoretical arguments that managed to account for many structural features of the strong interaction were developed, roughly speaking, while standard quantum-field-theory perturbative computations, i.e. perturbative renormalization methods⁵⁶, were essentially failing, due to the particularly high magnitude of this interaction (which is linked to the ‘strong force’ denomination). In 1973, Wilczek and Gross [251] and, independently, David and Politzer [252], theoretically described the so-called asymptotic freedom in quantum chromodynamics (QCD): at sufficiently small length scales, i.e. sufficiently high energies, quarks interact weakly, and eventually not at all in the limit of infinite energy, the so-called asymptotic freedom of quarks, which, in essence, makes perturbative computations work at such high-enough energies. This is in strong contrast with quantum electrodynamics (QED), where one has the opposite effect: the lower the typical energy of

⁵⁵Note that the weak force cannot either be described by a group of transformations preserving the norm of a single *naive* internal d.o.f.. The complexity of the weak force is described through the electroweak picture, see Paragraph 2.1.1.2.

⁵⁶See Appendix N for a general picture of perturbative renormalization theory.

the interaction, the better perturbative computations work⁵⁷, while at high energy, these perturbative computations fail, which was quickly pointed out by Landau in the early days of QED, in the 50's.

Now, while understanding such an asymptotic freedom enables to deal with high energies in QCD, the low-energy behaviour of the theory still requires to go beyond perturbative methods. Going beyond perturbative methods can be done with so-called lattice gauge theories (LGTs), which construct QFTs on a spacetime lattice. As we mentioned in the introduction, the seminal paper on LGTs is that of Wilson, in 1974 [27]. In this paper, Wilson shows that such a lattice construction of the theory, which avoids the problems of perturbation theory⁵⁸, enables to predict the confinement of quarks at low energy, a phenomenon for which the (hadron-)physics community was expecting a theoretical explanation since there was – and there is still – no evidence for free quarks in experiments⁵⁹. In a few years, the lattice picture quickly yielded many results, and LGTs are now standard.

2.2 Publication [3]: Quantum walks and non-Abelian discrete gauge theory

— ABSTRACT —

In this publication, we present a new family of 1D DTQWs which coincides, in the continuum limit, with the unidimensional Dirac dynamics of a relativistic spin-1/2 fermion coupled to a generic non-Abelian $U(N)$ Yang-Mills gauge field. The gauge-theory interpretation is extended beyond the continuum limit, by showing the existence of, (i) not only a $U(N)$ gauge invariance on the lattice, but also (ii) an associate lattice gauge-covariant quantity, which delivers, in the continuum, the field strength associated to a standard $U(N)$ Yang-Mills gauge field. We show, through numerical simulations, that classical, i.e. non-quantum phenomenology is recovered at short times.

The aim of this paper [3] is to extend the previous results on Abelian gauge fields to non-Abelian gauge fields. By simplicity, we have started this work in 1D, and the paper only deals with this case.

⁵⁷This is physically interpreted as a so-called *screening* of the electric charge by electron-positron pairs of the vacuum fluctuations surrounding the electric particle. While this is also the case for the color charge of quarks, the fact that gluons also carry a color charge, while photons do not, and the way they carry it, results in an opposite effect, called *antiscreening*, which accounts for quark confinement.

⁵⁸Which does not mean LGTs are free of other problems. Indeed, LGTs have other problems from the start, such as the loss of unitarity.

⁵⁹As we have seen in Paragraph 2.1.1.3, quarks were introduced by Gell-Mann and Zweig in 1964, as mathematical objects that greatly simplified the understanding of the hadronic classification and of the gauge-theory structure of the strong force. Two opposed visions emerged after the advent of the quark picture. Since there was no evidence for free quarks, Gell-Mann considered quarks were not real particles, but Feynman still thought the opposite, in the sense that quarks can be associated a classical trajectory through the path-integral framework; Feynman would refer to such ‘real quarks’ as *partons*, i.e. ‘parts of hadrons’. Such an opposition is still up to date.

2.2.1 Schematic picture of a non-Abelian Yang-Mills gauge theory

Before explaining how we build our DTQW with non-Abelian coupling, let us give a sum-up on the standard non-Abelian Yang-Mills gauge theory, which is the continuum-limit situation of our DTQW scheme, as we show in Section III of the paper.

2.2.1.1 Gauge-field-induced matter-field dynamics

Here is a simple picture of such a dynamics.

An Abelian gauge field (i.e. electromagnetic potential) influences the dynamics of a first-quantized matter field $\Psi(\mathbf{x}, t)$ ⁶⁰ by, *roughly speaking*, modifying its phase locally (i.e. depending on the spacetime location (\mathbf{x}, t)), and through a coupling between this dynamical phase modification and the external (i.e. position) degree of freedom (d.o.f.) of the field⁶¹. This phase (i) is an internal degree of freedom and (ii) is associated to⁶² the Abelian gauge group $U(1)$, so that it can be called Abelian or $U(1)$ internal degree of freedom. The magnitude of the interaction is characterized by a charge, specific to the considered field, called Abelian charge.

A non-Abelian gauge field influences the dynamics of the aforementioned matter field by modifying another internal d.o.f., called non-Abelian or $U(N)$ internal d.o.f., and through a coupling between this dynamical modification of the non-Abelian internal d.o.f. and the position d.o.f.. The magnitude of the interaction is given by an associated non-Abelian charge. As for any degree of freedom, the non-Abelian internal d.o.f. is formally implemented by tensorial product, which reduce to a multiplication in the Abelian case.

Such a gauge-field-induced matter-field dynamics is described, in the case of half-integer-

⁶⁰We make this presentation in n spatial dimensions for the sake of generality, although we will then limit ourselves to the 1D case, so that the Abelian field only contains an electric potential and no magnetic potential.

⁶¹A way to see this coupling is by applying the evolution operator that takes $\Psi(\mathbf{x}, t_1)$ to $\Psi(\mathbf{x}, t_2)$, which is a complex exponential of the Hamiltonian with (Abelian) gauge coupling: because the gauge field generically depends on position, it does not commute with the momentum, and this creates a non-trivial coupling between the internal $U(1)$ degree of freedom and the external one; this coupling becomes trivial if the gauge field does not depend on position but only on time.

Note that, as long as we keep it vague, this simple ‘physical’ picture holds whatever the nature of the field, i.e. whether its spin is half integer or integer: it can be a spin-1/2 field, in a relativistic or non-relativistic framework, but also an integer-spin field, such as the spinless (i.e. scalar) complex field, which, if it describes matter (as opposed to gauge fields), can only describe composite (i.e. non-elementary) particles.

See Appendix K to go beyond this simple vague picture and a discussion on the distinction between half-integer-spin and integer-spin (classical) fields.

⁶²The internal degree of freedom is arbitrary, i.e. fixed up to a transformation by an element of $U(1)$, in the absence of gauge field. This internal d.o.f. belongs to a half-integer-spin representation space of the $U(1)$ group.

spin (i.e. fermionic) matter, by the Dirac equation with Yang-Mills (minimal⁶³) coupling.

To have a better picture of both the Abelian and non-Abelian interactions, the geometrical framework of fiber bundles is useful, see Appendix H: the gauge field is a connection on the vector $U(N)$ -bundle. A necessary condition for the gauge field to be ‘Yang-Mills’ and not only ‘non-Abelian’, is that it belongs to the Lie algebra of the gauge group. An interesting epistemological paper about the geometrical foundations of classical Yang-Mills theory, by Catren, can be found at <http://www.sciencedirect.com/science/article/pii/S1355219808000166>⁶⁴.

2.2.1.2 Dynamics of the gauge field: matter field acting on a gauge field

The previous picture is not complete, because it does not take into account that matter influences the gauge-field dynamics.

Such a dynamics is described, in the case of an Abelian gauge field, by Maxwell’s equations. In the case of a non-Abelian gauge field, Maxwell’s equations generalize into the so-called “Yang-Mills field equations”. In our paper, we do not provide any DTQW equivalent for these equations. Yang-Mills field equations take a simple form when written in the framework of Cartan’s calculus (whose central ingredient is the exterior derivative), used covariantly on (Lie-algebra) principal $U(N)$ -bundles.

2.2.1.3 First-quantized (generically non-Abelian) Yang-Mills gauge theory of interactions

A generic first-quantized (non-Abelian) Yang-Mills gauge theory can thus be written compactly in 3 (non-scalar) equations:

- One dynamical equation for the matter field. For a spin-1/2 field, this is the Dirac equation with non-Abelian coupling, see below, Subsubsection 2.2.1.4.
- Two dynamical equations for the gauge field:

⁶³Non-minimal couplings have been considered essentially between the gravitational force and some other physical entity, that we describe by a field, either fermionic or bosonic. Such a non-minimal coupling arises naturally when describing the gravitational force by a curvature of spacetime, see the following discussion, <http://physics.stackexchange.com/questions/103892/minimal-vs-non-minimal-coupling-in-general-relativity>. The field that couples to gravity can be, e.g., a matter field [253, 254], an electromagnetic field [255], or an inflaton field [256, 257] in primordial cosmology. To give a global vague picture, we may say that such couplings have been introduced to tackle two important classes of theoretical problems in physics: (i) describing phenomena where the magnitude of the gravitational force is comparable to that of another given force, either the electromagnetic, the weak, or the strong one, and, (ii) understanding dark matter and dark energy, which have been invoked in cosmology to account for unexpected observations, as the unexpected galaxy rotation diagrams for dark matter, and the acceleration of universe’s expansion for dark energy. For information on modified gravity theories with non-minimal couplings to other fields, see, e.g., the following review of 2014 [258], the following same-year talk, http://www.cpt.univ-mrs.fr/~cosmo/SW_2014/PPT/Balakin.pdf, or this Master thesis, <https://fenix.tecnico.ulisboa.pt/downloadFile/395138327112/ThesisFinalN.pdf>, which is however less recent (2009).

⁶⁴This paper aims at going beyond the standard ‘physical’ argument underlying gauge theories, namely that physics must be local and that any degree of freedom of the system should not be constrained to have the same value at all spacetime points, but should actually be a field defined on spacetime, i.e. that (i) one should be able to modify the value of the parameter locally without being, at least immediately, affected by very distant objects, and that, (ii) one should still require the invariance property of the system with respect to changes of the degree of freedom once it is made local, by extended relativity principle, as Einstein did to go from special to general relativity.

1. The so-called *homogeneous* equations, which are (dynamical) constraints on the gauge field, independent of the presence of matter (the matter field does not enter this equation).
2. The so-called *inhomogeneous* equations, which describe how the presence of matter modifies the dynamics of the gauge field. The gauge-field part of this equation can be obtained from the homogeneous equation by Hodge duality.

For information on the solutions to this system, and their relevance to physics, see the following discussion, <http://physics.stackexchange.com/questions/27309/which-exact-solutions-of-the-classical-yang-mills-equations-are-known>, which contains many references.

2.2.1.4 Dynamics of the matter field, and non-Abelian gauge invariance: formalism

• Dynamical equation

The Dirac equation describing the dynamics of a spin-1/2 field Ψ of mass m , interacting with a non-Abelian $U(N)$ Yang-Mills gauge field, is:

$$[i\gamma^\mu \otimes D_\mu - m\mathbf{1}_{dN}] \Psi = 0, \quad (2.9)$$

where d is the dimension of the spin-representation space, and the index μ is summed over from 0 to n . The covariant derivative $D_\mu = \mathbf{1}_N \partial_\mu - iB_\mu$, where the B_μ 's are the $n+1$ spatiotemporal components of the gauge field. This gauge field is valued in the Lie algebra of $U(N)$, which is an N -dimensional vector space, and it can thus be decomposed as

$$B_\mu = B_\mu^k \tau_k, \quad (2.10)$$

where summation over k is implied, and where the τ_k 's are N^2 possible generators of $U(N)$, i.e. a possible basis of its Lie algebra⁶⁵. Here we have set the coupling constant to $g = -1$.

In one spatial dimension, the irreducible representations of the Clifford algebra have dimension 2, and we can choose $\gamma^0 = \sigma_1$ and $\gamma^1 = i\sigma_2$.

• Non-Abelian gauge invariance

Equation (2.9) is invariant under the following gauge transformation, which generalizes the Abelian one, i.e. Eq. (45):

$$\Psi \rightarrow \Psi' = (\mathbf{1}_d \otimes G) \Psi \quad (2.11a)$$

$$B_\mu \rightarrow B'_\mu = GB_\mu G^{-1} - i(\partial_\mu G)G^{-1}, \quad (2.11b)$$

where $G \in U(N)$ is the gauge transformation, that replaces the Abelian one $e^{-i\phi} \in U(1)$.

⁶⁵ $U(N)$ is both compact and connected; hence, if $U \in U(N)$, there exist a Hermitian matrix H such that $U = \exp[iH]$. Let us write $H_{ij} = a_{ij} + ib_{ij}$, where a_{ij} and b_{ij} are real numbers. H Hermitian means $a_{ji} = a_{ij}$ and $b_{ji} = -b_{ij}$. The number of b_{ij} 's that can be chosen arbitrarily is $(N^2 - N)/2$; indeed, to the N^2 arbitrary real numbers that define an arbitrary matrix, one must omit N since the diagonal elements of b must vanish ($b_{ii} = -b_{ii}$), and divide the whole by 2 because if all b_{ij} 's are chosen for, say, $i > j$, then those for $i' = j < j' = i$ are imposed. For a_{ij} , the reasoning is the same, and we must add, to $(N^2 - N)/2$, the diagonal elements, which can be given an arbitrary real value, so that the number of a_{ij} 's that can be chosen arbitrarily is $(N^2 - N)/2 + N$. The set of all Hermitian matrices of dimension N , which is the Lie algebra of $U(N)$, is thus a real vector space of dimension $(N^2 - N)/2 + [(N^2 - N)/2 + N] = N^2$.

The field strength, that generalizes the electromagnetic tensor (also called Faraday tensor), is given by

$$F_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu - i[B_\mu, B_\nu], \quad (2.12)$$

where the commutator vanishes in the Abelian case. This field strength is gauge covariant, i.e. its transformation under (2.11b) solely reflects the basis change in the non-Abelian internal-d.o.f. Hilbert space, due to the change of gauge: $F'_{\mu\nu} = GF_{\mu\nu}G^{-1}$. In geometric terms, $F_{\mu\nu}$ is the curvature of the vector $U(N)$ -bundle, of which the $U(N)$ part of the dN -component field Ψ (which also contains a spin part, in the notation we use) is a so-called section.

2.2.2 Walk operator for the 1D DTQW with non-Abelian coupling

The starting-point ingredient of our paper is the definition of a DTQW which (i) not only has the standard Yang-Mills matter dynamics as a continuum limit, Eq. (2.9), as already announced, but also (ii) satisfies a gauge invariance on the lattice, that generalizes the relations found in the Abelian case, Eqs. (1.5), and which delivers, in the continuum limit, the standard non-Abelian gauge invariance given by Eq. (2.11).

Actually, our 1D non-Abelian DTQW-operator satisfying the above conditions can be constructed by ‘straightforward’ extension of the Abelian case. Indeed, the 1D Abelian DTQW operator can be written (rewrite Eq. (1.2) as below, replacing the superscript ‘1D’ by ‘ $N = 1$ ’, which specifies the dimension of the gauge group):

$$W_j^{N=1} = C(\Delta\theta) \begin{bmatrix} e^{ia_j^+} & 0 \\ 0 & e^{ia_j^-} \end{bmatrix} S, \quad (2.13)$$

with

$$e^{ia_{j,p}^\pm} \equiv e^{i[\Delta\alpha_{j,p} \pm \Delta\xi_{j,p}]} \in U(1) \quad (2.14a)$$

$$\equiv e^{i[(a_0)_{j,p} \pm (a_1)_{j,p}]}, \quad (2.14b)$$

where the $(a_\mu)_{j,p}$ ’s are the Abelian gauge-field lattice-spacetime components, related to the standard Abelian gauge-field covariant continuum-spacetime components $(A_\mu)_{j,p}$ ’s by

$$a_\mu = \epsilon_A A_\mu, \quad (2.15)$$

where ϵ_A goes to zero in the continuum limit.

The 1D non-Abelian DTQW-operator is then ‘simply’ constructed as:

$$W_j^N = (C(\Delta\theta) \otimes \mathbf{1}_N) \begin{bmatrix} e^{ib_j^+} & 0 \\ 0 & e^{ib_j^-} \end{bmatrix} (S \otimes \mathbf{1}_N), \quad (2.16)$$

which acts on a $2N$ -component walker Ψ_j , with

$$e^{ib_{j,p}^\pm} \equiv e^{i[(b_0)_{j,p} \pm (b_1)_{j,p}]} \in U(N), \quad (2.17)$$

where the $(b_\mu)_{j,p}$ ’s are related to the standard non-Abelian Yang-Mills gauge-field covariant continuum-spacetime components $(B_\mu)_{j,p}$ ’s by (this is shown in Section III of our paper):

$$b_\mu = \epsilon_A B_\mu. \quad (2.18)$$

Eventually, the one-step evolution equation with non-Abelian DTQW operator (2.16) is invariant under the substitution $\Psi_{j,p} \rightarrow \Psi'_{j,p} = (\mathbf{1}_{d=2} \otimes G_{j,p}) \Psi_{j,p}$, provided that the gauge

field transforms as

$$e^{i(b^\pm)'_{j,p}} = G_{j+1,p} e^{ib^\pm_{j,p}} G_{j,p\pm 1}^{-1} .$$

This gauge transformation relates the exponentials of the gauge-field components, which are elements of $U(N)$, and cannot be reduced to a relation obtained by replacing, in the standard continuum transformation of the gauge-field components, Eq. (2.11b), the partial derivative, $\partial_\mu G$, by a discrete derivative, as in the Abelian case, see Eq. (1.5b). This is so because of the non-Abelian nature of the coupling, which implies that, if $e^{i\omega_1}$ and $e^{i\omega_2}$ are two elements of $U(N)$, then

$$e^{i\omega_1} e^{i\omega_2} \neq e^{i(\omega_1+\omega_2)} . \quad (2.19)$$

A related fact is that the natural quantities involved in the gauge invariance are not the lattice equivalents, b_μ 's, of the continuum gauge-field components B_μ 's, which both belong to the Lie algebra of $U(N)$, but the e^{ib^\pm} 's⁶⁶, which belong to the $U(N)$ group⁶⁷. Note however that we can write the lattice gauge transformation, (2.11), as a relation between the Lie-Algebra-valued quantities, b_μ 's, thanks to the Baker-Campbell-Hausdorff formula; this is *by far* more cumbersome, but can be useful to study the differences between the lattice and the continuum situations, and the passage from one to another.

2.2.3 Short but detailed review and comments

In Section III, we show that the continuum limit of our DTQW, i.e. the one-step evolution equation with the $U(N)$ walk operator (2.16), yields the standard non-Abelian Yang-Mills equation for matter, Eq. (2.9), and that the lattice gauge invariance, Eq. (2.19), yields the standard non-Abelian gauge invariance, Eq. (2.11b).

Now, a notable result of our paper is the finding, in Subsection II B, of a lattice gauge-covariant quantity, $\mathcal{F}_{j,p}$, which delivers, in the continuum (Section III), the standard field strength of non-Abelian Yang-Mills theory, see Eq. (14) of the paper. We have already mentioned, in the last paragraph of the previous subsection, that the lattice gauge transformation, Eq. (2.19), is not expressed naturally in the Lie algebra of $U(N)$ ⁶⁸, and that the natural quantities involved in this gauge transformation are manifestly the e^{ib^\pm} 's, which belong to the $U(N)$ group. It is thus natural to look for a lattice gauge-covariant quantity $\mathcal{F}_{j,p}$ by manipulating this quantities on the lattice; this is how we proceeded, and the result is Eq. (8). In the Appendix, we show that the $U(N)$ gauge field can be viewed as the combination of an $SU(N)$ and a $U(1)$ gauge field, and we show the precise connection with the Abelian case $U(1)$.

In Section II, we first check, in Subsection II B, the validity of our formal computation of the continuum limit, on an explicit solution, and, in Subsection II C, we show short-time-scale agreement with the classical, i.e. non-quantum situation, derived in [200].

⁶⁶And not even the e^{ib_μ} 's, because of (2.19).

⁶⁷In the Abelian case, the phase $\phi_{j,p}$ belongs to the Lie algebra of $U(1)$, while here $G_{j,p}$ belongs to $U(N)$.

⁶⁸Such a Lie-algebra-valued expression involves using several times the Baker-Campbell-Hausdorff formula, which is very cumbersome.

Quantum walks and non-Abelian discrete gauge theory

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A family of discrete-time quantum walks (DTQWs) on the line with an exact discrete $U(N)$ gauge invariance is introduced. It is shown that the continuous limit of these DTQWs, when it exists, coincides with the dynamics of a Dirac fermion coupled to usual $U(N)$ gauge fields in two-dimensional spacetime. A discrete generalization of the usual $U(N)$ curvature is also constructed. An alternate interpretation of these results in terms of superimposed $U(1)$ Maxwell fields and $SU(N)$ gauge fields is discussed in the Appendix. Numerical simulations are also presented, which explore the convergence of the DTQWs towards their continuous limit and which also compare the DTQWs with classical (i.e., nonquantum) motions in classical $SU(2)$ fields. The results presented in this paper constitute a first step towards quantum simulations of generic Yang-Mills gauge theories through DTQWs.

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I. INTRODUCTION

Discrete-time quantum walks (DTQWs) are unitary quantum automata and can be viewed as formal generalizations of classical random walks. They were first considered in a systematic way by Meyer [1], following the seminal work of Feynman and Hibbs [2] and Aharonov *et al.* [3]. DTQWs have been realized experimentally with a wide range of physical objects and setups [4–10], and are studied in a large variety of contexts, ranging from fundamental quantum physics [10,11] to quantum algorithmics [12,13], solid-state physics [14–17], and biophysics [18,19].

It has been shown recently that the continuous limit of several DTQWs coincides with the dynamics of Dirac fermions coupled to electromagnetic [20–22] and relativistic gravitational fields [23–26]. Though these fields are naturally gauge fields, they are not generic Yang-Mills gauge fields. Indeed, electromagnetism is based on the Abelian gauge group $U(1)$, while relativistic gravitational fields are not Yang-Mills gauge fields, since they are represented by a metric, and not by a connection. The aim of this paper is to exhibit and study DTQWs the continuous limit of which coincides with the dynamics of a fermion coupled to Yang-Mills $U(N)$ gauge fields.

To make things definite and as simple as possible, we focus on one-dimensional (1D) DTQWs. The minimal 1D DTQWs have a two-dimensional coin space. Their wave functions thus have two components, one propagating towards the left and one towards the right. To take into account the internal degrees of freedom associated to $U(N)$ gauge invariance, we consider 1D DTQWs with coin space of dimension $2N$, i.e., $2N$ -component wave functions. Half of the wave-function components propagates towards the left, and the other half towards the right. The so-called mixing operator advancing the walk in time is represented by a $2N \times 2N$ time- and space-dependent unitary matrix.

We introduce 1D DTQWs with $2N$ components which admit an exact discrete $U(N)$ gauge invariance and build for the DTQWs a discrete equivalent \mathcal{F} of the usual Yang-Mills curvature F . We then prove that the limit of these DTQWs, when it exists, coincides with the dynamics of Dirac fermions coupled to $U(N)$ gauge fields and that the discrete curvature \mathcal{F} tends towards F in the continuous limit.

These formal computations are complemented by numerical simulations. These address the convergence of the DTQWs towards their continuous limit and the correspondence with classical (i.e., nonquantum) trajectories in Yang-Mills fields [27]. The paper concludes by a brief summary and a discussion of the main results. Finally, the Appendix elaborates on the fact that a $U(N)$ gauge field can be viewed as the superposition of a $U(1)$ Maxwell field and an $SU(N)$ gauge field, and reinterprets our results in that alternate context.

II. THE DTQWS AND THEIR GAUGE INVARIANCE

A. The DTQWs

We consider DTQWs defined over discrete time and infinite discrete one-dimensional space. Instants are labeled by $j \in \mathbb{N}$ and space points are labeled by $p \in \mathbb{Z}$. The coin space of the DTQWs has dimension $2N$. Given a certain orthonormal basis in this space, the wave functions Ψ of the walks are represented by $2N$ components and we group these components into two N -component sets ψ^- and ψ^+ , which represent those parts of Ψ which propagate, respectively, to the left and to the right. The evolution equations read

$$\begin{bmatrix} \psi_{j+1,p}^- \\ \psi_{j+1,p}^+ \end{bmatrix} = \mathbf{B}(\theta, P_{j,p}, Q_{j,p}) \begin{bmatrix} \psi_{j,p+1}^- \\ \psi_{j,p-1}^+ \end{bmatrix}, \quad (1)$$

with

$$\begin{aligned} \mathbf{B}(\theta, P, Q) &= (\mathbf{C}(\theta) \otimes \mathbf{1}_N) \times \begin{bmatrix} P & 0 \\ 0 & Q \end{bmatrix} \\ &\equiv \begin{bmatrix} (\cos \theta) P & (i \sin \theta) Q \\ (i \sin \theta) P & (\cos \theta) Q \end{bmatrix}, \end{aligned} \quad (2)$$

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where \otimes is the so-called Kronecker (or tensorial) product for matrices, and P and Q are elements of $U(N)$. These walks are unitary, i.e., $\Pi_j = \sum_p |\Psi_{j,p}|^2$ is independent of j .

In the continuous limit, the parameter θ will code for the mass of the fermion and the matrices P and Q will code for the potential of the $U(N)$ gauge field to which the fermion is coupled.

B. Discrete $U(N)$ gauge invariance and discrete curvature

The DTQWs defined by Eq. (1) admit a discrete local $U(N)$ gauge invariance. Indeed, consider the local gauge transformation $\Psi_{j,p} = (\mathbf{1}_2 \otimes G_{j,p}^{-1}) \Psi'_{j,p}$, where $G_{j,p}$ is some matrix of $U(N)$. Equation (1) is kept invariant under this transformation, that is,

$$\begin{bmatrix} \psi'_{j+1,p} \\ \psi'_{j+1,p} \end{bmatrix} = \mathbf{B}(\theta, P'_{j,p}, Q'_{j,p}) \begin{bmatrix} \psi'_{j,p+1} \\ \psi'_{j,p-1} \end{bmatrix}, \quad (3)$$

provided that we set

$$\begin{aligned} P'_{j,p} &= G_{j+1,p} P_{j,p} G_{j,p+1}^{-1}, \\ Q'_{j,p} &= G_{j+1,p} Q_{j,p} G_{j,p-1}^{-1}. \end{aligned} \quad (4)$$

The above gauge invariance suggests that $R = (P, Q)$ is the discrete equivalent of the usual continuous $U(N)$ gauge potentials. This will be confirmed in Sec. III, where the continuous limit of Eq. (1) will be derived. We now wish to build out of R an object \mathcal{F} defined on the spacetime lattice, which generalizes for DTQWs the usual curvature (field-strength) tensor [28] F of standard gauge fields. This will be done by searching for an object whose transformation law under a change of gauge resembles the transformation law of F . Let

$$\begin{aligned} U_{j,p}(R) &= Q_{j,p}^\dagger P_{j,p}, \\ V_{j,p}(R) &= Q_{j,p} P_{j-1,p-1}, \end{aligned} \quad (5)$$

whose transformation under a change of gauge reads

$$\begin{aligned} U'_{j,p}(R') &= G_{j,p-1} U_{j,p}(R) G_{j,p+1}^\dagger, \\ V'_{j,p}(R') &= G_{j+1,p} V_{j,p}(R) G_{j-1,p}^\dagger, \end{aligned} \quad (6)$$

involving shifts of $G_{j,p}$ only in the spatial (temporal) dimension for $U_{j,p}(R)$ [$V_{j,p}(R)$], while these shifts were mixed in the transformation laws of Eq. (4). From these equations, we can write transformation laws involving the $2 \times 2 = 4$ discrete-spacetime neighbors of $G_{j,p}$:

$$\begin{aligned} U'_{j+1,p}(R') &= G_{j+1,p-1} U_{j+1,p}(R) G_{j+1,p+1}^\dagger, \\ U'_{j-1,p}(R') &= G_{j-1,p-1} U_{j-1,p}(R) G_{j-1,p+1}^\dagger, \\ V'_{j,p-1}(R') &= G_{j+1,p-1} V_{j,p-1}(R) G_{j-1,p-1}^\dagger, \\ V'_{j,p+1}(R') &= G_{j+1,p+1} V_{j,p+1}(R) G_{j-1,p+1}^\dagger, \end{aligned} \quad (7)$$

from which we can build

$$\mathcal{F}_{j,p}(R) = U_{j-1,p}^\dagger(R) V_{j,p-1}^\dagger(R) U_{j+1,p}(R) V_{j,p+1}(R), \quad (8)$$

whose transformation law reads

$$\mathcal{F}'_{j,p}(R') = G_{j-1,p+1} \mathcal{F}_{j,p}(R) G_{j-1,p+1}^{-1}. \quad (9)$$

As will become apparent in the next section, \mathcal{F} is a discrete equivalent to the curvature (field-strength) tensor of continuous gauge fields.

III. CONTINUOUS LIMIT

We now show that it is possible to choose θ , P , and Q in such a way that Eq. (1) admits a continuous limit identical to the Dirac equation for a fermion coupled to an arbitrary $U(N)$ gauge field.

In order to compute the continuous limit of Eq. (1), we first introduce a dimensionless time and space step ϵ , and consider that $\Psi_{j,p}$, $P_{j,p}$, and $Q_{j,p}$ are the values $\Psi(t_j, x_p)$, $P(t_j, x_p)$, and $Q(t_j, x_p)$ taken at spacetime point $(t_j = j\epsilon, x_p = p\epsilon)$ by a $2N$ -component wave function Ψ and two time- and spacetime-dependent matrices P and Q in $U(N)$. We then assume that Ψ , P , and Q are at least twice differentiable with respect to both space and time variables and let ϵ tend to zero.

As ϵ tends to zero, the wave functions on the left-hand side and on the right-hand side of Eq. (1) both tend towards $\Psi(t_j, x_p)$. Thus, the continuous limit of Eq. (1) can only exist if, in that limit, $B(\theta, P, Q)$ tends to unity at all points in spacetime. This is achieved by choosing an angle θ which tends to zero with ϵ and two matrices P and Q which tend to unity as ϵ goes to zero. We retain $\theta = -\epsilon m$, where m is a positive constant (as opposed to a function of t and x) which will play the role of a mass in the continuous limit. As for the matrices P and Q , we remark that $U(N)$ is a compact and connected Lie group. Thus, the exponential map generates the whole group [29], i.e., all elements $M \in U(N)$ can be written as

$$M = \exp \left(i \sum_k X_M^k \tau_k \right), \quad (10)$$

where the τ_k 's are N^2 generators of $U(N)$ and the X_M^k 's can serve as coordinates for M .

To ensure that both functions $P(t, x)$ and $Q(t, x)$ tend to unity when ϵ tends to zero, we choose $X_P^k(t, x) = \epsilon b_P^k(t, x)$ and $X_Q^k(t, x) = \epsilon b_Q^k(t, x)$, where $b_{P/Q}^k(t, x)$ are two real functions independent of ϵ .

Taylor expanding Eq. (1) at first order in ϵ and letting ϵ tend to zero then delivers

$$\begin{aligned} (\partial_0 - i b_0^k \tau_k) \psi^- - (\partial_1 - i b_1^k \tau_k) \psi^- &= -i m \psi^+, \\ (\partial_0 - i b_0^k \tau_k) \psi^+ + (\partial_1 - i b_1^k \tau_k) \psi^+ &= -i m \psi^-, \end{aligned} \quad (11)$$

where $\partial_0 = \partial_t$, $\partial_1 = \partial_x$,

$$\begin{aligned} b_0 &= (b_Q + b_P)/2, \\ b_1 &= (b_Q - b_P)/2, \end{aligned} \quad (12)$$

and summation over repeated index k is implied.

Equations (11) can be recast as

$$[i \gamma^\mu D_\mu - m] \Psi = 0, \quad (13)$$

where index μ is summed over from zero to one, with the gamma matrices $\gamma^0 = \sigma_1 \otimes \mathbf{1}_N$ and $\gamma^1 = i \sigma_2 \otimes \mathbf{1}_N$ and the covariant derivative $D_\mu = \partial_\mu - i b_\mu^k \tau_k$. Equation (13) is the flat-spacetime Dirac equation, with convention $[\eta^{\mu\nu}] = \text{diag}(+, -)$, for a spin-1/2 fermion of mass m coupled to a non-Abelian $U(N)$ potential $b_\mu^k \tau_k$ (with coupling constant

$g = -1$) [28] belonging to the Lie algebra of $U(N)$. Note that the b_μ^k 's are real-valued space- and time-dependent fields.

Taylor expanding Definition (8) for \mathcal{F} delivers

$$\mathcal{F}(t, x) = \mathbf{1}_N + 4\epsilon^2 F_{10}(t, x) + O(\epsilon^3), \quad (14)$$

where F_{10} is the only nonvanishing component of the antisymmetric curvature (field-strength) tensor $F_{\mu\nu}$ of the connection $B_\mu = b_\mu^k \tau_k$, defined by

$$F_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu - i[B_\mu, B_\nu], \quad (15)$$

with $[B_\mu, B_\nu] = B_\mu B_\nu - B_\nu B_\mu$. Note that the transformation law for $F_{\mu\nu}$ under a change of gauge reads

$$F'_{\mu\nu} = G F_{\mu\nu} G^{-1}, \quad (16)$$

which closely parallels Eq. (9).

IV. NUMERICAL SIMULATIONS OF U(2)-INVARIANT DTQWS

A. Simulated walk

As shown in the Appendix to this paper, $U(N)$ factorizes into the product of $U(1)$ and $SU(N)$. In physical terms, this means that a $U(N)$ gauge field can be seen as the superposition of a $U(1)$ Maxwell field and an $SU(N)$ gauge field. The effects of Maxwell fields on DTQWs have already been presented in several publications [20,21,24]. We want to focus on the effects of non-Abelian Yang-Mills fields and thus choose to simulate situations where the Maxwell field identically vanishes so that the $U(N)$ gauge field is then actually an $SU(N)$ gauge field. We also choose the simplest option $N = 2$. The group $SU(2)$ is compact and connected, and can thus be fully generated by the exponential map, from three generators $\bar{\tau}_k$, $k = 1, 2, 3$, belonging to its Lie algebra. We retain (see the Appendix) $\bar{\tau}_k = \sigma_k/2$ where the σ_k 's are the three Pauli matrices, and choose

$$\begin{aligned} \bar{\mathbf{X}}_0 &= (\bar{\mathbf{X}}_Q + \bar{\mathbf{X}}_P)/2 = (0, 0, 0), \\ \bar{\mathbf{X}}_1 &= (\bar{\mathbf{X}}_Q - \bar{\mathbf{X}}_P)/2 = (\epsilon E_{\text{YM}} t, 0, 0). \end{aligned} \quad (17)$$

The bar is used to distinguish the notations used for $SU(2)$ from those used for $U(N)$, including $U(2)$, in Sec. III. The boldface notation is used as a reminder that the Lie algebra of $SU(2)$ is of dimension 3. The continuous limit can be recovered by letting ϵ tend to zero (see Sec. III). In such a continuous limit, this potential, Eq. (17), generates a uniform and constant $SU(2)$ “electric” field E_{YM} in the $\bar{\tau}_1$ direction of the $SU(2)$ Lie algebra.

B. Convergence towards the continuous limit

To study numerically the convergence of a DTQW towards a solution of the Dirac equation, we choose an initial wave function and compare, for some given time j , its evolution $\psi_{QW}^u(t_j, \cdot) = \epsilon j, \cdot, u \in \{+, -\}$, through the DTQW to the evolution $\psi_D^u(t_j, \cdot)$ of the same initial condition through the Dirac equation. The comparison is carried out through the following mean relative difference:

$$\delta\psi_j^u = \sqrt{\frac{\langle |\psi_D^u(t_j, \cdot) - \psi_{QW}^u(t_j, \cdot)|^2 \rangle}{\langle |\psi_D^u(t_j, \cdot)|^2 \rangle}}, \quad (18)$$

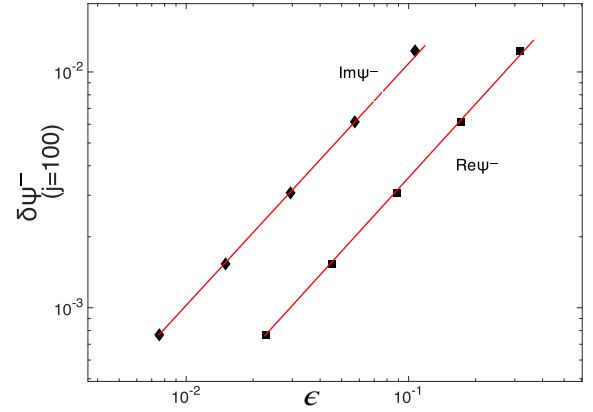


FIG. 1. Relative differences δf_j for $f = \text{Im } \psi^-$ and $f = \text{Re } \psi^-$ as functions of ϵ , at time $j = 100$, with $m = 0.1$ and $E_{\text{YM}} = 0.08$. The initial condition is given by Eq. (20) with $\sigma = 0.5$.

where

$$\langle f(t_j, \cdot) \rangle = \sum_{p=-p_{\text{max}}(\epsilon)}^{p_{\text{max}}(\epsilon)} f(t_j, x_p) \epsilon. \quad (19)$$

The numerical simulations are carried out over the space interval $[-x_{\text{max}}, x_{\text{max}}]$ with $x_{\text{max}} = 200$, and $p_{\text{max}}(\epsilon) \equiv x_{\text{max}}/\epsilon$. The maximal time over which we carry out the simulations, $t_{\text{max}} = 350$, is short enough so that the walker never reaches the spatial boundaries.

Note that $\delta\psi_j^u$ does not measure the difference between quantum states, for which phase differences are unimportant, but rather the difference between the functions ψ_D^u and ψ_{QW}^u . This is appropriate here because we want to test the convergence of a discrete scheme towards its formal continuous limit, and this convergence should be verified on both modulus and phase, i.e., on the whole complex function, and not only on the state it represents.

Since there is only a time dependence and no space dependence in the potentials (17), we can use as numerical solver for the Dirac equation standard pseudospectral methods [30,31], with resolution $2\pi/\epsilon$ in 2π -periodic boundary conditions. Time marching is performed using a second-order Runge-Kutta scheme. The original DTQW can also be simulated in spectral space using the standard translation operator in Fourier space.

Figure 1 shows that the mean relative differences δf_j for $f = \text{Im } \psi^-$ and $\text{Re } \psi^-$ scale as ϵ as expected: indeed, this scaling coincides with the theoretical expectation since, for a single time step, the discrepancy is theoretically of order ϵ^2 . Thus, after a fixed time $t = O(\epsilon^{-1})$, the discrepancy is of order $\epsilon^{-1}\epsilon^2 = \epsilon$. These results also confirm that the DTQW Eq. (1) with choice Eq. (17) can be used to simulate massive Dirac dynamics in a constant and uniform non-Abelian electric field E_{YM} .

C. Comparison with classical trajectories

Given a wave equation, it is well known [32] that the center of mass of a wave-packet solution follows classical trajectories. In the continuous-limit case described above in

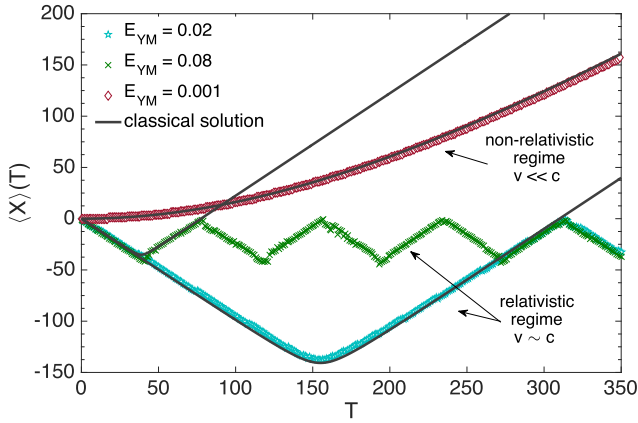


FIG. 2. Time evolution of the DTQW mean trajectory $\bar{x}(t)$ for a non-Abelian coupling constant $g = 1$ and different values of E_{YM} , vs classical trajectories (black solid line). Short-time agreement between quantum and classical dynamics is shown in the ultrarelativistic range $k_0^2 = 1$ (green and blue) and the nonrelativistic range $k_0^2 = 0$ (red). The initial condition is given by Eq. (20) with $\sigma = 0.5$ (green and blue), $\sigma = 1$ (red), and $m = 0.1$.

Sec. IV A, the corresponding classical equations have been explicitly derived in [27]. We now want to investigate whether the original DTQW also reproduces classical motions of the center-of-mass of wave packets.

We consider k_0 -centered Gaussian wave packets of positive-energy eigenvector $u_+(k)$ of the two-component [i.e., without $SU(2)$ internal degree of freedom] free Dirac Hamiltonian, tensorized with an equally weighted initial $SU(2)$ state:

$$\Psi(x) = \int dk e^{-\frac{(k-k_0)^2}{2\sigma^2} + i x k} [u_+(k) \otimes (1,1)^T / \sqrt{2}], \quad (20)$$

where superscript \top denotes the transposition, and

$$u_+(k) = \left[\frac{\sqrt{k^2 + m^2} - k}{\sqrt{(\sqrt{k^2 + m^2} - k)^2 + m^2}}, \frac{1}{\sqrt{\frac{(\sqrt{k^2 + m^2} - k)^2}{m^2} + 1}} \right]^T. \quad (21)$$

Figure 2 demonstrates the short-time agreement between solutions of classical particle trajectory equations (see [27]) and the centers of wave packets $\bar{x}(t)$ obtained from DTQW solutions, both in the nonrelativistic case, $k_0^2 = 0$, $m = 0.1$, and in the relativistic case, $k_0^2 = 1$, $m = 0.1$. When the agreement is lost, the oscillatory trajectory for $\bar{x}(t)$ is produced by the DTQW. Note that similar long-time oscillations are also found in the simple context of DTQWs corresponding to Dirac fermions coupled to electromagnetic fields [33].

V. CONCLUSION

We have introduced DTQWs on the line which exhibit an exact discrete $U(N)$ gauge invariance and the continuous limit of which coincides, when it exists, with the dynamics of Dirac fermions coupled to $U(N)$ gauge fields. We have also built a discrete generalization of the curvature tensor of the gauge fields. We have finally complemented these analytical results by numerical simulations which explore the convergence of

the DTQWs towards their continuous limit and compare the DTQWs with the dynamics of nonquantum particles in classical gauge fields. The interpretation of our results in terms of Maxwell fields superimposed to $SU(N)$ gauge fields is presented in the Appendix. The results presented in this paper constitute a first step towards quantum simulations of generic Yang-Mills gauge theories through DTQWs. Until now, only DTQWs with two-component wave functions have been realized experimentally [34]. But experimental procedures allowing the implementation of DTQWs with wave functions having more than two components have been proposed in [35,36]. In these procedures, the DTQWs are implemented with single photons or classical light, for example in optical cavities.

Let us now mention a few avenues open to future studies. The DTQWs presented in this paper should first be extended to $(1+2)$ and then to $(1+3)$ spacetime dimensions. Note that DTQWs modeling Dirac fermions coupled to $U(1)$ gauge fields have already been proposed in $(1+1)$ and $(1+2)$ dimensions [20–22]. Another possible extension would be the construction of DTQWs which are coupled, not only to $U(N)$ gauge fields but also to gravity. Until now, this has only been done for $N = 1$ and in $(1+1)$ spacetime dimensions [24]. Also, performing full quantum simulations of Yang-Mills gauge theories will require complementing the fermionic DTQW dynamics by dynamical equations for the discrete gauge fields, i.e., for matrices $P, Q \in U(N)$ which define the DTQW. The dynamical equations for the gauge field should be a set of finite difference equations relating the discrete curvature (field-strength) tensor \mathcal{F} introduced in the present paper to a discrete gauge-invariant fermionic current associated to the DTQW. This current has already been presented in [22] for $N = 1$ in $(1+2)$ spacetime dimensions, and the corresponding discrete Maxwell equations have also been written down. The procedure should now be extended to generic noncommutative discrete gauge fields. Finally, incorporating Yang-Mills fields to DTQWs defined on arbitrary graphs is certainly worth working on, if only for applications to quantum information.

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APPENDIX: ALTERNATIVE PHYSICAL INTERPRETATION

The Lie group $U(N)$ is the group of $N \times N$ unitary matrices, i.e., $N \times N$ matrices the determinant modulus of which equals unity. In particular, elements of $U(1)$ are complex numbers of the unit modulus, i.e., complex numbers of the form $\exp(i\beta)$, where β is an arbitrary real number. The group $U(N)$ is Abelian for $N = 1$ and non-Abelian for $N > 1$. Consider now an arbitrary element M of $U(N)$, its determinant $\det M = \exp(i\alpha)$, $\alpha \in]-\pi, +\pi]$, and we define the matrix $\tilde{M} = M/\delta$ where $\delta^N = \det M$. The matrix \tilde{M} has a unit determinant and is thus an element of the special unitary group $SU(N)$. The group $U(N)$ can therefore be factorized into the direct product of $U(1)$ and $SU(N)$. This

factorization is not unique because δ is not uniquely defined by the equation $\delta^N = \det M$. Indeed, this equation has the N distinct solutions $\delta_k = \exp[i(\alpha + 2k\pi)/N]$, $k = 0, \dots, N-1$, and each solution defines a different factorization. Note also that imposing a factorization which depends continuously on M is only possible if one makes a cut along the negative real axis in the complex plane of $\det M$, i.e., if one does not define the factorization for matrices M the determinant of which corresponds to the value $\alpha = \pi$ (and is thus equal to -1).

To make all computations definite, we now choose $k = 0$ in the above definition of δ_k . This defines unambiguously a factorization of $U(N)$ into the direct product of $U(1)$ and $SU(N)$. This factorization is not continuous for matrices M with $\det M = -1$, but that should not be a practical problem when one is working on a spacetime lattice. In the continuous limit, all $U(N)$ matrices considered in this paper tend to unity. Their determinant is thus close to unity and the retained factorization is thus defined and continuous for all these matrices.

In physical terms, the existence of the factorization means that a $U(N)$ gauge field can be interpreted as the superposition of a $U(1)$ Maxwell field and an $SU(N)$ gauge field. Now, $SU(N)$ is itself a compact and connected Lie group, so the whole group is generated from the identity by the exponential map. The above factorization can thus be used to write all matrices $M \in U(N)$ as

$$M = \delta_M \bar{M} = \exp(iY_M) \exp\left(i \sum_k \bar{X}_M^k \bar{\tau}_k\right), \quad (\text{A1})$$

where the $\bar{\tau}_k$'s are the $N^2 - 1$ generators of $SU(N)$. This point of view is adopted in Sec. IV A. Note that the factorization of $U(N)$ also shows that the DTQWs presented in this paper coincide, for $N = 1$, with the DTQWs already proposed to simulate Dirac fermions coupled to arbitrary electric fields [20].

The discrete curvature \mathcal{F} also factorizes into a curvature for the Maxwell field and a curvature for the $SU(N)$ gauge field.

One finds indeed that

$$\mathcal{F}_{j,p}(R) = \mathcal{F}_{j,p}(\delta_R) \mathcal{F}_{j,p}(\bar{R}) \quad (\text{A2})$$

where $\delta_R = (e^{iY_P}, e^{iY_Q})$ and $\bar{R} = (\bar{P}, \bar{Q})$. The $SU(N)$ curvature $\mathcal{F}_{j,p}(\bar{R})$ is given by Eq. (8) and the $U(1)$ Abelian curvature reads

$$\mathcal{F}_{j,p}(\delta_R) = \exp[2i(\mathcal{I}f_{10})_{j,p}], \quad (\text{A3})$$

where

$$(f_{10})_{j,p} = (d_1 Y_0)_{j,p} - (d_0 Y_1)_{j,p}, \quad (\text{A4})$$

with

$$\begin{aligned} Y_0 &= (Y_Q + Y_P)/2, \\ Y_1 &= (Y_Q - Y_P)/2, \end{aligned} \quad (\text{A5})$$

$$d_0 = (L_0 - \Sigma_1), \quad d_1 = \Delta_1, \quad (\text{A6})$$

and

$$\begin{aligned} (L_0 K)_{j,p} &= K_{j+1,p}, \\ (\Sigma_1 K)_{j,p} &= (K_{j,p+1} + K_{j,p+1})/2, \\ (\Delta_1 K)_{j,p} &= (K_{j,p+1} - K_{j,p+1})/2, \end{aligned} \quad (\text{A7})$$

where K is an arbitrary quantity which depends on j and p . Operator \mathcal{I} is defined in terms of L_0 and L_1 by

$$\mathcal{I} = 1 + L_0^{-1} L_1^{-1}. \quad (\text{A8})$$

This form of $\mathcal{F}_{j,p}(\delta_R)$ is interesting because $(f_{10})_{j,p}$ and operators d_0 and d_1 have already been introduced in [22] in the context of DTQWs exhibiting a $U(1)$ gauge invariance.

Choosing $Y_\mu = \epsilon A_\mu$, $\bar{X}_{P/Q}^k = \epsilon \bar{b}_{P/Q}^k$ and Taylor expanding Eq. (A2) at second order in ϵ delivers

$$\mathcal{F}_{j,p}(R) = \mathbf{1}_N + 4\epsilon^2(f_{10}\mathbf{1}_N + \bar{F}_{10}) + O(\epsilon^3), \quad (\text{A9})$$

where \bar{F}_{10} is given by Eq. (15) after substitution $B \rightarrow \bar{B}$, and $f_{10} = \partial_1 A_0 - \partial_0 A_1$ is the (10) component of the usual Abelian curvature tensor.

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Part II

DTQWs interacting with gravitational fields

One-dimensional DTQWs in gravitational fields

Contents

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MOTIVATIONS

The aim of this introductory material to the second part of the manuscript, is to give a pedagogical, general, and essential view of the results of Refs. [91, 90], that is, of how to make a DTQW propagate in a (1+1)D curved spacetime, to speak in vague but pointful terms, that must be clarified later. The publication on which the next, third and last chapter is based, is an extension of the results presented in this introductory material.

ii.1 Quantum walks as Dirac fermions in (1+1)D curved spacetime

ii.1.1 General relativity and gravitation-induced advecting speed field

In general relativity, the gravitational field experienced by a particle, due to surrounding mass-energy sources, is encoded in the spacetime deformation¹, which is mathematically described by a pseudo-Riemannian space with signature $(+, -, \dots, -)$, with as many minus signs as the spatial dimensions. In this curved spacetime, the particle follows geodesics, i.e. is a free particle, subject to no force, since the gravitational force is *already* encoded in the curvature of space. Projecting this spacetime deformation, with the tetrad formalism, on some flat, i.e. Minkowskian spacetime, which can be chosen as the local inertial spacetime

¹Deformation with respect to the standard Euclidean spacetime.

of the particle (i.e., the spacetime which is tangent to the worldline), gives the particle a *spacetime-varying* speed (in this flat spacetime), i.e. an *acceleration*, consequence of the gravitational force produced by the projection of the original-spacetime curvature on the flat spacetime. If we take the non-relativistic limit, such a spacetime variation of the speed is that induced by the *Newtonian* gravitational force.

Equation (35b) tells us that ψ^\downarrow is transported at (dimensionless) speed 1 (algebraically on the line), with a deformation induced by the mass-coupling source term $-im\psi^\uparrow$ (the mass m couples ψ^\uparrow and ψ^\downarrow).

Indeed, forget about the mass-coupling source term for a moment, and consider the following standard (deformationless) advection equation for an arbitrary quantity $u(t,x)$, at constant and uniform speed v :

$$(\partial_t + v\partial_x)u = 0. \quad (\text{ii.1})$$

Any function $f(x - vt)$ is a solution of this equation, and the equation thus describes the transport of the function f at speed v ; this transport mechanism is homogeneous, i.e. is the same at every spacetime point because so is v .

Imagine now that v is spacetime dependent, i.e. $v(t,x)$, as induced by a gravitational field. Again, any solution of the form $f(x - v(t,x)t)$ is solution of this equation²: the equation thus describes the transport of the function f at speed $v(t,x)$; this transport mechanism is inhomogeneous, i.e. depends on the spacetime point (t,x) through $v(t,x)$.

ii.1.2 **Standard DTQWs cannot yield any spacetime-dependent advecting speed field in the continuum limit**

ii.1.2.1 **The DTQW must be inhomogeneous**

Our question is how to obtain the spacetime-dependent transport described by Eq. (ii.1) with local speed $v(t,x)$, for the wavefunction of a quantum particle, in the continuum limit of some DTQW. Technically, the question is how to obtain a spacetime-dependent speed $v(t,x)$ in front of ∂_x in, e.g., Eq. (35b), instead of the constant speed 1.

Considering a standard DTQW, see Eq. (10), homogeneous, i.e. whose coin operation does not depend on the (1+1)D spacetime-lattice point (j,p) , means that the discrete transport mechanism is the same at each (j,p) , and this holds in some possibly-existing continuum limit, i.e. the latter cannot describe any spacetime-dependent transport such as that we wish to obtain.

ii.1.2.2 **The standard ‘one-step’ continuum limit of inhomogeneous DTQWs does not do the job either**

Here we present a quick technical sum-up of why such a continuum limit will not work.

Consider a coin operation (5) with spacetime-dependent entries, $q_{j,p} = ((q_s)_{j,p})_{s=1,4} = (\alpha_{j,p}, \theta_{j,p}, \xi_{j,p}, \zeta_{j,p})$, that we allow to read

$$(q_s)_{j,p} = (q_s^0)_{j,p} + \epsilon_q (\bar{q}_s)_{j,p} + \mathcal{O}(\epsilon_q^2), \quad (\text{ii.2})$$

²This is true provided that $v(t,x)$ itself satisfies the equation, i.e. provided that its convective derivative vanishes, $\frac{dv}{dt} \equiv (\partial_t + v\partial_x)v = 0$, which merely states that v is an imposed field, having no dynamics, and that if a point particle is embedded in it at point (t,x) , it will move with speed $v(t,x)$.

which is merely a sufficient condition for the coin operation to have a limit in the continuum, i.e. when the spacetime-lattice step $\epsilon_l = \epsilon_q$, goes to zero. Consider now the Taylor expansion in ϵ_l of the DTQW one-step evolution equation, Eq. (10), with spacetime-dependent coin operation $U^{\text{Euler}}(q(t,x))$, $t = j\epsilon_l$, $x = p\epsilon_l$. The derivatives $\partial_x \psi^{\uparrow\downarrow}$ can only come from the multiplication of the *first-order* terms $\partial_x \psi^{\uparrow\downarrow}$ by a spacetime-dependent quantity function of the *zeroth-order* angles, $(q_s^0)_{j,p}$. But we know that there is a zeroth-order constraint for the continuum limit to exist, namely $U^{\text{Euler}}(q^0(t,x)) = \mathbf{1}_2$, that is to say,

$$e^{i(\alpha^0 + \xi^0)} \cos \theta^0 = 1 \quad (\text{ii.3a})$$

$$e^{i(\alpha^0 - \xi^0)} \cos \theta^0 = 1 \quad (\text{ii.3b})$$

$$e^{i(\alpha^0 + \zeta^0)} \sin \theta^0 = 0 \quad (\text{ii.3c})$$

$$e^{i(\alpha^0 - \zeta^0)} \sin \theta^0 = 0. \quad (\text{ii.3d})$$

$$(\text{ii.3e})$$

For such constraints to be satisfied, all four zeroth-order angles must be *independent of the spacetime point*. Hence, no standard DTQW can yield any spacetime-dependent transport in the continuum limit we have considered.

ii.1.3 k -step continuum limit and DTQW in curved spacetime

The previous ‘one-step’ continuum limit does not allow for any sharp variation of the (j,p) -dependent quantities, even on spacetime scales of the order of a few spacetime-lattice sites, because we demand that these (j,p) -dependent quantities coincide with smooth functions at *each* spacetime point. Let us take a coarser look and lower this requirement by demanding a coincidence every k spacetime points, k being an integer superior or equal to 2. This defines a larger class of continuum limits, which contains the one-step class. This means that the evolution equation whose Taylor equation we are going to perform is not anymore the one-step equation, Eq. (10), but the k -step one, i.e.

$$\langle p | \begin{pmatrix} |\psi_{j+k}^{\uparrow}\rangle \\ |\psi_{j+k}^{\downarrow}\rangle \end{pmatrix} \rangle = \langle p | \underbrace{\begin{bmatrix} e^{i\xi_j} \cos \theta_j & e^{i\zeta_j} \sin \theta_j \\ -e^{-i\zeta_j} \sin \theta_j & e^{-i\xi_j} \cos \theta_j \end{bmatrix}}_{U^{\text{Euler}}(q_j)} \begin{bmatrix} \sum_p |p-1\rangle \langle p| & 0 \\ 0 & \sum_p |p+1\rangle \langle p| \end{bmatrix} \rangle^k \begin{pmatrix} |\psi_j^{\uparrow}\rangle \\ |\psi_j^{\downarrow}\rangle \end{pmatrix}, \quad (\text{ii.4})$$

where we have used the suitable notation of a quantum state which is explicit in spin space but implicit in position space.

The zeroth-order constraint for such a k -step continuum limit to exist is $(U^{\text{Euler}}(q_{j,p}^0))^k = \mathbf{1}_2$. This stroboscopic view of DTQWs has been introduced by Di Molfetta et al. in [91], and the zeroth-order constraints for the continuum limit to exist have been fully examined for $k = 2$ in [90].

We can show that the following coin [91, 90],

$$B(\theta) = \begin{bmatrix} -\cos \theta & i \sin \theta \\ -i \sin \theta & \cos \theta \end{bmatrix}, \quad \theta(t,x), \quad (\text{ii.5})$$

which satisfies the zeroth-order constraint for $k = 2$ (but *not* for $k = 1$), yields a DTQW whose 2-step continuum limit describes the dynamics of a (massless) Dirac fermion in a (1+1)D curved spacetime with signature $(+,-)$, with a speed

$$v(t,x) \propto \cos^2 \theta(t,x), \quad (\text{ii.6})$$

where t is, as in the one-step case, the continuum-limit time corresponding to the discrete one j , i.e. $t_j = j\epsilon_t \rightarrow t$ when $\epsilon_t \rightarrow 0$. The PDE of such a dynamics can be written in the following compact form,

$$\gamma^{(a)} \left[e_{(a)}^\mu \partial_\mu \Phi + \frac{1}{2} \frac{1}{\sqrt{-G}} \partial_\mu \left(\sqrt{-G} e_{(a)}^\mu \right) \Phi \right] = 0, \quad (\text{ii.7})$$

where $\mu \in \{t, x\}$, $a \in \{0, 1\}$, $e_{(a)}^\mu$ are the components of the diad, i.e. orthonormal basis, ($e_0 = e_t$, $e_1 = (\cos \theta) e_x$), on the original coordinate basis (e_t, e_x) , $\Phi = \Psi \sqrt{\cos \theta}$ is the spinor which lives in the curved spacetime, $[G_{\mu\nu}] = \text{diag}(1, -1/\cos^2 \theta)$ is the metric tensor of the curved spacetime, $G = \det [G_{\mu\nu}]$, and the (flat) gamma matrices are given, as usually chosen in our work, by $\gamma^{(0)} = \sigma_1$, $\gamma^{(1)} = i\sigma_2$. (We know put round brackets around the indices labelling the coordinates on the locally-flat spacetime.)

ii.2 Application: radial motion of a DTQW in a Schwarzschild blackhole

In Refs. [91, 90] is shown an application of the previous result to a (1+1)D metric associated to a time and a radial coordinate of a Schwarzschild blackhole. If the walker, which, remember, carries as spin-1/2, starts on the horizon of the blackhole, half of its occupation probability (or density) will collapse on the singularity, while the other half will remain localized on the horizon. If the walker starts below the horizon, i.e. inside the blackhole, it will not escape from it; more precisely, half of its density (i.e. one branch), will end on the singularity at some instant, while the other branch will also end on this singularity, but later. If the walker starts outside the blackhole, one branch will still collapse on the singularity, while the other branch will escape from the blackhole.

Two-dimensional DTQWs in gravitational fields (Publication [4])

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3.1.1 Short but detailed review and comments	105

3.1 Publication [4]: Quantum walks and gravitational waves

— ABSTRACT —

In this publication, we present a new family of 2D DTQWs which coincides, in the continuum limit, with the Dirac dynamics of a relativistic spin-1/2 fermion in a generic (1+2)D curved spacetime. We then focus on the particular case where this spacetime corresponds to the polarization plane of a gravitational wave (GW). We show how the probability of presence of the DTQW in this plane is affected by a pure shear GW. In the continuum limit, the GW modifies the eigen-energies of the walker by an anisotropic factor which is computed exactly. For wavelengths close to the spacetime-lattice step, the probability of presence is modified non trivially; the minimal comment on such an influence is that the net effect of the GW is maximal for short wavelengths, comparable to the spacetime-lattice step.

3.1.1 Short but detailed review and comments

This paper, Ref. [4], begins by a 2D generalization of the 1D formal results obtained in Ref. [91]: indeed, we introduce a 2D DTQW whose continuum limit yields the dynamics of a spin-1/2 Dirac fermion propagating in an arbitrary (1+2)D curved spacetime, see Section III of the paper. The construction is based on the 1D 2-step construction, see Section ii.1 for a sum-up, and is discussed in depth in Section II of the paper. For a general technical presentation of the Dirac equation in curved spacetime, see Appendix M.

We then consider the particular case where the 2D curved space is that corresponding to a polarization plane of a (linear and plane) gravitational wave (GW), see Section IV, and we focus on pure shear GWs in Section V, where we present and discuss the dispersion relation

of the DTQW, in Fig. 1. It is important to have in mind that the (1+2)D curved spacetime can be interpreted as such only in the continuum situation, because we have not made any link with a proper notion of curvature on the lattice. The curved metric corresponding to the aforementioned GW is usually treated, in the standard continuum situation, as a small metric deformation of the flat-spacetime Minkowskian metric. We proceed in the same way for the DTQW evolving on the lattice, and all computations are made at first order in the metric perturbation, whose perturbative nature is traced by the small parameter ξ .

In Section VI, we analyse two case-studies in this pure-shear-GW background:

- The first case-study, Subsection VI A, presents the continuum situation, i.e. how the pure shear GW modifies the flat-spacetime dynamics of a 2D spin-1/2 Dirac fermion. Such a continuum situation is reached, from the DTQW lattice situation, by making the spacetime-lattice step, ϵ_l , go to zero, or equivalently, by taking to zero the quasimomentum of the quantum walker, namely $\mathbf{q} = \epsilon_l \mathbf{Q}$, where \mathbf{Q} is the momentum of the associated Dirac fermion of the continuum situation¹. We give the corrections to the free (i.e. flat-spacetime) dynamics, due to the metric curvature induced by the GWs. We give the corrections (i) to the one-step Dirac evolution operator, see Eq. (32), and (ii) to the eigen-elements of this Dirac operator, see Eqs (33) and (34). In particular, the effect of the pure shear GWs on the usual relativistic dispersion relation of Dirac fermions, of the form energy = \pm momentum, is the addition of an anisotropic correction, i.e. whose magnitude depends on the direction in the polarization plane, see Eq. (35).
- The second case-study, Subsection VI B, goes beyond the continuum-limit situation, i.e., to speak in a lattice terminology, explores the whole Brillouin zone, and not only small quantum-walker wavevectors. The problem we are interested in is the modification, by the GW, of an interferential DTQW matter distribution located in some polarization plane of the wave. In Appendix L are given technical details and motivations for such a study. We limit ourselves to the modification after a single time step, which is best seen on the relative matter-distribution change, between the initial time and that after one time step, defined by Eq. (37) and given, after an analytical computation, by Eq. (38). Since such a quantity is position dependent in the polarization plane, and we are interested in the maximum effect of the wave, we look for the maximum value, in the polarization plane, of the relative matter-distribution change, see Eq. (40). Such a quantity is maximum for matter modes whose wavelength is comparable to a few lattice steps, see Fig. 4, i.e. the effect of the wave is stronger at small spatial scales comparable to the lattice step, than in the continuum large-scale situation.

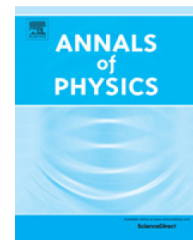
¹Note that, even if ϵ_l (and thus \mathbf{q}), goes to zero, \mathbf{Q} can have an arbitrarily big modulus.



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Quantum walks and gravitational waves



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H I G H L I G H T S

- Explicit construction of quantum walks coupled to $(1 + 2)$ D gravitational fields.
- Study of $(1 + 2)$ D quantum walks coupled to gravitational waves.
- Interference patterns of quantum walks in gravitational waves.

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A B S T R A C T

A new family of discrete-time quantum walks (DTQWs) propagating on a regular $(1 + 2)$ D spacetime lattice is introduced. The continuum limit of these DTQWs is shown to coincide with the dynamics of a Dirac fermion coupled to an arbitrary relativistic gravitational field. This family is used to model the influence of arbitrary linear gravitational waves (GWs) on DTQWs. Pure shear GWs are studied in detail. We show that on large spatial scales, the spatial deformation generated by the wave induces a rescaling of the eigen-energies by a certain anisotropic factor which can be computed exactly. The effect of pure shear GWs on fermion interference patterns is also investigated, both on large scales and on scales comparable to the lattice spacing.

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1. Introduction

Discrete-time quantum walks (DTQWs) are unitary quantum automata. They are not stochastic but can be viewed nevertheless as formal quantum analogues of classical random walks. They were first introduced by Feynman [1,2] in the 1940s and later re-introduced, as ‘quantum random walks’ by Aharonov et al. [3], and in a systematic way by Meyer [4]. DTQWs have been realized experimentally with a wide range of physical objects and setups [5–11], and are studied in a large variety of contexts, ranging from fundamental quantum physics [6,12] to quantum algorithmics [13,14], solid-state physics [15–18] and biophysics [19,20].

It has been shown recently that the continuum limit of several DTQWs defined on regular $(1 + 1)$ D spacetime lattices coincides with the dynamics of Dirac fermions coupled, not only to electric fields [21,22], but also to arbitrary non-Abelian Yang–Mills gauge fields [23] and to relativistic gravitational fields [24–27]. Gravitational waves (GWs) [28] are of great interest, both theoretically and experimentally, and their effects on DTQWs are thus worth investigating. The interest about GWs has been renewed by their recent direct detection [29]. Linear GWs resemble electromagnetic waves. In particular, GWs can be expanded as a superposition of plane waves and each plane wave as a superposition of two polarization states, both polarizations being perpendicular to the direction of propagation. The effect of these plane GWs on matter is thus typically studied in the polarization plane and it makes little sense to envisage the action of GWs on $(1 + 1)$ D DTQWs. Performing a valid study of how GWs influence DTQWs thus requires building DTQWs coupled to $(1 + 2)$ D gravitational fields.

We start by presenting a new family of $(1 + 2)$ D DTQWs whose continuum limit coincides with the dynamics of a Dirac fermion coupled to arbitrary $(1 + 2)$ D gravitational fields. The construction of this family is inspired by the $(1 + 1)$ D construction presented in [25]. The DTQWs in the $(1 + 2)$ D spacetime depend on two parameters, which code for the mass of the walker and for the finite spacing of the lattice, and on four time- and space-dependent angles. We then show how to choose these four angles to describe linear GWs. A generic linear GW on the lattice can be considered as the superposition of three waves: two compression waves along the directions of the lattice and a shear wave coupling directly two directions of the lattice through non-diagonal metric components. Shear effects are of particular interest in relativistic gravitation and are present in generic solutions of Einstein equations [30]. We thus focus on pure shear GWs and examine in detail their action on the DTQWs. Our main results are the following. On large spatial scales, pure shear GWs rescale locally the eigen-energies by an anisotropic factor, to make up for the space deformation induced by the wave, and the eigen-polarizations are modified as well. On smaller scales comparable to a few lattice spacings, both polarizations and energies are modified in a non-trivial way; this has the effect of changing significantly the interference pattern of two fermion eigen-modes. A final section discusses the construction of the DTQWs and mentions several avenues open to further study.

2. DTQWs in $(1 + 2)$ dimensions

Consider a quantum walker moving on a two-dimensional lattice (discrete space) with nodes labeled by $(p_1, p_2) \in \mathbb{Z}^2$. Let $j \in \mathbb{N}$ label discrete time and (b_-, b_+) be a certain time- and position-independent basis of the two-dimensional coin Hilbert space of the walker, that we identify to $((1, 0)^\top, (0, 1)^\top)$, where \top denotes the transposition. The state of the walker at time j and point (p_1, p_2) is described by a two-component wave function $\Psi_{j,p_1,p_2} = \psi_{j,p_1,p_2}^- b_- + \psi_{j,p_1,p_2}^+ b_+$. The collection $(\Psi_{j,p_1,p_2})_{(p_1,p_2) \in \mathbb{Z}^2}$ will be denoted by Ψ_j .

The time evolution of Ψ_j is fixed by a time-dependent unitary operator V_j :

$$\Psi_{j+1} = V_j \Psi_j. \quad (1)$$

This unitary operator involves two real positive parameters, ϵ and m , and four time- and space-dependent angles θ^{11} , θ^{12} , θ^{21} and θ^{22} ; it consists essentially in a combination of rotations in spin space and of translations in physical space, along the two directions of the lattice. The operator V_j consists in a rather complicated combination of rotations in spin space and of translations in physical

space along the two directions of the lattice. It is defined as follows:

$$V_j = \mathbf{\Pi}^{-1} \left[\mathbf{W}_1(\theta_j^{12}) \mathbf{W}_2(\theta_j^{22}) \right] \mathbf{\Pi} \left[\mathbf{W}_2(\theta_j^{21}) \mathbf{W}_1(\theta_j^{11}) \right] \mathbf{Q}(\epsilon(m - T_\epsilon(\boldsymbol{\theta})/4)), \quad (2)$$

where $\theta_j^{kl} = (\theta_{j,p_1,p_2}^{kl})_{(p_1,p_2) \in \mathbb{Z}^2}$ for $(k, l) \in \{1, 2\}^2$, and $\boldsymbol{\theta} = (\theta_j^{kl})_{(k,l,j) \in \{1,2\}^2 \times \mathbb{N}}$. The operator $\mathbf{\Pi}$ is

$$\mathbf{\Pi} = \frac{1}{\sqrt{2}} \begin{bmatrix} -i & 1 \\ -1 & i \end{bmatrix}. \quad (3)$$

The operators $\mathbf{W}_k(\theta_j)$, $k \in \{1, 2\}$, are defined by

$$\mathbf{W}_k(\theta_j) = \mathbf{R}^{-1}(\theta_j) \left[\mathbf{U}(\theta_j) \mathbf{S}_k \mathbf{U}(\theta_j) \mathbf{S}_k \right] \mathbf{R}(\theta_j), \quad (4)$$

where \mathbf{S}_k is the spin-dependent translation operator in the k spatial direction, while $\mathbf{R}(\theta_j)$ and $\mathbf{U}(\theta_j)$ are rotations in the coin Hilbert space:

$$\begin{aligned} (\mathbf{S}_1 \Psi_j)_{p_1,p_2} &= \begin{bmatrix} \psi_{j,p_1+1,p_2}^- \\ \psi_{j,p_1-1,p_2}^+ \end{bmatrix} \\ (\mathbf{S}_2 \Psi_j)_{p_1,p_2} &= \begin{bmatrix} \psi_{j,p_1,p_2+1}^- \\ \psi_{j,p_1,p_2-1}^+ \end{bmatrix}, \end{aligned} \quad (5)$$

$$\begin{aligned} (\mathbf{R}(\theta_j) \Psi_j)_{p_1,p_2} &= \mathbf{r}(\theta_{j,p_1,p_2}) \Psi_{j,p_1,p_2} \\ (\mathbf{U}(\theta_j) \Psi_j)_{p_1,p_2} &= \mathbf{u}(\theta_{j,p_1,p_2}) \Psi_{j,p_1,p_2}, \end{aligned} \quad (6)$$

with

$$\begin{aligned} \mathbf{u}(\theta) &= \begin{bmatrix} -\cos \theta & i \sin \theta \\ -i \sin \theta & \cos \theta \end{bmatrix} \\ \mathbf{r}(\theta) &= \begin{bmatrix} i \cos(\theta/2) & i \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2) \end{bmatrix}. \end{aligned} \quad (7)$$

Finally

$$\mathbf{Q}(M) = \begin{bmatrix} \cos(2M) & -i \sin(2M) \\ -i \sin(2M) & \cos(2M) \end{bmatrix}, \quad (8)$$

and

$$T_\epsilon(\boldsymbol{\theta}) = \sum_{k=1}^2 (C^{k2} D_0^\epsilon (C^{-1})^{1k} - C^{k1} D_0^\epsilon (C^{-1})^{2k}), \quad (9)$$

with $(D_0^\epsilon K)_{j,p_1,p_2} = (K_{j+1,p_1,p_2} - K_{j,p_1,p_2})/\epsilon$ for any quantity K_{j,p_1,p_2} defined on the spacetime lattice, and

$$[C^{kl}] = [\cos \theta^{kl}]. \quad (10)$$

Let us now comment on the construction of the operator V_j . The new $(1+2)$ D DTQWs defined by (1) are inspired by the $(1+1)$ D DTQWs introduced in [24]. As shown in this earlier work, the coupling of a DTQW with a gravitational field in $(1+1)$ D can only be obtained if the walker performs at each time step not one, but two jumps in the spatial direction. Thus, one would expect that coupling DTQWs with gravitational fields in $(1+2)$ D could be obtained by letting the walker perform two jumps in each spatial direction at each time-step. These jumps are represented by the operators $\mathbf{W}_1(\theta_j^{11})$ and $\mathbf{W}_2(\theta_j^{22})$ which we will discuss in more detail below. These 2×2 jumps however do not suffice and do not take into account the shear generated by generic gravitational fields. This shear couples directions and manifest itself by non-diagonal metric coefficients which do not vanish identically. To take the

shear into account, the quantum walker has to perform two extra jumps in each direction at each time step. These two extra jumps are represented by the operators $\mathbf{W}_1(\theta_j^{12})$ and $\mathbf{W}_2(\theta_j^{21})$. We are interested in DTQWs whose continuum limit coincides with the Dirac equation. Choosing a given representation of the $(1+2)$ D Clifford algebra to write down Dirac equation in explicit form introduces an apparent symmetry breaking between the two space directions x and y , even in flat spacetime. The operator Π enters the definition of the DTQWs to account for this apparent symmetry breaking. The operators $\mathbf{W}_k(\theta_j)$ themselves deserve some more comments. Each operator involves two jumps, represented by the operators \mathbf{S}_k 's, and two mixing operators, represented by the $\mathbf{U}(\theta_j)$'s. As shown in [24] for the $(1+1)$ D, involving only these operations would deliver the correct Dirac dynamics in the continuum limit, but not in a standard 'fixed' spin basis. The operators $\mathbf{R}^{-1}(\theta_j)$ and $\mathbf{R}(\theta_j)$ compensate for this basis difference.

The operator $\mathbf{Q}(\epsilon(m - T_\epsilon(\theta))/4)$ is included (i) to endow the DTQW with the mass m (see the continuum limit presented in the next section), (ii) to provide the 'mass-like' extra term $-T_\epsilon(\theta)$ which is present in the $(1+2)$ D Dirac equation (see next section and Appendix B). Note that $T_\epsilon(\theta)$ (i) is non local in the time j and (ii) vanishes if $[C^{kl}]$ is either diagonal, antidiagonal, or independent of j .

It is convenient to introduce two three-dimensional objects, $[e_{(a)}^\mu]$ and $[e_\mu^{(a)}]$, $(a, \mu) \in \{0, 1, 2\}^3$, whose spatial parts coincide respectively with C^{kl} and $(C^{-1})^{kl}$. More precisely, we define $e_{(0)}^0 = e_0^{(0)} = 1$, $e_{(1)}^0 = e_1^{(0)} = e_{(0)}^1 = e_0^{(1)} = e_{(2)}^0 = e_2^{(0)} = e_{(0)}^2 = e_0^{(2)} = 0$ and $e_{(l)}^k = C^{kl}$, $e_l^{(k)} = (C^{-1})^{kl}$, for $(k, l) \in \{1, 2\}^2$. These two objects allow to rewrite $T_\epsilon(\theta)$ in the more compact form (see Appendix A for a derivation):

$$T_\epsilon(\theta) = -\varepsilon^{abc} \eta_{cd} e_{(a)}^\mu D_b^\epsilon e_\mu^{(d)}, \quad (11)$$

where $[\eta_{ab}] = \text{diag}(1, -1, -1)$, ε^{abc} is the totally antisymmetric symbol, with $\varepsilon^{012} = 1$, and the finite difference operator $(D_b^\epsilon) = (D_0^\epsilon, D_1^\epsilon, D_2^\epsilon)$ can be given arbitrary spatial components D_1^ϵ and D_2^ϵ , since the terms containing D_1^ϵ and D_2^ϵ vanish in Eq. (11), see Appendix A. The Einstein summation convention has also been adopted in (11).

In the continuum limit, the four time- and space-dependent angles will code for the components of a curved metric in $(1+2)$ D spacetime. The $e_{(a)}^\mu$'s will then code for a 3-bein or triad, the $e_\mu^{(a)}$'s will code for its dual and ϵ will go to zero like the temporal and spatial steps of the spacetime lattice.

3. Continuum limit

To investigate the continuum limit of walk (1), we proceed as in [22–24,31] and first interpret Ψ_{j,p_1,p_2} and $\theta_j^{11}, \theta_j^{12}, \theta_j^{21}, \theta_j^{22}$ as the values taken by a wave function Ψ and by four functions $\theta^{11}, \theta^{12}, \theta^{21}, \theta^{22}$ at spacetime point $(x_j^0 = j\epsilon, x_{p_1}^1 = p_1\epsilon/2, x_{p_2}^2 = p_2\epsilon/2)$. The factor $1/2$ is necessary to make the continuum limit match with the standard form of the Dirac-equation. The limit $\epsilon \rightarrow 0$ is then obtained by Taylor expanding (1) at first order in ϵ . The zeroth-order terms cancel each other, and the first-order terms deliver a Schrödinger-like equation for Ψ (see Appendix C for a derivation):

$$i\partial_0\Psi = H\Psi, \quad (12)$$

where

$$H = \sum_{k=1}^2 \left[-i \left(B^k \partial_k + \frac{1}{2} \partial_k B^k \right) \right] + Q, \quad (13)$$

with

$$B^k = e_{(a)}^k \gamma^{(0)} \gamma^{(a)} \quad (14a)$$

$$Q = (m - T_0/4) \gamma^{(0)} \quad (14b)$$

$$T_0 = -\varepsilon^{abc} \eta_{cd} e_{(a)}^\mu \partial_b e_\mu^{(d)}, \quad (14c)$$

and

$$\begin{aligned}\gamma^{(0)} &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \gamma^{(1)} &= \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \\ \gamma^{(2)} &= \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}.\end{aligned}\quad (15)$$

We show in [Appendix B](#) that Eq. (12) is the Hamiltonian form [32] of the Dirac equation for a spin-1/2 fermion of mass m in a $(1+2)$ D spacetime equipped with metric

$$g_{\mu\nu}(x^0, x^1, x^2) = \eta_{ab} e_{\mu}^{(a)}(x^0, x^1, x^2) e_{\nu}^{(b)}(x^0, x^1, x^2). \quad (16)$$

The $e_{(a)}^{\mu}$'s are the components of the 3-bein or triad $(e_{(a)}) = (e_{(1)}, e_{(2)}, e_{(3)})$ on the coordinate basis $(\partial_{\mu}) = (\partial_0, \partial_1, \partial_2)$ in the tangent space, and the $e_{\mu}^{(a)}$'s are the components of the dual triad $(e^{(a)}) = (e^{(1)}, e^{(2)}, e^{(3)})$ on the dual coordinate basis $(\partial^{\mu}) = (\partial^0, \partial^1, \partial^2)$.

All components of the dual triad with one and only one of the indices equal to the time index 0 vanish, and $e_0^{(0)} = 1$, so that:

$$[g_{\mu\nu}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & g_{11} & g_{12} \\ 0 & g_{21} & g_{22} \end{bmatrix}, \quad (17)$$

where

$$\begin{aligned}g_{12} = g_{21} &= -e_2^{(1)} e_1^{(1)} - e_1^{(2)} e_2^{(2)} \\ g_{11} &= -(e_1^{(1)})^2 - (e_1^{(2)})^2 \\ g_{22} &= -(e_2^{(2)})^2 - (e_2^{(1)})^2.\end{aligned}\quad (18)$$

Also of interest is the explicit expression of the matrices B^1 and B^2 in terms of the angles defining the DTQW:

$$\begin{aligned}B^1 &= \begin{bmatrix} -\cos \theta^{11} & -i \cos \theta^{12} \\ i \cos \theta^{12} & \cos \theta^{11} \end{bmatrix} \\ B^2 &= \begin{bmatrix} -\cos \theta^{21} & -i \cos \theta^{22} \\ i \cos \theta^{22} & \cos \theta^{21} \end{bmatrix}.\end{aligned}\quad (19)$$

4. DTQWs coupled to GWs

GWs represent weak gravitational fields propagating in spacetime. Technically, they are particular solutions of Einstein equations linearized around the vacuum. After the proper choice of coordinate system (gauge), these Einstein equations linearized around the vacuum essentially simplify into Poisson equations for two independent metric components. GWs can thus be expanded in Fourier modes. Hence, of particular interest are the plane GWs. In the so-called traceless gauge with coordinates (t, x, y, z) , the metric of a monochromatic plane GW of pulsation ω propagating along the z direction takes the standard form $g_{\mu\nu} = \eta_{\mu\nu} + \xi h_{\mu\nu}$ with

$$h_{\mu\nu}(t, z) = e^{i\omega(t-z)} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \bar{F}(t-z) & \bar{G}(t-z) & 0 \\ 0 & \bar{G}(t-z) & -\bar{F}(t-z) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (20)$$

Here, the $\eta_{\mu\nu}$'s are the components of the Minkowski metric in inertial coordinates (with signature convention $(+, -, -, -)$), \bar{F} and \bar{G} are two arbitrary functions which represent two polarization

states, and ξ is a small parameter which traces the perturbative nature of the waves. In other words, ξ is merely introduced as a reminder that the $\xi h_{\mu\nu}$ is considered small with respect to $g_{\mu\nu}$; all results will be henceforth presented as first-order Taylor expansion in ξ . The GW affects the metric only in planes of constant z parallel to the (x, y) plane and it is therefore customary to study its effect on matter located in these planes. The reduced $(1 + 2)$ D metric in a plane of constant z , say $z = 0$, takes the form:

$$ds^2 = dt^2 - (1 - \xi F(t)) dx^2 - (1 + \xi F(t)) dy^2 + 2\xi G(t) dx dy, \quad (21)$$

where $F(t) = \exp(i\omega t)\bar{F}(t)$ and $G(t) = \exp(i\omega t)\bar{G}(t)$.

Let K and K' be two arbitrary real constants and perform the following change of coordinates:

$$\begin{aligned} T &= t \\ X &= x \left(1 - \xi \frac{K}{2} \right) \\ Y &= y \left(1 - \xi \frac{K'}{2} \right). \end{aligned} \quad (22)$$

Since GWs are perturbative solutions of Einstein equations valid only at first order in ξ , the components of the metric in the new coordinate system (T, X, Y) need only be computed at the same order in ξ and one finds:

$$ds^2 = dT^2 - (1 - \xi (F(T) - K)) dX^2 - (1 + \xi (F(T) + K')) dY^2 + 2\xi G(T) dXdY. \quad (23)$$

We can choose the triad $(e_{(a)})_{a=1,2,3}$ in such a way that its only non-vanishing components on the coordinate basis $(\partial_T, \partial_X, \partial_Y)$ are $e_{(a=1)}^X = 1 + \xi (F(T) - K)/2$, $e_{(a=2)}^Y = 1 - \xi (F(T) + K')/2$, and $e_{(a=1)}^Y = e_{(a=2)}^X = \xi G(T)$. Identify now (x^0, x^1, x^2) introduced in the preceding section with (T, X, Y) . A $(1 + 2)$ D DTQW presented in Section 2 will simulate, in the continuum limit, a Dirac fermion propagating in the metric (23), if

$$\cos \theta^{11} = 1 + \xi (F(T) - K)/2 \quad (24a)$$

$$\cos \theta^{22} = 1 - \xi (F(T) + K')/2 \quad (24b)$$

$$\cos \theta^{12} = \cos \theta^{21} = \xi G(T). \quad (24c)$$

Since ξ is an infinitesimal and we are working at first order in ξ , the third equation can be solved immediately by choosing $\theta^{12} = \theta^{21} = \pi/2 - \xi G(T)$. Now, if we had not introduced the constants K and K' and had identified directly the coordinates t, x , and y introduced earlier with the continuum-limit coordinates x^0, x^1 , and x^2 , Eqs. (24a) and (24b) could not be solved simultaneously, because the absolute value of both cosines must be smaller than one. Let us explain how introducing these two constants enables us to overcome this difficulty. Linear GWs are defined as perturbations of the flat-space time geometry. Treating the metric (23) as a perturbation to the flat Minkowski metric only makes sense if $F(T)$ is bounded. One can then always find K and K' which make both $-(F(T) - K)$ and $(F(T) + K')$ positive. Eqs. (24a) and (24b) are then solved by choosing $\theta^{11} = (-\xi(F(T) - K))^{1/2}$ and $\theta^{22} = (\xi(F(T) + K'))^{1/2}$. We will now focus on pure shear GWs, for which $F(t) = 0$. We also retain the simple choice $K = K' = 0$.

5. DTQWs and pure shear GWs

The DTQWs are entirely defined by the single angle $\theta^{12} = \theta^{21} = \pi/2 - \xi G(T)$, the mass parameter m and the value of ϵ . To make the discussion definite, we set $m = 0$ and $\epsilon = 1$. Since $\epsilon = 1$, (i) the continuum limit is recovered by considering wave functions which vary only on scales much greater than unity, and (ii) the coordinates used in the continuum limit, T, X and Y , are related to the lattice integer coordinates, $j, p_1 = p_X$ and $p_2 = p_Y$, by

$$T = T_j = j, \quad X = p_X/2, \quad Y = p_Y/2. \quad (25)$$

Since the advancement operator V_j depends only on the time T and not on X and Y , the DTQWs are best analyzed in Fourier space. Let $A(T, X, Y)$ be an arbitrary function defined on the infinite lattice. One can write (see [21]):

$$A(T, X, Y) = \frac{1}{\sqrt{2\pi}^2} \int_{k_X=-\pi}^{\pi} \int_{k_Y=-\pi}^{\pi} \tilde{A}(T, k_X, k_Y) \exp(i(k_X p_X + k_Y p_Y)) dk_X dk_Y, \quad (26)$$

with the Fourier transform on the lattice defined by

$$\tilde{A}(T, k_X, k_Y) = \frac{1}{\sqrt{2\pi}^2} \sum_{(p_X, p_Y) \in \mathbb{Z}^2} A(T, X, Y) \exp(-i(k_X p_X + k_Y p_Y)). \quad (27)$$

Each Fourier mode $\tilde{A}(T, k_X, k_Y)$, $(k_X, k_Y) \in [-\pi, \pi]^2$, is dynamically independent of the other ones. Its evolution between time j and $j+1$ is fixed by the operator V_j in Fourier representation, that depends on $\mathbf{k} = (k_X, k_Y)$ through exponentials which describe in Fourier space the translations in physical space. Since the DTQWs perform pairs of jumps in each direction (see (4)), the time-evolution operator in Fourier space is best conceived as a function of $q_X = 2k_X$ and $q_Y = 2k_Y$. We will denote this operator by $W(\xi, G(T_j); q_X, q_Y)$, making also explicit the dependence with respect to ξ and $G(T_j)$. The wave-vector $\mathbf{q} = (q_X, q_Y)$ is actually the one to work with in the continuum-limit because $\mathbf{k} \cdot \mathbf{p} = \mathbf{q} \cdot \mathbf{R}$, where $\mathbf{p} = (p_X, p_Y)$ and $\mathbf{R} = (X, Y)$.

Note that the Brillouin zone in k -space is $[-\pi, +\pi[$ and that the Brillouin zone in q -space is therefore $[-2\pi, +2\pi[$.

A straightforward computation at first order in ξ delivers $W(\xi, G(T); q_X, q_Y) = W^{(0)}(q_X, q_Y) + \xi G(T) W^{(1)}(q_X, q_Y)$, with

$$W^{(0)}(q_X, q_Y) = \begin{bmatrix} e^{iq_X} \cos q_Y & -e^{-iq_X} \sin q_Y \\ e^{iq_X} \sin q_Y & e^{-iq_X} \cos q_Y \end{bmatrix} \quad (28)$$

and

$$W^{(1)}(q_X, q_Y) = \begin{bmatrix} e^{iq_X} A(q_X, q_Y) & -e^{-iq_X} B(q_X, q_Y) \\ e^{iq_X} B^*(q_X, q_Y) & e^{-iq_X} A^*(q_X, q_Y) \end{bmatrix}, \quad (29)$$

where the superscript $*$ denotes complex conjugation, and

$$\begin{aligned} A(q_X, q_Y) &= \frac{1}{\sqrt{2}} e^{i\frac{\pi}{4}} \bar{A}(q_X, q_Y) \\ B(q_X, q_Y) &= \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{4}} \bar{B}(q_X, q_Y), \end{aligned} \quad (30)$$

with

$$\begin{aligned} \text{Re } \bar{A}(q_X, q_Y) &= -\cos(q_X - q_Y) + \cos q_Y - \sin q_Y + \sin 2q_Y \\ \text{Re } \bar{B}(q_X, q_Y) &= +\sin(q_X + q_Y) - \sin q_Y + \cos q_Y - \cos 2q_Y \\ \text{Im } \bar{A}(q_X, q_Y) &= -\cos(q_X + q_Y) + \cos q_Y + \sin q_Y \\ \text{Im } \bar{B}(q_X, q_Y) &= +\sin(q_X - q_Y) + \sin q_Y + \cos q_Y - 1. \end{aligned} \quad (31)$$

The operator W controls the entire DTQW dynamics. In particular, at time T_j , the energies corresponding to any given (q_X, q_Y) are logarithms of the eigenvalues of $W(\xi, G(T_j); q_X, q_Y)$ and the associated eigenvectors define the eigen-polarizations of the spin-1/2 fermion. Thus, a generic shear GW changes in a time-dependent way the polarization and the energy of the quantum walker. The only modes which are not affected by pure shear GWs are those for which both $A(q_X, q_Y)$ and $B(q_X, q_Y)$ vanish. A direct computation shows that, in the q -space Brillouin zone $[-2\pi, 2\pi[$, both functions vanish simultaneously for two different finite sets of values of (q_X, q_Y) . The first set is $(q_X, q_Y) = 2\pi(r_X, r_Y)$ with $(r_X, r_Y) = (0, 0), (0, -1), (0, 1), (-1, 0), (1, 0), (-1, -1), (-1, 1), (1, -1), (1, 1)$, for which the unperturbed (i.e. ‘free’) operator $W^{(0)}$ coincides with unity, so that these

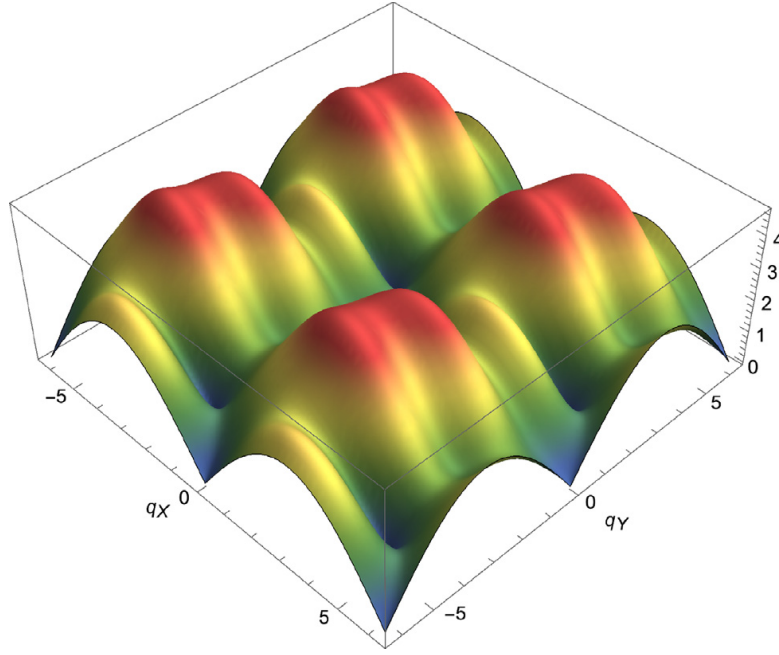


Fig. 1. (Color online) Modulus $\rho(q_X, q_Y)$ of the eigenvalues of $W^{(1)}(q_X, q_Y)$.

modes are unaffected by the free DTQW. The second set is $(q_X, q_Y) = (-\pi/2, \pi/2) + 2\pi(s_X, s_Y)$ with $(s_X, s_Y) = (0, 0), (0, -1), (1, 0), (1, -1)$, for which $W^{(0)}$ coincides with $-i\sigma_1$, so that the spin components of these modes are flipped at each time step by the free DTQW (and shifted by a global phase $-i$). Thus, at first order in the wave perturbation, the modes on which this pure shear GW has no influence correspond to modes for which the probability of presence of the walker, $|\psi_{j,p_1,p_2}^-|^2 + |\psi_{j,p_1,p_2}^+|^2$, is unaffected by the free DTQW. All these modes are ‘small-scale’ (i.e. of the same order of magnitude as the lattice spacing) except the $(0, 0)$ mode, which corresponds to a uniform wave function. This mode cannot be populated if space is infinite.

The operator $W^{(1)}(q_X, q_Y)$ can be further characterized by its eigenvalues. They are complex conjugate to each other and have as common modulus $\rho(q_X, q_Y) = (|A(q_X, q_Y)|^2 + |B(q_X, q_Y)|^2)^{1/2}$. The function $\rho(q_X, q_Y)$ is plotted in Fig. 1. It admits four absolute maxima of identical amplitude approximately equal to 4.69826. These maxima are located at (q_X^a, q_Y^b) with $a, b = \pm$ and $q_X^+ \simeq 2.1423$, $q_X^- \simeq -4.14088$, $q_Y^+ \simeq 2.81949$, $q_Y^- \simeq -3.46369$. Generally speaking, the higher ρ , the greater the influence of GWs on DTQWs. Thus, pure shear GWs that have a maximal influence on DTQWs on ‘small’ scales comparable to a few lattice steps (a mode with $|\mathbf{q}| = 2\pi$ has a period of $2\pi/|\mathbf{k}| = 4\pi/|\mathbf{q}| = 2$ lattice steps).

We will now present in detail two case-studies. The first one investigates perturbatively how the eigen-energies and eigenvectors behave for large-scale modes, i.e. modes which vary on scales much larger than the lattice spacing. The other study is not restricted to large-scale modes, and shows how the interference pattern between two fermion eigen-modes is changed by a GW.

6. Two case-studies

6.1. Large-scale fermion modes

Large scales are those relevant to the continuum limit and correspond to values of q_X and q_Y close to zero. One finds, at first order in q_X and q_Y :

$$W(\xi, G(T); q_X, q_Y) = \begin{bmatrix} 1 + i(q_X + \xi G(T) q_Y) & -(q_Y + \xi G(T) q_X) \\ q_Y + \xi G(T) q_X & 1 - i(q_X + \xi G(T) q_Y) \end{bmatrix}. \quad (32)$$

One can check that this is the walk operator obtained in the continuum limit, see Section 3 and Appendix C.

The eigenvalues $\lambda_{\pm}(\xi, G(T); q_X, q_Y)$ of this operator read, at first order in ξ ,

$$\lambda_{\pm}(\xi, G(T); q_X, q_Y) = 1 \mp i \left(1 + 2\xi G(T) \frac{q_X q_Y}{|\mathbf{q}|^2} \right) |\mathbf{q}|. \quad (33)$$

Associated eigenvectors $V_{\pm}(\xi, G(T); q_X, q_Y)$ can also be expanded in ξ :

$$V_{\pm}(\xi, G(T); q_X, q_Y) = V_{\pm}^{(0)}(q_X, q_Y) + \xi G(T) V_{\pm}^{(1)}(q_X, q_Y), \quad (34)$$

but exact expressions are quite involved and depend on the sign of q_X . One finds for example

$$V_{+}^{(0)}(q_X, q_Y) = \begin{bmatrix} -i \frac{q_Y}{q_X + |\mathbf{q}|} \\ 1 \end{bmatrix} \quad (35a)$$

$$V_{+}^{(1)}(q_X, q_Y) = -i \frac{q_X}{q_X + |\mathbf{q}|} \begin{bmatrix} q_X - \frac{q_Y^2 \left(1 + 2 \frac{q_X}{|\mathbf{q}|} \right)}{q_X + |\mathbf{q}|} \\ 0 \end{bmatrix} \quad (35b)$$

for positive values of q_X .

The eigen-energies $E_{\pm}(\xi, G(T); q_X, q_Y)$ are by definition related to the eigenvalues $\lambda_{\pm}(\xi, G(T); q_X, q_Y)$ by $\lambda_{\pm}(\xi, G(T); q_X, q_Y) = \exp(-iE_{\pm}(\xi, G(T); q_X, q_Y))$. At first order in $|\mathbf{q}|$, one finds:

$$E_{\pm}(\xi, G(T); q_X, q_Y) = \pm \left(1 + 2\xi G(T) \frac{q_X q_Y}{|\mathbf{q}|^2} \right) |\mathbf{q}|. \quad (36)$$

On large scales, the lowest-order effect of the pure shear GWs is thus an anisotropic deformation of spatial scales by a factor $(1 - 2\xi G(T) q_X q_Y / |\mathbf{q}|^2)$, the eigen-energies being changed accordingly by the inverse factor, since they are linear in the momentum in free space.

6.2. Interference pattern modified by GWs

We now wish to study the effect of pure shear GWs on all modes, and not only on large-scale ones. GW has been first observed directly using interference with light [29] but detectors based on interference with matter waves are still considered as a viable alternative (see for example [33]). It is thus natural, in the context of the present article, to study the effect of GWs on interference patterns of the walker. To be definite, we consider how GWs modify interference patterns between two energy eigen-modes of the free DTQW which share the same energy, thereby ensuring that the interference pattern of these modes is stationary in the absence of GWs.

Consider for example the two wavevectors $(q_X^1 = q^1 > 0, q_Y^1 = 0)$ and $(q_X^2 = 0, q_Y^2 = q^2 > 0)$, and the two initial polarizations

$$\begin{aligned} \psi^1 &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ \psi^2 &= \begin{bmatrix} i \\ -\frac{1}{\sqrt{2}} \\ 1 \\ \frac{1}{\sqrt{2}} \end{bmatrix}. \end{aligned} \quad (37)$$

The first is an eigen-polarization of $W^{(0)}(q^1, 0)$, associated to the eigenvalue $\exp(-iq^1)$ and the second is an eigen-polarization of $W^{(0)}(0, q^2)$, associated to the eigenvalue $\exp(-iq^2)$. In particular, both eigenvalues are the same if $q^1 = q^2 = q$ and the free DTQW then does not modify the interference pattern of the two fermion eigen-modes. This is not so anymore in the presence of a GW, which changes the interference pattern at each time step j by a contribution proportional to $\xi G(T_j)$.

Let $N_0(q, X, Y)$ be the initial density of an equal superposition of the two interfering fermion eigenmodes, i.e. $N_0(q, X, Y) = \Psi_0^\dagger(q, X, Y)\Psi_0(q, X, Y)$, where $\Psi_0(q, X, Y) = \Psi^1 \exp[iqX] + \Psi^2 \exp[iqY]$, and let $N_1(\xi, G(T_{j=1}); q, X, Y)$ be the density after one time step of the DTQW. The interesting quantity is the relative density variation Δ after one time-step per unit of $\xi G(T)$,

$$\Delta(q, X, Y) = \frac{1}{\xi G(T_{j=1})} \frac{N_1(\xi, G(T_{j=1}); q, X, Y) - N_0(q, X, Y)}{N_0(q, X, Y)}. \quad (38)$$

A direct computation shows that

$$N_0(q, X, Y) = 2 + \sqrt{2} \cos\left(\frac{q}{2}(p_X - p_Y)\right), \quad (39)$$

and

$$\Delta(q, X, Y) = \frac{2\sqrt{2}}{N_0(q, X, Y)} \cos\left(\frac{q}{2}(p_X - p_Y - 2)\right) \sin^2 q. \quad (40)$$

Fig. 2 shows the contours of $N_0(q, X, Y)$ and $\Delta(q, X, Y)$ in the (X, Y) plane for $q = q_{\max}$, for which the effect of the GW is maximum (see the discussion below). Both $N_0(q, X, Y)$ and $\Delta(q, X, Y)$ depend on X and Y only through $u = p_X - p_Y = 2(X - Y)$. Fig. 3 shows how the profile of $\Delta(q, u)$ as a function of u changes with q . The profiles are periodic functions of u , and are plotted over two periods.

The net effect of the GW can be measured by $\Delta_M(q) = \max_u |\Delta(q, u)|$. This function is π -periodic in q and also obeys:

$$\Delta_M(q) = \begin{cases} f(q) & \text{if } q \in [0, \pi/2[\\ f(\pi - q) & \text{if } q \in [\pi/2, \pi], \end{cases} \quad (41)$$

with

$$f(q) = \frac{2\sqrt{2} \sin^2(q) \sqrt{1 - \sin^2(q)/2}}{2 + \sqrt{2} \cos(q) \sqrt{1 - \sin^2(q)/2} - \sin^2(q)}. \quad (42)$$

Fig. 4 displays $\Delta_M(q)$ on $[0, \pi]$, which is half of the positive half of the q -space Brillouin zone. The absolute minimum is zero and occurs for $q = 0$ and π . The absolute maximum is approximately 2.48161 and is reached for 2 values of q , $\pi - q_{\max}$ and $q_{\max} \simeq 1.97504$, which correspond respectively to the following two values of the wavelength $\lambda(q) = 2\pi/|k| = 4\pi/|q|$: 10.7722 and 6.3626. There is also a local minimum reached for $q = \pi/2$, whose value is 2.

7. Discussion

We have introduced a new two-dimensional DTQW whose continuum limit coincides with the dynamics of massive spin-1/2 Dirac fermions propagating in a curved spacetime. We have then shown how to use these DTQWs to simulate the influence of GWs on Dirac fermions. We have finally focused on pure shear GWs and investigated in detail how these influence DTQWs on both large and small scales. On large spatial scales, pure shear GWs locally rescale the eigen-energies anisotropically, to make up for the space deformation induced by the wave, and the eigen-polarizations are modified as well. On smaller scales typically comparable to two or three lattice steps, both polarizations and energies are modified in a non-trivial way; for instance, this has the effect of significantly changing the interference pattern of a superposition of two flat-spacetime eigen-modes.

There exist another way to build DTQWs simulating the interaction of a Dirac field with a gravitational one. This other construction was presented in [26] for the $(1+1)$ D case and an extension to higher spacetime dimensions has just been completed [34]. This extension also allows fermions to have internal degrees of freedom.

Both constructions use a regular lattice, but they differ in nearly all other aspects. The construction of DTQWs used in this paper is Taylor-made to deliver DTQWs whose continuum limit coincides with

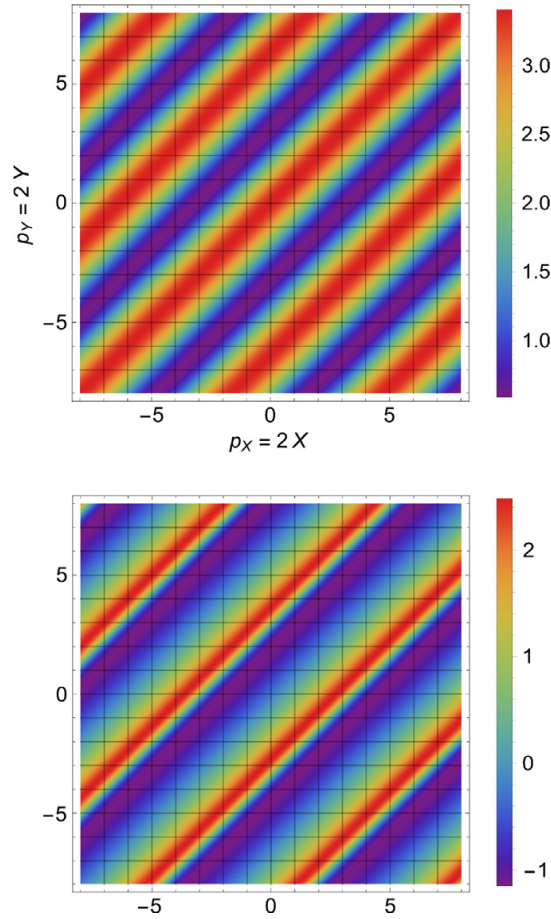


Fig. 2. (Color online) Density $N_0(q_{\max}, X, Y)$ (top) and relative density variation $\Delta(q_{\max}, X, Y)$ (bottom) in the (X, Y) plane. The mesh represents the 2D lattice on which the DTQW is defined, p_X and p_Y are the integer coordinates used to label the nodes of this lattice, while X and Y are those defined to recover, in the continuum limit, the standard form of the Dirac equation in curved spacetime, Eq. (12).

the Dirac equation. The other construction is based on Paired Quantum Walks which admit a whole class of PDEs as continuum limits, including the Dirac equation. As a consequence, each construction has its pros and cons, which we shall now discuss.

As apparent from the above material, our construction works only in synchronous coordinate systems, for which all mixed time–space metric components identically vanish and the time–time component is identical to unity. This does not restrict the gravitational fields one can take into account, since all gravitational fields admit local synchronous coordinates. But it forces the lattice to be regular in precisely these synchronous coordinates, whereas the other construction allows the lattice to be regular in arbitrary coordinates.

On the other hand, the time-advancement operator V_j used in our construction only involves gauge-invariant i.e. intrinsic aspects of the gravitational fields, while the time-advancement operator used in the other construction mixes both gauge-invariant and gauge-dependent aspects of the gravitational field. Thus, if one adopts the construction used in this paper, the operator V_j itself can be viewed as a discrete gauge-invariant gravitational field. The gauge dependence of standard continuous physics then manifests itself only in the choice of coordinates when one performs the continuum limit i.e. in the correspondence between the continuous coordinates x^μ and the lattice indexes. On the other hand, the other construction encodes both the gauge-invariant aspects of the gravitational fields and a choice of coordinates into a single object i.e. in the time-advancement operator. And one is still free to choose continuous coordinates as one wishes.

Also, the other construction originally required doubling the number of components of the wave function, but an implementation using only $U(2)$ operators, shifts and swaps has now been presented [34].

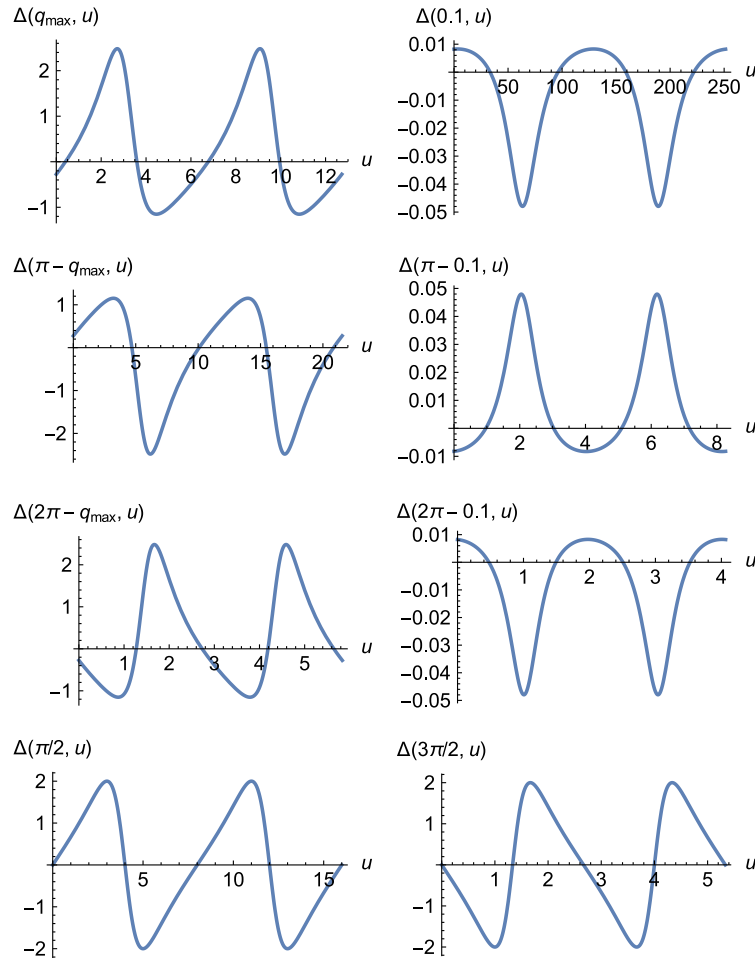


Fig. 3. (Color online) Profiles of the relative density variation $\Delta(q, u = p_x - p_y)$ as a function of u for various values of q . The profiles are plotted over two rather than one period for a better visual appreciation.

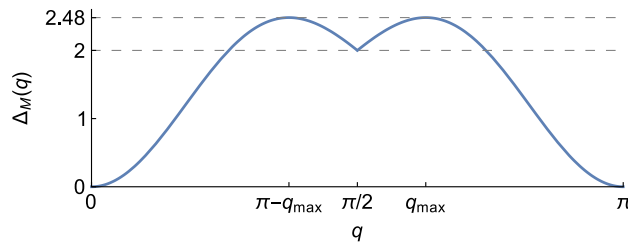


Fig. 4. (Color online) Maximum of the relative density variation induced by a GW on the interference pattern between two fermion eigen-modes, as a function of the common wavevector of these modes, q , plotted on half of the positive half of the q -space Brillouin zone, namely $[-2\pi, 2\pi]$.

All in all, it seems that both constructions have their own strong and weak points. The construction used in this paper is perhaps more physically grounded and the other one may be of a more mathematical nature.

Let us finally mention of few extensions of this work. The first one is rather straightforward and consists in allowing the operators \mathbf{u} and \mathbf{r} to be arbitrary members of $SU(2)$. The extra angles which will appear code for arbitrary discrete electromagnetic fields (see [25]). The other extension consists in incorporating in the model extra internal dimensions. This should in particular deliver DTQWs where the time-advancement operator unifies arbitrary discrete Yang–Mills fields with discrete gravitational fields (see [23] for $(1 + 1)$ D DTQWs simulating Dirac fermions in arbitrary Yang–Mills fields).

In a different direction, the influence of gravitational fields on DTQWs should be systematically studied, with possible applications ranging from fundamental physics to quantum algorithmics.

Acknowledgments

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Appendix A. Compact form of the mass-like term

In this appendix, we show that $T_\epsilon(\theta)$ given by Eq. (9) can be put under the form of Eq. (11). By definition of the $e_{(a)}^\mu$'s and because $(\eta_{ab}) = \text{diag}(0, -1, -1)$,

$$\begin{aligned} T_\epsilon(\theta) &= e_{(2)}^k D_0^\epsilon e_k^{(1)} - e_{(1)}^k D_0^\epsilon e_k^{(2)} \\ &= \varepsilon^{0bc} e_{(b)}^k D_0^\epsilon \eta_{cd} e_k^{(d)} \\ &= \varepsilon^{0bc} e_{(b)}^\mu \eta_{cd} D_0^\epsilon e_\mu^{(d)} \\ &= -\varepsilon^{b0c} e_{(b)}^\mu \eta_{cd} D_0^\epsilon e_\mu^{(d)} \end{aligned} \quad (\text{A.1})$$

where the Einstein summation convention has been used and ε^{abc} is the completely antisymmetric symbol. The third line is obtained from the second one by taking into account that all 3-bein and inverse 3-bein components with one spatial index and the time index 0 identically vanish.

Consider now $K^i = \varepsilon^{ibc} e_{(b)}^\mu \eta_{cd} D_i^\epsilon e_\mu^{(d)}$ with $i \in \{1, 2\}^2$ where the D_i^ϵ are arbitrary finite differences operators which deliver zero when applied to spatially constant objects. The quantity ε^{ibc} is non vanishing only if b or c is equal to zero. The term with $c = 0$ gives a vanishing contribution to K^i because η_{cd} then enforces $d = 0$ and the only non-vanishing inverse 3-bein component $e_\mu^{(0)}$ is $e_0^{(0)} = 1$ and $D_0^\epsilon e_0^{(0)} = 0$. The only possibly non-vanishing contribution to K^i thus comes from the term where $b = 0$. But the only non-vanishing 3-bein component $e_{(0)}^\mu$ is $e_{(0)}^0 = 1$. Now, the only non-vanishing inverse 3-bein component $e_0^{(d)}$ is $e_0^{(0)} = 1$ and $D_0^\epsilon e_0^{(0)} = 0$.

The K^i 's thus vanish identically and this completes the proof of (11). Note that Eq. (11) is true independently of the definition of the spatial 'discrete derivative' operators D_1^ϵ and D_2^ϵ .

Appendix B. Mass-like term in the (1 + 2)D Dirac equation

Consider a spacetime of dimension $(1 + d)$ equipped with metric g . The Hamiltonian form of the Dirac equation is (see Eq. (35) of [32]):

$$i\partial_0|\Psi\rangle = \hat{H}|\Psi\rangle, \quad (\text{B.1})$$

with

$$\hat{H} = \sum_{k=1}^d \left[-i \left(\hat{B}^k \partial_k + \frac{1}{2} \partial_k \hat{B}^k \right) \right] + \hat{M} + \hat{A}(d), \quad (\text{B.2})$$

where

$$\hat{B}^k = \hat{\alpha}^{(i)} \frac{e_{(i)}^k}{e_{(0)}^0} + e_{(0)}^k, \quad (\text{B.3})$$

$$\hat{M} = \frac{m}{e_{(0)}^0} \hat{\gamma}^{(0)}, \quad (\text{B.4})$$

and $\hat{\alpha}^{(k)} = \hat{\gamma}^{(0)} \hat{\gamma}^{(k)}$. As in the main sections of this article, the $e_{(a)}^\mu$ are the components of a $(1 + d)$ -bein on a coordinate basis. The components of the inverse $(1 + d)$ -bein will be denoted by $e_\mu^{(a)}$. The hat designates operators, as opposed to their representation in a given spin basis.

In $d = 3$, the term $\hat{A}(d)$ reads

$$\hat{A}(d = 3) = -\frac{i}{2} \hat{\gamma}_5 \hat{\alpha}^{(a)} \tilde{\mathcal{B}}_{(a)}, \quad (\text{B.5})$$

with $\hat{\gamma}_5 = \hat{\gamma}_{(0)} \hat{\gamma}_{(1)} \hat{\gamma}_{(2)} \hat{\gamma}_{(3)}$ and

$$\tilde{\mathcal{B}}_{(a)} = \frac{1}{e_{(0)}^0} \left(\frac{1}{2} \varepsilon_{(a)(b)(c)(d)} e^{(b)\mu} e^{(c)\nu} \partial_\mu e_\nu^{(d)} \right), \quad (\text{B.6})$$

where $\varepsilon_{(a)(b)(c)(d)}$ is the antisymmetric symbol. The notation $\tilde{\mathcal{B}}$ matches the one used in Ref. [32]. In (B.5), we can permute $\hat{\gamma}_5$ and $\hat{\alpha}^{(a)} = \hat{\gamma}^{(0)} \hat{\gamma}^{(a)}$ because $\hat{\gamma}_5$ anticommutes with all $\hat{\gamma}^{(a)}$'s, and we obtain

$$\hat{A}(d = 3) = -\frac{i}{2} \hat{\gamma}^{(0)} \hat{\gamma}^{(a)} \hat{\gamma}_5 \times \left[\frac{1}{e_{(0)}^0} \left(\frac{1}{2} \varepsilon_{(a)(b)(c)(d)} e^{(b)\mu} e^{(c)\nu} \partial_\mu e_\nu^{(d)} \right) \right], \quad (\text{B.7})$$

where \times denotes the multiplication. After a cyclic, hence odd permutation of the four indices, (B.7) reads

$$\hat{A}(d = 3) = -\frac{\hat{\gamma}^{(0)}}{8e_{(0)}^0} \underbrace{\left[-2i\varepsilon_{(b)(c)(d)(a)} \hat{\gamma}^{(a)} \hat{\gamma}_5 \right]}_{\hat{J}_{(b)(c)(d)=3}} e^{(b)\mu} e^{(c)\nu} \partial_\mu e_\nu^{(d)}. \quad (\text{B.8})$$

The expression of $\hat{J}_{(b)(c)(d)}$ given above is only valid in $(1 + 3)$ dimensional spacetimes. In arbitrary dimension $(1 + d)$, it reads (Eq. (25-c) of [32]):

$$\hat{J}_{(b)(c)(d)} = \{\hat{\gamma}_{(b)}, \hat{S}_{(c)(d)}\}, \quad (\text{B.9})$$

where

$$\hat{S}_{(c)(d)} = \frac{i}{2} [\hat{\gamma}_{(c)}, \hat{\gamma}_{(d)}]. \quad (\text{B.10})$$

Now, $\hat{J}_{(b)(c)(d)}$ is obviously antisymmetric in (c, d) , but we can show by an explicit computation that it is also antisymmetric in (b, c) , which is a consequence of the Clifford algebra satisfied by the gamma matrices. Hence, if one of the indices is repeated, $\hat{J}_{(b)(c)(d)}$ vanishes. This shows that $\hat{J}_{(b)(c)(d)}$ vanishes in $(1 + 1)D$ spacetimes, so that

$$\hat{A}(d = 1) = 0. \quad (\text{B.11})$$

In $(1 + 2)$ dimension, there are 6 non vanishing components of $\hat{J}_{(b)(c)(d)}$:

$$\begin{aligned} \hat{J}_{012} &= -\hat{J}_{102} \\ \hat{J}_{201} &= -\hat{J}_{021} \\ \hat{J}_{120} &= -\hat{J}_{210}. \end{aligned} \quad (\text{B.12})$$

In representation (14), we can check that

$$J_{012} = J_{201} = J_{120} = 2 \times \mathbf{1}_2 = 2, \quad (\text{B.13})$$

where $\mathbf{1}_2$ is the 2×2 identity matrix. The previous equalities are then valid in any representation (trivial to check). Hence, a compact and generic expression for $\hat{J}_{(\beta)(\rho)(\sigma)}$ in $d = 2$ is:

$$\hat{J}_{(b)(c)(d)} = 2\varepsilon_{(b)(c)(d)}, \quad (\text{B.14})$$

where $\varepsilon_{(b)(c)(d)}$ is the 3D antisymmetric symbol. Thus, a generic expression for the term $\hat{A}(d)$ in $(1+2)$ dimensions is

$$\hat{A}(d=2) = -\frac{1}{4e_{(0)}^0} \underbrace{\left(\varepsilon_{(b)(c)(d)} \underbrace{e^{(b)\mu} e^{(c)\nu} \partial_\mu e_\nu^{(d)}}_{\tau_{(b)(c)(d)}} \right)}_{T_0} \hat{\gamma}^{(0)}. \quad (\text{B.15})$$

Observe that $\hat{A}(d=2)$ has, in the spin Hilbert space, the same structure as the mass term (B.4). We have

$$T_0 = \tau^{012} - \tau^{102} + \tau^{201} - \tau^{021} + \tau^{120} - \tau^{210}. \quad (\text{B.16})$$

If we take a dual 3-bein of the form

$$[e_\mu^{(\alpha)}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & e_1^{(1)} & e_2^{(1)} \\ 0 & e_1^{(2)} & e_2^{(2)} \end{bmatrix}, \quad (\text{B.17})$$

then

$$T_0 = e^{(1)\nu} \partial_0 e_\nu^{(2)} - e^{(2)\nu} \partial_0 e_\nu^{(1)}, \quad (\text{B.18})$$

which, after a small calculation (the same as that of Appendix A but replacing the D_b 's by ∂_b 's), can be shown to coincide with Eq. (14c). This finalizes the proof that the $(1+2)$ D Dirac equation in representation (14) can be put under the form of Eq. (12).

Appendix C. Detailed computation of the continuum limit

We are going to show that the first-order expansion of the walk operator reads $V_j = 1 - i\epsilon H$ with H given by (13).

We define $\mathcal{M}_\epsilon = m - T_\epsilon(\theta)/4$. At first order in ϵ ,

$$\mathbf{Q}(\epsilon \mathcal{M}_\epsilon) = 1 - i\epsilon \mathcal{M}_0 \sigma_1, \quad (\text{C.1})$$

where \mathcal{M}_0 is the limit of \mathcal{M}_ϵ when ϵ goes to zero, and σ_1 the first Pauli matrix.

The spin-dependent shift operators can be written

$$\mathbf{S}_k = e^{i\epsilon P_k \sigma_3}, \quad (\text{C.2})$$

with the momentum operator

$$P_k = -i\partial_k. \quad (\text{C.3})$$

Thus

$$\mathbf{S}_k = 1 + i\epsilon P_k \sigma_3, \quad (\text{C.4})$$

from which one obtains

$$\mathbf{W}_k(\theta_j) = 1 - i\epsilon \mathbf{H}_k(\theta_j), \quad (\text{C.5})$$

where the ‘1D Hamiltonians’ $\mathbf{H}_k(\theta_j)$ read

$$\mathbf{H}_k(\theta_j) = -\frac{1}{2} \mathbf{R}^{-1}(\theta_j) \mathbf{U}(\theta_j) \{ \mathbf{U}(\theta_j), P_k(\sigma_3) \mathbf{R}(\theta_j) \} \star. \quad (\text{C.6})$$

Here $\{A, B\} = AB + BA$ and the notation $P_k(O_j \star)$ means that P_k applies to $O_j \Psi_j$ and not only to $O_j : (j, p_1, p_2) \mapsto O_{j, p_1, p_2}$, which is any operator acting on Ψ_j , i.e.

$$P_k(O_j \star \Psi_j) \equiv P_k(O_j \Psi_j), \quad (\text{C.7})$$

so that $\mathbf{H}_k(\theta_j)\Psi_j$ reads

$$\begin{aligned}\mathbf{H}_k(\theta_j)\Psi_j &= -\frac{1}{2}\mathbf{R}^{-1}(\theta_j)\mathbf{U}(\theta_j)\mathbf{U}(\theta_j)P_k(\sigma_3\mathbf{R}(\theta_j)\Psi_j) \\ &\quad - \frac{1}{2}\mathbf{R}^{-1}(\theta_j)\mathbf{U}(\theta_j)P_k(\sigma_3\mathbf{U}(\theta_j)\mathbf{R}(\theta_j)\Psi_j).\end{aligned}\quad (\text{C.8})$$

The previous expressions lead to

$$V_j = 1 - i\epsilon\mathbf{H}, \quad (\text{C.9})$$

with

$$\mathbf{H} = \sum_{k=1}^2 \mathbf{K}(\theta_j^{k1}, \theta_j^{k2}) + \mathcal{M}_0\sigma_x, \quad (\text{C.10})$$

where

$$\mathbf{K}(\theta_j^{k1}, \theta_j^{k2}) = \mathbf{H}_k(\theta_j^{k1}) + \mathbf{\Pi}^{-1}\mathbf{H}_k(\theta_j^{k2})\mathbf{\Pi}. \quad (\text{C.11})$$

We will now show that \mathbf{H} is identical to H given by (13). We can immediately check that the mass term $\mathcal{M}_0\sigma_x$ is the one given by (B.4). We therefore need to show that $\mathbf{K}(\theta_j^{k1}, \theta_j^{k2})$ is identical to the term in square brackets from Eq. (13). The total Hamiltonian \mathbf{H} is linear in the $\mathbf{H}_k(\theta_j^{kl})$. It is convenient to compute first each $\mathbf{H}_k(\theta_j^{kl})$ separately and then combine all results into \mathbf{H} . For each given (j, k, l) , one can safely use the simplified notations

$$U = \mathbf{U}(\theta_j^{kl}) \quad \text{and} \quad R = \mathbf{R}(\theta_j^{kl}). \quad (\text{C.12})$$

Eq. (C.6) leads to

$$\begin{aligned}\mathbf{H}_k(\theta_j^{kl}) &= -\frac{1}{2}R^{-1}U[UP_k(\sigma_3 + P_k(\sigma_3U)R\star) \\ &= \frac{i}{2}R^{-1}U[U\partial_k(\sigma_3R\star + \partial_k(\sigma_3UR\star)],\end{aligned}\quad (\text{C.13})$$

which delivers

$$\mathbf{H}_k(\theta_j^{kl}) = \frac{i}{2}R^{-1}U[\{U, \sigma_3\}(R\partial_k + \partial_k R) + \sigma_3(\partial_k U)R]. \quad (\text{C.14})$$

Now, we have

$$\{U, \sigma_3\} = -2c\mathbf{1}_2, \quad (\text{C.15})$$

where $\mathbf{1}_2$ is the 2×2 identity matrix and

$$c = \cos\theta_j^{kl}, \quad (\text{C.16})$$

and

$$R^{-1}UR = -\sigma_3. \quad (\text{C.17})$$

Hence,

$$\mathbf{H}_k(\theta_j^{kl}) = -i\left(-c\sigma_3\partial_k + \frac{1}{2}\Omega\right), \quad (\text{C.18})$$

with

$$\Omega = R^{-1}U(2c\partial_k R - \sigma_3(\partial_k U)R). \quad (\text{C.19})$$

We have

$$-c\sigma_3 = D^{kl} = \begin{bmatrix} -\cos\theta_j^{kl} & 0 \\ 0 & \cos\theta_j^{kl} \end{bmatrix}, \quad (\text{C.20})$$

and a straightforward computation involving only matrix products and derivations shows that

$$\Omega = \partial_k D^{kl}, \quad (\text{C.21})$$

so that

$$\mathbf{H}_k(\theta_j^{kl}) = -i \left(D^{kl} \partial_k + \frac{1}{2} \partial_k D^{kl} \right). \quad (\text{C.22})$$

Now, we have

$$\mathbf{\Pi}^{-1} \mathbf{H}_k(\theta_j^{kl}) \mathbf{\Pi} = -i \left(A^{kl} \partial_k + \frac{1}{2} \partial_k A^{kl} \right), \quad (\text{C.23})$$

where the antidiagonal matrix is given by

$$A^{kl} = \mathbf{\Pi}^{-1} D^{kl} \mathbf{\Pi} = \begin{bmatrix} 0 & -i \cos \theta_j^{kl} \\ i \cos \theta_j^{kl} & 0 \end{bmatrix}. \quad (\text{C.24})$$

Note that Eqs. (C.21)–(C.24) are all written at fixed (j, k, l) and thus involve in particular no summation over k .

Combining (C.21) and (C.24) leads to

$$\sum_{k=1}^2 \mathbf{K}(\theta_j^{k1}, \theta_j^{k2}) = -i \left(B^k \partial_k + \frac{1}{2} \partial_k B^k \right), \quad (\text{C.25})$$

where summation over k is implied in the right-hand side. This completes the proof.

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Conclusion & perspectives

The conclusion of the research work on which this thesis is based is essentially twofold.

In Part I, it has been shown that DTQWs can be used to discretize certain first-quantized Yang-Mills gauge theories [1, 2, 3], which extends previous results in lower spacetime and coin-space dimensions [92, 93, 90]. The starting point of these discretizations is, indeed, the discretization of the fermionic matter-field dynamics – i.e., typically, the Dirac equation for spin-1/2 fermions – under the form of a DTQW, which was seminaly introduced by Feynman in 1+1 dimensions [29, 97]. In addition to deliver the aforementioned field theories in the continuum limit – which is the minimal requirement for a discretization of such field theories – the DTQWs-based discretizations suggested in the present work, not only (i) ensure, by construction, a unitary dynamics on the lattice², but also (ii) preserve, at the lattice level, both (ii.a) Yang-Mills gauge invariance and (ii.b) ‘continuity’, i.e. the conservation of the Yang-Mills charge current, and (iii) can be associated a lattice gauge-invariant quantity³ – which of course delivers the standard Yang-Mills field strength in the continuum. By combining (iii) with (ii), one can eventually construct a lattice equivalent to the gauge-field dynamics⁴.

Let us be more precise on the achievements of this work. The DTQWs-based discretization program described in the previous paragraph, has indeed been achieved for an Abelian Yang-Mills gauge theory in 1+2 dimensions [1, 2], see Chapter 1, and there is work in progress on the Abelian (1+3)D case. In the non-Abelian case, a (1+1)D scheme has been suggested, which couples the matter dynamics to a generic non-Abelian $U(N)$ Yang-Mills gauge field [3], see Chapter 2. While this scheme verifies by construction property (ii.a), which was a necessary starting point to eventually achieve (iii)⁵, point (ii.b) is still an open question, as well as the possibility to design a lattice equivalent for the gauge-field dynamics.

In Part II, it has been shown that it was possible to extend to 1+2 dimensions [4] previous (1+1)D results [91, 90] demonstrating that DTQWs can be used to discretize Dirac dynamics in curved spacetime, while preserving unitarity by construction. This (1+2)D scheme has been used to study how linear plane gravitational waves influence a transverse fermionic matter distribution, while the (1+1)D scheme had been used to simulate fermionic radial motion in a Schwarzschild blackhole. Higher-dimensional extensions of DTQWs-based fermionic dynamics in curved spacetime have also been achieved by Arrighi et al. [193], by pairing DTQWs. The differences between both schemes are discussed in both publications, [4] and [193].

²Regarding unitarity in standard LGTs, see Appendix O.

³In the non-Abelian case, this quantity is gauge *covariant*.

⁴The *matter-induced*, i.e. *inhomogeneous*, lattice gauge-field dynamics, indeed combines (iii) with (ii), while the *homogeneous* gauge-field dynamics, i.e. the dynamical constraints, simply combine (iii) with (ii.a). To be more precise, the lattice equivalent suggested for the matter-induced gauge-field dynamics ensures (ii.b).

⁵This was much more complicated to achieve than in the Abelian case.

Let us now comment on the specificities of the DTQWs-based discretizations of QFTs presented in Part I of this manuscript, with respect to other works on the quantum simulation of QFTs.

While D’Ariano et al. [59] and Arrighi et al. [60] have suggested lattice substitutes for Lorentz invariance of standard continuum QFTs, an issue which is not addressed in the present research work, the latter instead provides, not only (i) a lattice equivalent for the Yang-Mills gauge invariance of standard continuum QFTs, but also (ii) a lattice gauge-invariant associated quantity⁶, and (iii) lattice Maxwell’s equations ensuring the conservation of the charge current on the lattice, as detailed above. This whole issue of Yang-Mills gauge invariance is not addressed by either Arrighi et al. nor D’Ariano et al.⁷

Recall that, while Yang-Mills gauge invariance is standardly associated, through Noether’s theorem, to the (Yang-Mills) current conservation, the spacetime-translation subgroup of Poincaré invariance is associated to the conservation of the total energy and momentum, and the Lorentz subgroup is associated to the conservation of the total angular momentum. Generally speaking, the interest of designing a discrete dynamical model satisfying conservation laws, is twofold. If the discrete model is used in order to reproduce a continuum theory, preserving the continuum conservation laws on the lattice makes it unnecessary to compensate for the discrepancies arising otherwise, and which can lead to physical aberrations. Now, independently of the continuum limit of such discrete models, designing them in the perspective of making them satisfy discrete conservation laws – which are a pillar in all physical theories – a priori endow these discrete models with, if not a great one, at least some versatility, i.e. makes them, a priori, suitable for various applications, not necessarily connected, at least explicitly, to a continuum situation, but do connected to the conservation of physical quantities, on a discrete background.

In standard LGTs, Yang-Mills gauge invariance was seminaly implemented on the lattice by Wilson [27]. Indeed, he constructed a gauge-invariant action on the lattice for both the matter field and the gauge field. In particular, the lattice gauge-invariant gauge-field kinetic term yields, in the continuum, essentially the standard ‘square of the field strength’, as needed. Let us now comment on the on-shell dynamics on the lattice. To obtain this lattice on-shell dynamics of either the matter field or the gauge field, one ultimately needs, starting from Wilson’s original LGT, to define a variational principle on the lattice, to be applied directly to Wilson’s lattice gauge-invariant action. Now, one month after Wilson submitted his seminal paper, Kogut submitted a Hamiltonian formulation of LGT [259], which discretizes spatially the Hamiltonian of the system, while keeping time continuous. To obtain the on-shell dynamics of either the matter field or the gauge field with such a formulation, one simply needs to omit from the full Hamiltonian, which describes both the matter-field and the gauge-field dynamics, the irrelevant term for the desired on-shell dynamics. For more information on the differences between Wilson and Kogut’s LGT, see Appendix O. While many suggestions for the either analog [13] or digital [260, 261, 13] quantum simulation of LGTs, also ensure Yang-Mills gauge invariance on the lattice and implement lattice gauge-invariant Hamiltonians, a difficulty related to the on-shell gauge-field dynamics was first addressed by Jordan et al. [261] and Wiese [13], and then in *extensive* detail by Zohar et al. in 2015 [262]. By nature, this difficulty contains both

⁶In the non-Abelian case, this quantity is gauge *covariant*.

⁷However, D’Ariano et al. integrate, to their axiomatic presentation, the seminal work of Bialynicki-Birula which provides a unitary discretization of Maxwell’s equations that ensures energy conservation on the lattice [186].

energy-conservation and current-conservation aspects.

This difficulty, that we shall briefly clarify soon, has been one of the experimental challenges that had to be met to achieve the recent tracking of “Real-time dynamics of lattice gauge theories with a few-qubit quantum computer”, led last year at the University of Innsbruck by Martinez et al. [24]. This experiment digitally quantum simulates the quantum-electrodynamical Schwinger model, i.e. the creation of electron-positron pairs by vacuum fluctuations. Because such a seminal experimental work deals with a Yang-Mills gauge theory which is Abelian, the gauge-field on-shell dynamics corresponds to Maxwell’s equations, and, because the model is considered in the minimal spacetime dimension, namely 1+1, these Maxwell’s equations reduce to Ampère’s law without magnetic field⁸ and Gauss’s law; while the former is indeed a dynamical equation, the latter is a non-dynamical constraint. The aforementioned theoretical and experimental challenge is the implementation of Gauss’s law in this minimal quantum simulation of LGT. Martinez et al.’s experimental work is the concretisation of a large number of theoretical works on the quantum simulation of standard LGTs [263, 260, 261, 13, 262]. Note the tensor-network reformulation [264] of the theory contained in Martinez et al.’s experiment [24]. See the following talk given in 2013 by Reznik, on his joint work with Zohar and Cirac, <http://www.lattice2013.uni-mainz.de/presentations/Plenaries%20Tuesday/Reznik.pdf>. One of the next steps to take is certainly to experimentally quantum simulate non-Abelian $U(N)$ and $SU(N)$ Yang-Mills gauge theories, based on recent theoretical work, still in the framework of standard LGTs [14, 15].

Let us highlight some differences between (standard⁹) LGTs and the DTQWs-based discretizations of (first-quantized) QFTs that have been discussed in the present manuscript [2, 3], that we will call DTQW-GTs in the following discussion. As in LGTs, the lattice gauge fields essentially appear, in DTQW-GTs, as exponentials of their continuum counterparts, which reflects the periodicity induced by the lattice, and makes it sufficient to limit both the *lattice* quasimomenta and gauge fields¹⁰ – which deliver the standard momenta and gauge fields in the continuum –, to the spacetime Brillouin zone¹¹. While on the one hand, as Wilson seminally pointed out [27], such an exponentiation ensures, in LGTs, the local gauge invariance on the lattice, starting from a *standard* finite differentiation of the continuum free theory, the lattice gauge invariance in DTQW-GTs is on the other hand, as the exponentials, in-built¹², essentially because of an *in-built (time-evolution) unitarity* which is directly constructed at the level of the evolution operator with no need to define a Hamiltonian. Regarding the question of unitarity in LGTs, see Appendix O. This remark leads us to the following important difference: while, in LGTs, the gauge-field exponential is implemented in the Lagrangian [27] or the Hamiltonian [259], it is implemented at the level of the evolution operator in DTQW-GTs. This difference is reminiscent of that between tight-binding models and DTQWs schemes regarding the implementation of gauge fields, which has been underlined when discussing the ‘third’ electromagnetic interpretation of

⁸We may rather call this a degenerate (general) Ampère’s law, since speaking of this law in such terms, i.e. “Ampère’s law”, usually implies the presence of a magnetic field (and sometimes even forgets about the electric field time variation). With no magnetic field, this law simply states that the charge current is given by the time variation of the electric field.

⁹We shall omit the word ‘standard’ in the following discussion, for the sake of brevity.

¹⁰In argument of the exponentials.

¹¹The denomination ‘Brillouin zone’ usually refers to the spatial zone, while the temporal zone is often referred to as the ‘Floquet zone’.

¹²Provided we consider a sufficiently broad family of inhomogeneous DTQWs.

electromagnetic DTQW schemes, in Subsection 1.2.1.

Another difference must be evoked, between the gauge-field exponentials appearing in LGTs and those appearing in DTQW-GTs. In DTQW-GTs, the gauge fields are, as matter fields, defined on the sites of the lattice, while in LGTs the gauge fields are defined on the links of the lattice. As the aforementioned exponentiation in LGTs, this is necessary to ensure the gauge invariance of the basic finite-differentiated free kinetic term of the continuum theory, which involves products of fields at different lattice sites. More technically, one needs, in order to build the lattice gauge field, to perform an integral of the continuum gauge field over the link before exponentiating it; this yields a so-called parallel transporter, that replaces the continuum gauge field in the lattice theory [27, 259, 265, 266, 28]. This integration over the links is not introduced, at least explicitly, in DTQW-GTs. Note eventually that the ‘discrete differential operators’ involved in DTQW-GTs are *not* standard finite differences.

Eventually, discretizing fermionic fields is notoriously difficult in LGTs [267, 266, 28]. We have mentioned in the discussion of Ref. [1] that the scheme presented in this publication exhibits *fermion doubling* since, although the discretization is not done by standard finite-differentiation, it is still a *symmetric discretization*. This is the case of all DTQW-GTs presented in this manuscript¹³. Regarding this matter, among others, I would like to mention the paper of 2016 by Brower et al. [268], which constructs finite elements suited for lattice formulations of QFT on curved backgrounds, based on standard LGTs; the construction mixes standard finite-element methods to Regge calculus.

Let us finally sum up possible directions for further studies.

1. Second quantization

LGTs are fully second quantized, while no second quantization of DTQW-GTs has been suggested yet. Indeed, although several works have suggested canonical second quantizations for DTQWs, none of them implements, to the best of my knowledge, gauge invariance on the lattice. These works use the framework of QCA to describe multiparticle states, and the standard DTQW is derived has the one-particle case, see, e.g., Refs. [269, 270, 59], as well as the PhD manuscript of T. C. Farrelly [44]¹⁴.

2. Mapping between LGTs and DTQW-GTs

It would be interesting to investigate to which extent it is possible to map these two a priori different spacetime discretizations of Yang-Mills gauge theories, if there is a mapping at all. Whatever the answer may be, one should discuss the pros and cons of each discretization, with respect to the other. Let us list several items to be investigated regarding those questions.

¹³In Ref. [44] is suggested a way of removing fermion doubling in DTQWs.

¹⁴Today, 22 August 2017, I am reading this document for the first time – it is not open-access yet, but should be in a few days. In this work, various paths actually converge, all together, towards the QCA-based second quantification of DTQWs (although there is still work to be done), with a gauge-invariance implementation – which seems to be the same as ours, see Section 3.4.2 of [44] – but in the Abelian case only, while we have suggested a non-Abelian gauge-invariant scheme [3]. From what I have seen, no gauge-invariant quantity is suggested, while we have suggested gauge-invariant (or gauge-covariant) quantities in both the Abelian and the non-Abelian case [2, 4], as well as lattice equivalents to Maxwell’s equations [2]. Farrelly’s PhD manuscript is based on four publications: two of them indeed deal with DTQW and QCA schemes for fermions [271, 272], while the two others deal with quantum thermodynamics. I strongly recommend the reading of Ref. [44].

(a) *Lagrangian vs. Hamiltonian LGTs*

There are two standard formulations of LGTs: (i) the Lagrangian formulation, seminally introduced by Wilson (W) in 1974 [27], which is naturally associated to the path-integral formalism¹⁵, and (ii) the Hamiltonian formulation, seminally introduced by Kogut and Susskind (KS) in 1975¹⁶ [259], which is naturally associated to the canonical formalism¹⁷. In KS-LGTs, the time-evolution unitarity is manifest, as in DTQW-GTs, whereas this unitarity is far from manifest in W-LGTs. We refer the reader to Appendix O for a few more comments regarding this matter¹⁸. Eventually, it is straightforward to derive, from KS-LGTs, the lattice on-shell dynamics of either the matter field or the gauge field: one indeed simply needs to omit from the full Hamiltonian the irrelevant terms. If one works instead with W-LGTs, one ultimately needs to define a variational principle on the lattice to achieve such a purpose.

(b) *Link variables*

In LGTs, the gauge fields are naturally associated to the links of the lattice. In DTQW-GTs, they have been defined on the nodes [2, 3]. In LGTs, each spin component can be transported in both directions on a given lattice axis¹⁹, while in DTQW-GTs, the upper component is always transported in the same direction along a given axis of the spatial lattice, and the lower component is transported along the other direction along this axis; this is obvious given that the transport is determined by the spin-dependent shift. Now, the gauge field is implemented, in DTQW-GTs, by the spin-dependent phase. Let us write Eq. (1) of [2] in the case of vanishing mixing angles θ^+ and θ^- ²⁰:

$$\psi_{j+1,p,q}^- = e^{(\alpha_2)_{j,p,q}} e^{(\alpha_1)_{j,p,q+1}} \psi_{p+1,q+1}^- \quad (3.1)$$

$$\psi_{j+1,p,q}^+ = e^{-(\alpha_2)_{j,p,q}} e^{-(\alpha_1)_{j,p,q-1}} \psi_{p-1,q-1}^+, \quad (3.2)$$

with

$$(\alpha_\mu)_{j,p,q} = i\epsilon q (A_\mu)_{j,p,q}, \quad (3.3)$$

where ϵ is the lattice spacing, the electric charge equals -1 in [2], and $(A_\mu)_{j,p,q}$ is the covariant μ component of the continuum gauge field, but defined only on the nodes of the lattice. In our scheme, ψ^- goes left in time and ψ^+ goes right. Now, notice that the gauge field can be associated to the links, exactly as in LGTs. Indeed, let us *define*

$$U_{(j,p,q) \rightarrow (j,p+1,q)} \equiv (U_{\mu=1})_{j,p,q} \equiv e^{i\epsilon q (A_{\mu=1})_{j,p,q}} \quad (3.4)$$

$$U_{(j,p,q) \rightarrow (j,p,q+1)} \equiv (U_{\mu=2})_{j,p,q} \equiv e^{i\epsilon q (A_{\mu=2})_{j,p,q}}, \quad (3.5)$$

¹⁵The scattering-matrix elements are viewed as statistical-physics correlators through a Wick rotation.

¹⁶Both papers were submitted to Phys. Rev. D one month apart.

¹⁷The scattering-matrix elements are computed as in canonical quantum physics, with Hermitian operators acting on multiparticle Hilbert spaces (so-called Fock spaces).

¹⁸Recall that the lattice is a possible regulator for field theories, but not the only one.

¹⁹See, e.g., Eqs. (12) and (13) in [273] (1D case): for each spin component, the Hermitian-conjugate term of (12) accounts for the propagation in the other direction.

²⁰For the scheme to deliver Dirac propagation, these angles must have value $\pm\pi/4$ at zeroth order in the step of the lattice, i.e. they cannot vanish as we consider here. The present consideration has *only* a pedagogical purpose, since it enables to see how the spin-dependent phase is related to the spin-dependent shift, in *both* directions, putting aside the spin coupling.

where the arrow has been defined according to the opposite of the time evolution of the matter field, which is the same as in LGTs²¹. These two expressions match exactly with Eq. (5.18) of [28]. We now see that link variables can be considered in DTQW-GTs, which are the same as in LGTs^{22,23}. With the help of such a formulation, it may be possible to view the differences between LGTs and DTQW-GTs as a choice of which transporters we choose to apply to build the time evolution, and in which order we choose to apply them, that is, a choice in the way we connect the nodes by the links, from a given instant to the next one. This may as well be another way of viewing the fact that the differences between LGTs and DTQW-GTs substantially lie in the way one discretizes the Dirac equation.

(c) *Evolution-operator vs. Hamiltonian gauge invariance*

In KS- (resp. W-) LGTs, the gauge-field exponentials are introduced in the Hamiltonian (resp. Lagrangian). This enables to preserve gauge invariance at the level of the spacetime-discretized Hamiltonian (resp. Lagrangian). In DTQW-GTs, these exponentials are introduced in the evolution operator, so that what appears in the effective Hamiltonian²⁴ is the argument of the exponential, i.e. what will give the gauge field in the continuum. This makes DTQW-GTs a priori more natural in the sense that the fact that one has gauge-field exponentials is only due to the time-evolution unitarity; in other words, one does not need to exponentiate the continuum gauge field to ensure gauge invariance; this gauge invariance is instead ensured by an appropriate definition of the DTQW operator in terms of a product of well-chosen unitaries.

3. Mappings between tight-binding condensed-matter systems and DTQW schemes

(a) *An application of Item 2*

If a mapping is found between LGTs and DTQW-GTs, the present item, 3, can be seen as an application of such a hypothetical result. Indeed, there are already well-established correspondences between LGT prescriptions to implement gauge fields and the so-called Peierls substitution to implement a magnetic field in (condensed-matter) tight-binding Hamiltonians (TBHs). Now, some of these TBHs can be engineered with several quantum setups, such as, e.g., cold atoms in optical lattices [80, 81]. A seminal experimental proposal in the field of the quantum simulation of TBHs with cold atoms coupled to synthetic gauge fields, by Osterloh et al. [274], makes it fully explicit this correspondence between LGTs and cold-atom engineered systems – in the case of a 2D lattice and for a particular non-Abelian SU(2) gauge field. These correspondences have now

²¹Indeed, in LGTs, a non-daggered transporter $p \rightarrow p+1$ is conventionally associated, in the gauge-matter coupling term of the Hamiltonian, to a particle annihilation at $p+1$ and a particle creation at p . See, e.g., Eqs. (12) and (13) in [273].

²²Up to (i) the fact that time is continuous in KS-LGTs, and (ii) the difference mentioned in the next item.

²³Similar gauge-field link variables are also described in Section 3.4.2 of [44].

²⁴This effective Hamiltonian is generically obtained from the evolution operator, defined as a product of unitaries, by using the Baker-Campbell-Hausdorff formula.

been extended to very generic TBHs [262], and underlie all current proposals to quantum simulate high-energy lattice QFTs with low-energy engineered systems.

(b) **Weaker mappings**

One can also directly try to simulate TBHs with DTQWs, without trying to map, at least explicitly, DTQW-GTs to LGTs. To achieve such a purpose, one may want to build intuition from the quantum simulation of TBHs with LGTs. Notice that TBHs are non-relativistic, while DTQWs are intrinsically relativistic. This is a priori a notable difference, since, from a given instant to the next one, there is, in the relativistic case, a bounded causal neighborhood, while this is not the case in TBHs, i.e. there is a non-vanishing probability that a particle moves of an arbitrary big distance from a given instant to the next one^{25,26}. One may need to take a non-relativistic limit as in Strauch’s paper (infinitely-strong mass coupling, i.e. $\theta \rightarrow \pi/2$ in Eq. (5).) [124], so that the time coordinate of DTQWs and that of TBHs would not be the same. The question would then be how to obtain a TBH from the non-relativistic limit of a DTQW, instead of obtaining the space-discretized Schrödinger equation as in [124]. Indeed, while mappings between DTQWs and TBHs have been suggested, these connections are only phenomenal, i.e. there is no rigorous connection between both; see, e.g., [275] and http://science.gu.se/digitalAssets/1581/1581243_tosini.pdf. Let us recall several applications of the coupling of TBHs to gauge fields:

i. *Abelian case*

These are TBHs with a superimposed electromagnetic field. This system has a myriad of applications, e.g., all the quantum Hall effects. Regarding quantum Hall effects, the two following very complete references may be consulted: [276, 277].

ii. *Non-Abelian case*

A well-known condensed-matter non-Abelian gauge theory is that of the Rashba coupling, which describes how the Pauli spin-orbit term affects TBHs [203]. Notice that the spin-orbit coupling contributes to the energy gaps in the bandstructure of solids; in the case of graphene, e.g., this spin-orbit coupling accounts for a (very) small gap [278], that can be neglected in a first approximation, which delivers the well-known graphene Dirac ‘strict’ i.e. ‘massless’ cones. Eventually, an idea regarding the interpretation of the overlap integrals of TBHs in terms of the DTQW parameters is mentioned at the end of Appendix E, which could be investigated further.

²⁵This fact was reminded me by A. Alberti. The result is also recalled, and proved, in the introduction (Chapter 1) of Farrelly’s PhD manuscript [44]. In the sense that they preserve the relativistic causal neighborhood, DTQWs seem to be models a priori more suited to the discretization of continuum-spacetime relativistic dynamics than KG-LGTs, which, since essentially implementing TBHs in continuous time, do not preserve the above-mentioned causal neighborhood. In his introduction, Farrelly reviews several arguments in favor of – but also some against – time discretization in quantum simulations of QFTs [44].

²⁶Although this probability must, on average, decrease with distance, above some distance threshold.

Publications, internships & communications

Publications

1. Pablo Arnault and Fabrice Debbasch.
Landau levels for discrete-time quantum walks in magnetic fields.
Physica A, 443:179–191, 2015.
Received 12 December 2014, Revised 24 July 2015, Available online 15 September 2015, Published 1 February 2016.
<https://doi.org/10.1016/j.physa.2015.08.011>.
2. Pablo Arnault and Fabrice Debbasch.
Quantum walks and discrete gauge theories.
Phys. Rev. A, 93:052301, 2016.
Received 28 July 2015, Revised manuscript received 16 October 2015, Published 2 May 2016.
<https://doi.org/10.1103/PhysRevA.94.012335>.
3. Pablo Arnault, Giuseppe Di Molfetta, Marc Brachet and Fabrice Debbasch.
Quantum walks and non-Abelian discrete gauge theory.
Phys. Rev. A, 94:012335, 2016.
Received 6 May 2016, Published 19 July 2016.
<https://doi.org/10.1103/PhysRevA.94.012335>.
4. Pablo Arnault and Fabrice Debbasch.
Quantum walks and gravitational waves.
Ann. Physics, 383:645–661, 2017.
Received 8 September 2016, Accepted 7 April 2017, Available online 27 April 2017.
<https://doi.org/10.1016/j.aop.2017.04.003>.

Internships

1. **April and May 2016: 2-month internship** in the team of Dieter Meschede and Andrea Alberti, at the Institute for Applied Physics (IAP), Bonn, Germany, with a grant from the group; I am indebted to Dieter Meschede and Andrea Alberti for both their invitation and financial support. Ongoing collaboration on 2D DTQWs coupled to magnetic fields, with a focus on topological magnetic phases and the bulk-edge correspondance. In-progress experiment, with an analog quantum simulator consisting of pseudo-spin-1/2 cold atoms trapped in a 2D periodic potential generated with laser beams; one can drive the atoms on the 2D lattice, left or right and up or down, according to their pseudo-spin. For details on both (i) the study of topological effects with DTQWs (in the absence of magnetic field), and (ii) on the experimental setup,

see the paper by Thorsten Groh et al. [279]. More details on the experimental setup are available on the website of the group, <http://quantum-technologies.iap.uni-bonn.de/en/quantum-walks/2d-quantum-simulator.html>.

2. **July and August 2016: 2-month internship** in the team of Yutaka Shikano, at the Center for Integrative Molecular Systems (Cimos), Okazaki, Japan, thanks to a grant of the JSPS Summer Program; I warmly thank both the JSPS for their support, and Yutaka Shikano for his invitation and additional support. In-progress theoretical work on both (i) a DTQW self-induced curved metric, started by Giuseppe Di Molfetta, and (ii) a close examination of the interference terms in the feed-forward DTQW, which is used for the quantum simulation of anomalous diffusion [280], with an eventual collaboration with Norio Konno and Etsuo Segawa.

Communications

1. **Poster** on publications [1] and [2], at the First International Conference for Young Quantum-Information Scientists (YQIS), November 2015, Institut d'Optique Graduate School (IOGS), Palaiseau, France. The book of abstracts is available at https://yqis15.sciencesconf.org/conference/yqis15/pages/BoA_YQIS2015_IOGS_2.pdf.
2. **Poster** on the research projects I was involved in at that time, during the introduction week of the JSPS Summer Program 2016. Don't hesitate to visit the JSPS website for information on its activities and fellowships, at <http://www.jsps.go.jp/english/programs/index.html>. For one-page-long texts, each sharing a personal experience, of the French fellows of the JSPS Summer Program 2016, and older ones, go to <http://jsps.unistra.fr/les-bourses-de-la-jsps/summer-program/>.
3. **25-min talk** covering all the publications I coauthored as a PhD student [1, 2, 3, 4], at the Workshop on Quantum Simulation and Quantum Walks (WQSQWs), November 2016, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Prague, Czech Republic. The book of abstracts is available at <http://wqsqw2016.phys.cz/WQSqw-abstracts.pdf>.
4. **Poster** giving a compact presentation of the state-of-the-art ongoing construction of DTQW-based lattice gauge theories, at the conference Atomes Froids et Technologies Quantiques (AFTQ), Decembre 2016, École Normale Supérieure, Paris, France. For an abstract of the poster, go to <https://aftq16.sciencesconf.org/126422/document>. For an abstract of the poster by Muhammad Sajid, which describes the in-progress work of the Meschede-Alberti group on quantum-Hall physics with the 2D DTQW analog simulator, go to <https://aftq16.sciencesconf.org/126328/document>.

Appendix

Causal neighborhoods

Given a certain time interval Δt , let us define the *relativistic causal neighborhood* around a point P in physical space as the P -centered sphere of radius $R_{\text{rel}} = c \Delta t$, c being the speed of light. R_{rel} is much bigger than many usual macroscopic scales. Let us define a *mesoscopic-transport (or continuum-medium) causal neighborhood* around a point P in some medium, as the P -centered sphere of radius $R_{\text{mes}} = v \Delta t$, where v is the typical speed modulus of the matter of which the medium is made of. v depends on the initial conditions and on the diverse phenomena which take place within the medium¹.

The simple qualitative picture accounting for the possibility to consider mesoscopic samples of matter as pointlike, is the following. There are microscopic particles, namely atoms and molecules, which are either (i), in the case of fluids, subject to many collisions between each other, due to particular thermodynamical conditions such that the mean free path between two collisions is precisely below the mesoscopic scale, or (ii) well arranged, as in solids, and oscillate around their equilibrium position, with an amplitude which is also (much) below the mesoscopic scale considered. This makes it possible to consider that, on sufficiently short time scales Δt , a microscopic particle located at the center of some mesoscopic volume cannot escape it^{2,3}. If, moreover, Δt is much bigger than the time scale T of the studied phenomenon, then mesoscopic particles keep their integrity during the phenomenon. It is actually not necessary, for the mesoscopic-particle or continuum-medium picture to hold, that these mesoscopic particles strictly keep their integrity all along the mesoscopic and macroscopic dynamics, but only that the average displacement of atoms which is induced by the microscopic dynamics be smaller than the average displacement of

¹These phenomena can be, e.g., convection, viscosity diffusion or heat diffusion. It is often useful to consider a different v for each phenomenon. The terminology ‘typical speed’ used above is actually obscure. One must distinguish between characteristic speeds and average speeds. Convection and diffusion are not related to any characteristic speeds, but one can associate to these phenomena average speeds by $v = d / \Delta t$, where d is the mean displacement induced by the considered phenomenon over Δt .

²In the case of solids, Δt is actually infinite if the considered system is isolated.

³The following examples are instructive. A point P in vacuum can be reached, within a time interval $\Delta t = 1$ s, by any photon located within the P -centered sphere of radius $R_{\text{rel}} \simeq 3 \times 10^8$ m. Consider now that this point P is in a sufficiently dense medium, such as, e.g., the Sun, which is essentially made of Hydrogen, and Helium at its center. Photons collide with the molecules of the medium. Assume that after each collision the new direction of the photon is random. If P is in the radiative zone, it can only be reached by photons contained within the P -centered sphere of radius $R_{\text{mes,rad}} = \sqrt{c \Delta t d} \simeq 145$ m, where $d \simeq 7 \times 10^{-5}$ m is the mean free path of a photon in the Sun (i.e. the distance between two collisions). For details on this phenomenon, see, e.g., https://media4.obspm.fr/public/AAM/pages_proba/exo-soleil.html. In the convective zone, the energy carried by photons is mainly transported by convection of the hydrogen plasma: a point P in the convective zone can only be reached by photons contained within the P -centered sphere of radius $\max\{R_{\text{mes,rad}}, R_{\text{mes,conv}}\}$, where $R_{\text{mes,conv}} = v_{\text{conv}} \Delta t$ and v_{conv} is the average plasma-convection speed.

the physical quantity described by the mesoscopic-transport equation⁴.

The atomistic collisional picture for fluids was initially developed by Boltzmann in the late 19th century, while the existence of atoms was far from widely accepted yet. If one takes into account special relativity, it is a natural idea to combine this collisional picture with the relativistic locality to which atoms are subject, in order to derive relativistic mesoscopic-transport equations; that being said, achieving this is far from straightforward. This point is briefly developed in the rest of the introduction, i.e. after the reference to this appendix in the introduction.

⁴These quantities can indeed be (i) the speed of the mesoscopic samples of matter, but also (ii) the temperature, with no macroscopic or mesoscopic matter displacement, or (iii) the density, which may be transported on distances much bigger than those on which matter is transported; this is typically the case of density waves in continuum media. (It may be more intuitive to think of this as a transport of the *spatial variations*, i.e. the *gradient* of these quantities.)

On computers

This appendix aims at mentioning a (very) few important milestones, both theoretical and experimental, in the history of both computation and computers, first classical, and then quantum. The appendix will end with the difficulties that have to be overcome in order to achieve the construction of a universal quantum computer.

B.1 Classical computer

B.1.1 Abstract classical computer

In his 1936 seminal paper [70, 71], Turing described both (i) a-machines (for ‘automatic machines’), now called *Turing machines* (TMs), and (ii) the now-called *universal Turing machines* (UTMs).

B.1.1.1 Specific-task abstract classical computer: the Turing machine

A TM is an abstract machine, i.e. a mathematical object, let us call it T , that models a hypothetical actual machine that would implement an algorithmic task, which we first informally define as a given series of unambiguous operations, triggered by an input belonging to a certain set of possible inputs¹. The TM always produces an output – i.e. it always ‘halt’ – entirely determined by the input (and is in this sense deterministic). A TM can thus be viewed as implementing – thanks to several ‘ingredients’ and in a certain *way* – a mathematical function, and, again, the TM is viewed as a model for an actual machine implementing this mathematical function. The *way* this function is implemented by the TM is encoded in the so-called ‘action table’ of the TM, which indicates which operation should be done at each step². The action table lists all the possible configurations that the TM may encounter given the set of all possible inputs, and specifies the action to be performed for each of those configurations, in order to eventually make the TM produce the desired output. To implement the instructions of its action table, a hypothetical actual TM only needs to be able to perform 6 elementary operations, called *primitives*. These concrete primitives are *right*, *left*, *print*, *scan*, *erase*, and *nothing/halt*³.

We have above informally defined the notion of algorithm. Actually, the notion of TM historically enabled to give a proper *mathematical definition* of an algorithm: the latter is, in this perspective, any series of operations that can either (i) directly be performed by a TM, or (ii) at least reducible to Turing-machine-performable operations. Indeed, Turing eventually came up with the notion of TM by requiring it to capture and be able to realize

¹We code these inputs essentially with binary numbers, i.e. with a series of zeros and ones.

²There are in general several possible action tables to compute the same function, and the question of the simplest one naturally arises.

³One could say that the notion of TM makes this ‘black box’ which is introduced to teach the notion of function to young students, (*more* than) white.

any task that we intuitively view as an algorithm. Grounded on this notion of TM which, although still abstract, is more than strongly underlaid by a concrete realization, the field of algorithmics quickly developed. In such an abstract-algorithmics context, the Turing-machine primitives often translate into *logical gates*, i.e. elementary logical operations with which one can build any algorithm.

To sum up, an actual automatic machine (i.e. automaton) realizing a certain task triggered by an input which can be encoded in a series of zeros and ones, that we may call specific-task (classical) computer, can always be described, theoretically, by a certain TM (i.e. having a certain action table and a certain set of possible inputs). The Turing-machine model is thus essentially the most general mathematical model for a specific-task (classical) computer.

From this theoretical point of view, the first legacy of Turing and his Turing-machine model may be, as several authors suggest, to have given the proper way of thinking algorithmically, i.e. the way to design practical mathematical algorithms, that could all be implemented on machines through the same principles, with, if not none, at least only a few technical modifications. I make this remark because the architecture of actual current computers is way more sophisticated and differs, in several aspects, from the too basic one defined by TMs (or, rather, UTMs), as we briefly underline further down.

B.1.1.2 Universal abstract classical computer

• The universal Turing machine

The obvious limitation of an automaton based on a certain TM is that it can only perform the task encoded in the action table. To perform other TM-type tasks, one has either to (i) build another automaton which realizes another action table, or, if possible, to (ii) reprogram the automaton with another action table.

Turing thus proposed, in the same above-mentioned 1936 seminal paper [70], the now-called UTMs. A UTM U takes as input a certain TM T and a possible input i for T . By encoding the action table of T as a standard Turing-machine input, i.e. as a series of one's and zero's, and by (abstractly) storing it in its memory, U can then, by reading this encoded action table together with the input i , produce the same output as T would produce with input i , which is noted $U(T, i) = T(i)$.

It is important to note that a UTM is not more than a TM in terms of the ingredients it is made of, i.e. a UTM is a TM, with additional functioning specifications *only*. More relevantly: once we have mathematically defined the notion of TM, it is a theorem that there exist a certain TM, that we call UTM, which does the job of any TM – that we give the UTM as an encoded input – *as efficiently as the TM itself*⁴. In the discussions about computational power, we will thus from now on often drop the ‘U’ in ‘UTMs’.

• Other models of computation

As implicitly suggested at the end of Subsubsection B.1.1.1, one can conceive other models of computation than the TM. Let us try to give both an intuitive and general picture of what a *computational model* is.

⁴See, e.g., Theorem 2 in the following notes, <https://homes.cs.washington.edu/~anuprao/pubs/CSE531Winter12/lecture1.pdf>. The notion of *efficiency* has a precise meaning in computer science.

★ **Computational model.** A computational model may be viewed as the given of (i) a set of *elementary operations*, called *primitives*, such as that of the TM, listed above, or such as logical gates, and (ii) a *background*, such as the whole TM setup, described above, or a graph, on which one positions and relates the primitives according to some *rules*. All these elements are defined in order for the computational model to achieve a certain *class of computational aims*.

★ **Universal computational model.** The computational model is considered *universal* when the class of computational aims it can fulfill is sufficiently broad according to some *criteria*, or *requirements of reference*. Designing a universal computational model thus demands to find both a set of primitives and a way of chaining them that enable to meet the universality requirements. A standard universality requirement – and thus definition – is that the computational model have (at least) the same computational power as a (U⁵)TM, in which case the model is said Turing-complete⁶. Other universality criteria may be useful, depending one's computational aims. Taking the TM as a reference is, in particular, underlaid by the so-called *Church-Turing thesis*, which states that TMs should be able to implement any type of 'automatic task'. Because the notion of 'automatic task' is not (meant as being) mathematically defined in the Church-Turing thesis and its extensions, these theses are not mathematical claims that call for mathematical proofs or disproofs, but rather philosophical or metamathematical claims that call for mathematical definitions for notions such as 'automatic task' or 'computation'⁷.

An example of widespread computational model is the *circuit model*. This model is not Turing-complete, but its extension, the *circuit-family model*, is more than Turing-complete, i.e. a circuit family (CF) may compute a broader class of tasks than a TM. By the denomination 'circuit model', one sometimes refers to the circuit-family model, since, being not Turing-complete, the mere circuit model is not of sufficient interest. There is a subclass of CFs which is equivalent to (polynomial-time) TMs, namely, *uniform CFs*.

B.1.2 Actual classical computer

B.1.2.1 Specific-task actual classical computer

An example of such a machine is the Turing (electromechanical) bomb, which was build by Turing himself, together with Welchman, in order to decrypt the encrypted messages created by the Nazis during World War II thanks to Enigma machines, which are another example of specific-task computer.

Specific-task computers were later also designed to treat and store the data generated by scientific experiments, e.g., in radioastronomy.

B.1.2.2 Universal actual classical computer

The theoretical description of such machines, i.e. the so-called 'stored-program (abstract) computer', is strongly reminiscent of the UTM, although it differs from it in several aspects.

⁵In the discussions about computational power, we will from now on definitely drop the 'U'.

⁶'Having the same computational power as' means (i) 'being able to realize the same tasks as' and (ii) 'as efficiently as'.

⁷This leads to classifying computational models into equivalence classes of robust computability notions, i.e. computability notions which are frequently found to be equivalent from one computational model to the other.

The essence of stored-program computers is contained in the so-called ‘Von Neumann architecture’, seminally introduced in 1945⁸, and both terminologies are sometimes used as synonyms. Stored-program computers encode the input instructions describing a program⁹ as standard data which is stored in their main (or primary) memory, the RAM i.e. random-access memories¹⁰, and then read and execute these data as a standard input, as UTMs do with input TMs. The encoding and the execution of the source code – which is written in a ‘human’ language (usually, english) – can be performed successively as a single block by an *interpreter*. In this case, the interpreter stores the encoded source code in the RAM before executing it. The encoding and the execution can also be separated tasks. In this second case, the encoding is done by a *compiler*, and the compiled i.e. encoded source code is stored in the so-called ‘data memory’ (to be ‘opposed’ to the RAM), for ‘future’ execution; the file containing the compiled code is directly executable by the computer, whenever wished.

B.2 Quantum computer

B.2.1 Abstract quantum computer

B.2.1.1 Specific-task abstract quantum computer

- The quantum Turing machine

The notion of *quantum TM* (QTM) was seminally introduced in Deutsch’s 1985 paper, ‘Quantum theory, the Church-Turing principle and the universal quantum computer’, see http://old.ceid.upatras.gr/tech_news/papers/quantum_theory.pdf. The notion of QTM enables, in particular, to capture *quantum algorithms* (see below) in action tables, and may shed light on the implementation of quantum algorithms by an actual quantum computer.

- Quantum algorithms

As in the classical case, quantum algorithms may be designed according to other *models of quantum computation* than QTMs (see below). That being said, all quantum algorithms share the following characteristics. Instead of manipulating *binary data*, they manipulate what we may call *quantum binary data*, i.e. (i) the (*logical*¹¹) *bits* are replaced by *qubits*, which can be in any superposition of zeros and ones, and which we could call *superposed bits*, (ii) the *bit strings* are replaced by *entangled qubit strings* and (iii) the *classical gates* are replaced by *quantum gates*.

Two important quantum algorithms, developed in the 90’s, are Shor’s [36, 37], for prime-number factorization, and Grover’s [38], for database search.

⁸This architecture was seminally described in the *First draft on the EDVAC*, a reproduction of which is available at <https://web.archive.org/web/20130314123032/http://qss.stanford.edu/~godfrey/vonNeumann/vnedvac.pdf>. Von Neumann explicitly mentioned UTMs as a source of inspiration.

⁹A ‘program’ can be seen as either a less-abstract version of an ‘algorithm’, or simply as a different terminology to refer to algorithms.

¹⁰This memory must be quickly accessible by the processor, or CPU (Central Processing Unit), since it stores encoded programs that should be accessible to be run *at an arbitrary time and from an arbitrary location*, hence the denomination ‘random access’.

¹¹To be opposed to *physical* qubits. We will drop the precision ‘logical’ from now on in this paragraph, but it is implicit since we are in an abstract context.

B.2.1.2 Universal abstract quantum computer

- **The universal quantum Turing machine**

The notion of *universal QTM* was, together with that of QTM, also naturally introduced in Deutsch's seminal work (see above). Note that this is three years after Feynman's seminal 1982 paper [42], which was about universal quantum *simulation* – of (local) physics.

- **Other models of universal quantum computation**

Quantum algorithmics has, from Deutsch's seminal work, developed enough for several realistic theoretical models of *universal* quantum computation to be suggested within the last 10 years, other than universal QTMs. Examples of such models are that by Childs, based on CTQWs [9, 10], or that by Lovett et al., based on DTQWs [158], which is the DTQW version of the first paper Childs [9].

There is also a quantum counterpart to classical circuit families (CFs), namely *quantum CFs* (QCFs). The following review work on the “computational equivalence between QTMs and QCFs”, <http://www.math.ku.dk/~moller/students/chrW.pdf>, ends with the following conclusion: “Finitely-generated QCFs are thus an intermediate of polynomial-time uniformly generated QCFs and uniform QCFs, such that their computational power exactly matches that of polynomial-time QTMs.” This makes me believe that the computational power of QCFs relative to QTMs is lower than that of CFs relative to TMs, since uniform CFs are equivalent to (polynomial-time) TMs. That being said, I am currently not enough qualified to be certain about such a statement, and even if this statement is true, I currently do not master well enough the various concepts I have introduced to speak further about this.

B.2.2 Actual quantum computer

B.2.2.1 Specific-task actual quantum computer

These computers are currently developing. They work at best with, in average, a few tens of physical qubits. The company IBM has given online free access to a five-qubit quantum computer, see <https://quantumexperience.ng.bluemix.net/qx/editor>, and it also offers online access to a 16-qubit one, for the use of which one has to pay.

B.2.2.2 Universal actual quantum computer

The current difficulty in achieving the construction of a universal quantum computer is essentially a technical one, namely, scalability. Scalability is the scale-up potential of a device. The scalability of current quantum-computing devices is poor, if one aims at beating classical computers. This is essentially due to the difficulty of increasing the size of memories, i.e. the difficulty to manipulate a high number of qubits coherently.

Standard (personal) current (universal) classical computers, use several Gigabytes of RAM, i.e. tens of millions of physical bits to store programs to be executed, let us say around 100 million physical bits.

The following lines have been produced essentially after reading the broad-audience untechnical article ‘Quantum Computing: How Close Are We?’, by E. Cartlidge [Cart], see https://www.osa-opn.org/home/articles/volume_27/october_2016/features/quantum_computing_how_close_are_we/. With current quantum gate fidelity and quantum error tolerance (see below), Martinis et al. [281] estimate that around 100 million physical *qubits*, manipulated coherently, would be needed to carry out Shor’s factoring algorithm on a 2000-bit number in around a day, which is a task “far beyond the reach of today’s best supercomputers” [Cart].

Several technological candidates currently compete in the design of future universal quantum computers (the physical architecture of such machines may involve several of these techniques, but there will likely be a predominant one). Four of such candidates are summed-up in [Cart]: spin qubits, superconducting circuits, ion traps, and integrated photonic circuits. Cold atoms in optical lattices, which are not in the list, have also been considered for large-scale quantum computation, e.g. by Inaba et al. in 2014 [282] (see also the larger-audience paper at <https://phys.org/news/2014-03-entangling-atoms-optical-lattice-quantum.html>).

On so-called quantum non-locality

We remind the reader that the doubled quotation marks are used to quote other authors. These quotes are always followed by the reference from which they have been extracted.

In their well-known 1935 paper, Einstein, Podolsky and Rosen (EPR) [283] exposed a certain quantum-mechanical thought experiment that they considered as paradoxical, the so-called EPR paradox. According to them, this paradox implied the incompleteness of quantum mechanics (QM) as a theoretical tool to predict results about Nature. By incompleteness, they explicitly meant that there are “elements of the physical reality” [283] which have no “counterpart” [283] in the theory, i.e. to which no “physical quantity” [283] is associated in the theory. It is suitable for the purpose of the present discussion to rephrase EPR’s statement as follows: there is information in Nature that QM is unable to capture, *while it obviously should*. The current overwhelmingly-dominant vision, that progressively emerged out of the analysis of many experiments of increasing both subtlety and precision, is that this obviousness was simply not, and that QM introduces an intrinsic limit¹ to knowledge, to which the classical-physics approximation is blind².

When introducing EPR’s paradox, the above-mentioned obviousness is often presented, following EPR’s line of argument, as grounded on a certain conception of “reality” [283]. Indeed, EPR’s paper seems to hope to convince the reader by, essentially, elaborating on a “reasonable” [283] definition of reality, that they attempt to give³. Throughout the paper, their concept of reality is basically used as a physical characteristic that can take two values, either ‘real’ or ‘unreal’. That being said, such a presentation of EPR’s paradox, which strictly follows EPR’s formal presentation, structured around the notion of reality by an extensive use of logical inferences, tends to overlook the background on which the paper was conceived, which is quite enlightening.

One of the key aspects of EPR’s issue is that the axioms of quantum mechanics give no information about the physical quantity under consideration before it is measured. Let us call this epistemic characteristic (*pre-measurement*) *undetermination*. We shall come back to it further down. Another key aspect of EPR’s issue is the axiom of quantum mechanics which

¹This feature is indeed a limit in certain cases, see below, but it can also be used as a resource, e.g. for secure communication.

²A ‘*preview*’ to what follows in this appendix. This intrinsic limit is due to the possibility of encoding information non-locally, i.e. the fact that some information is sometimes not accessible locally, where the word ‘locally’ is understood in a sense which is *stronger* than the relativistic one, and which is that of ‘local measurement’, seminally defined by local hidden variables, see further down, and later extensively discussed [53, 284]. Indeed, if we set aside universe’s expansion, the information we are speaking about is *always* locally accessible in a relativistic sense, since during the entangled-state preparation, each of the two subsystems must be within the light cone of the other, so that this remains true afterwards. Although, for the sake of simplicity, we just identified *quantum non-locality*, which I may also call *non-localizability*, to entanglement, there are actually some non-entangled states that can also encode non-local information. Conversely, one can show that maximal entanglement does not always provide maximal quantum non-locality [285, 286, 287].

³Bohr criticized the vagueness of the concepts developed by EPR.

states that, instantaneously or extremely quickly after measuring the system, the state of the system changes and becomes that of the outcome. Let us call this axiom the *state-reduction axiom*. In the Copenhagen interpretation of QM, largely conceived by Bohr and Heisenberg around 1930, this axiom is viewed as a “kind of action” [288], i.e. as accounting for a physical process, the so-called *wavepacket collapse*, which must be superluminal, although Heisenberg also quickly pointed out that this kind of action “can never be utilized for the transmission of signals so that it is not in conflict with the postulates of the theory of relativity” [288]. Einstein criticized such an interpretation and referred to it as a “spooky action at a distance”, reminiscent of the old gravitational and electromagnetic actions at a distance.

Now, I still need to investigate about the following two historical possibilities. Either, first possibility, EPR were actually rather convinced by Heisenberg’s no-signaling (or no-communication) claim, and were already advocating, in their paper, for the so-called *local realism*⁴; in that case, their main concern would indeed have been pre-measurement undetermination. Or, second possibility, EPR were not convinced by no-signaling claims because no fully convincing proof of this result had been developed yet; in that second case, QM was, in EPR’s thought experiment, breaking causality essentially *because it was breaking relativistic locality*, where, here, ‘relativistic locality’ stands at least for slower-than-light propagation of energy, if not for Lorentz invariance⁵. Both EPR’s paper and the way the paradox is presented mainly suggests the first historical possibility, but EPR’s line of argument is both subtle and vague enough to suggest that both concerns might have intertwined more than often presented.

Whatever concern was the dominant one to EPR, one can for sure say that the incompleteness of QM was to them unavoidable if one wished to preserve causality, whatever the meaning we assign to the word causality.

Let me again follow the second historical possibility. It might be that incompleteness was EPR’s answer to a result that they view as paradoxical, not that much because of their vision of reality, but rather because of their vision of what a physical theory must be⁶. Indeed, it might be that EPR could not admit that the state-reduction axiom was not physical in the usual sense, as Heisenberg suggested: because, to EPR, if one was willing to introduce this axiom, it had to be physical in the usual sense, then it was, in some situations, such as that they present in their paper, actually breaking relativistic locality and could not be a good or at least sufficient axiom. I follow this maybe unconventional line of thought because one might say that EPR’s conception of reality was, essentially, merely that of a *causal reality ensured by relativistic locality*. The no-signaling theorem ensures that this vision *is still in order nowadays*. But rigorous proofs of the no-signaling theorem are rather subtle, and this result might not have been as firmly grounded at EPR’s time, so that they could not be convinced by it. To prove the no-signaling theorem, indeed, one needs to fundamentally reconsider what a measurement actually is; it demands to realize that it involves both ‘microscopical’ and ‘macroscopical’ or ‘topological’ aspects [53, 284].

In his well-known 1964 paper⁷ [Bell1964], i.e. 29 years after EPR’s paper, Bell still concluded that there is some signal that “must propagate instantaneously” [Bell1964], if

⁴Note that this terminology is not used in their paper.

⁵This meaning will be used throughout the rest of this appendix

⁶Regarding this matter, EPR’s concept of completeness is precisely developed in the perspective of setting constraints on what a physical theory should be.

⁷A scan of the paper is available at http://www.drchinese.com/David/Bell_Compact.pdf.

his thought experiment happened to be verified, as he believed it would. Bell also added that this would imply that QM “could not be Lorentz invariant” [Bell1964]. The above-mentioned local-realist vision was developed between EPR and Bell’s papers. A *local realist theory* is, technically, a *strict synonym* for a *local hidden-variables theory*⁸. It is a *much stronger* requirement than the sole respect of relativistic locality. At that time, however, it might be that this requirement was seen as, if not equivalent, at least not that stronger than the requirement of relativistic locality. For sure, the local-realist requirement was seen as needed to preserve slower-than-light propagation *at least for this exotic action at a distance*⁹.

It seems, as the introduction of Bell’s paper suggests, that one of the important triggers for this paper was Bell’s realization that one could introduce hidden variables similar to those informally suggested by EPR, as shown by Bohm [289, 290], but that, instead of reducing EPR’s concern, this seemed to actually ‘naturally’ augment what was viewed as a tangible “gross” [Bell1964] non-locality that violated slower-than-light propagation. We shall clarify these concepts and arguments below.

Several experiments are viewed as demonstrating, with an increasing precision, the violation of Bell’s inequalities¹⁰. This is viewed as a proof of the so-called *non-locality* of the information carried by (quantum) physical systems, which can be summed-up as followed. Consider a certain physical system S_1 ; then, provided this system interacts *in a certain way* with another one S_2 at some instant t_0 , and provided the quantum coherence of both S_1 and S_2 is ensured for $t > t_0$, then S_1 will, for any $t > t_0$, contain information about S_2 , *regardless of any future interaction with S_2* (and vice versa). This fundamental property disappears with decoherence. Not to confuse it with relativistic locality, we may rather use the terminology *non-localizability* instead of *quantum non-locality*.

The terminology ‘quantum non-locality’ is sometimes almost used as a synonym for the *non-separability* of entangled systems, although this non-localizability can appear in separable systems¹¹. Quantum non-locality sometimes only refers to the type of non-locality which appears in Bohm’s interpretation of quantum mechanics, which is actually rather rare in the Copenhagen interpretation, although it can happen¹².

A trace of no-signaling in QM is that the state evolution is described by a PDE, namely the Schrödinger equation, which by the way had already been given relativistic counterparts when EPR’s paper was published, namely the Klein-Gordon and Dirac equations.

In the light of the no-signaling theorem, the Aharonov-Bohm effect can be viewed as

⁸Local hidden variables were mathematically defined by Bell, and somehow tailored to prove its well-known inequalities. Bell theoretically proved that no local hidden-variable theory can reproduce the full range of QM predictions.

⁹I need to investigate on how grounded was the no-signaling theorem at that time. If it was firmly grounded, then local realism was seen as needed *only* for the exotic action at a distance of the wavepacket collapse to be subluminal. If not, then local realism was, *more largely, seen as actually needed to firmly ground no-signaling*. This historical question is not obvious. Indeed, while there were for sure already several claims for no-signaling, why then, if this no-signaling was already firmly grounded, insisting on introducing an exotic signal that conveys no information?

¹⁰In his paper, Bell underlined that it was “crucial” [Bell1964] to realize “experiments of the type proposed by Bohm and Aharonov” [Bell1964], “in which the settings [of the measuring devices] are changed during the flight of the particles” [Bell1964]. The first experiment of this kind was realized by Aspect et al. in 1982 [291].

¹¹Regarding these questions, one may first read Wikipedia’s dedicated article, Section 2, at https://en.wikipedia.org/wiki/Quantum_nonlocality

¹²See the following discussion: <https://physics.stackexchange.com/questions/197530/non-locality-vs-non-realism-arbitrary-choice>.

a manifestation of the non-localizability of information: within such an interpretation, the electromagnetic potential should not be regarded as ‘more physical than the electromagnetic field’, a picture sometimes conveyed, but as ‘containing non-local information’, in the same way quantum entanglement can do [\[292\]](#).

Aharonov's quantum random walks

D.1 Generic scheme (or protocol)

D.1.1 Definition (one-step scheme)

Aharonov's scheme [32] takes as input a ket belonging to the position (or external) Hilbert space, that we will call 'external ket' $|\psi_j\rangle_p$, where the subscript 'p' is for 'position', and outputs, after one time step, another external ket $|\psi_{j+1}\rangle_p$ given by

$$|\psi_{j+1}\rangle_p = \hat{A}_j^\pm |\psi_j\rangle_p, \quad (\text{D.1})$$

where I define the Aharonov operator by

$$\hat{A}_j^\pm = \hat{M}_j^\pm \hat{W}_j^a \hat{T}_j. \quad (\text{D.2})$$

As formally written, the scheme is the succession of three operations:

1. The preparation of the spin in a given superposition along some direction. This superposition can be time dependent (this is not the case in the original paper though), which can always be viewed as, *e.g.*, keeping the original superposition but along a time-dependent direction, with a possible overall phase change. This operation corresponds to tensorizing the external input ket with the prepared superposition, and reads:

$$\hat{T}_j = \begin{pmatrix} c_j^+ \\ c_j^- \end{pmatrix} \otimes, \quad (\text{D.3})$$

with the basis

$$|+\rangle_c = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle_c = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (\text{D.4})$$

where the subscript 'c' indicates that the kets belong to the coin Hilbert space.

2. A DTQW one-step operation, combination of a spin-dependent shift and a coin operation:

$$\hat{W}_j^a = \hat{C}_j^a \hat{S}^a = e^{i\omega_j} \underbrace{\begin{bmatrix} \alpha_j & \beta_j \\ -\beta_j^* & \alpha_j^* \end{bmatrix}}_{\in \text{SU}(2)} \begin{bmatrix} e^{-i\hat{P}} & 0 \\ 0 & e^{i\hat{P}} \end{bmatrix}, \quad (\text{D.5})$$

where \hat{P} is the momentum operator, that acts on the external ket. The superscript 'a' is to indicate the use of the 'Aharonov' convention, in which, although the shift is applied before the coin operation, as in the convention used in this thesis and on the contrary to the standard convention (see Appendix G), the shift however shifts the spin up to the right, and the spin down to the left, as in the standard convention and on the contrary to that used in this thesis. In the original scheme, the coin operation does not depend on time.

The spin-dependent shift operation, \hat{S}^a , entangles the spin and external degrees of freedom of the initially non-entangled input state, given by

$$|\Psi_j\rangle \equiv \hat{T}_j |\psi_j\rangle_p. \quad (\text{D.6})$$

Both an upper case psi letter and no subscript associated to the ket mean that the ket belongs to the full Hilbert space, tensorial product of the coin and position Hilbert spaces. One can view generic position-spin entanglement as making a spin state depend on position, which generates two probability amplitudes, that for spin up and that for spin down. The spin-dependent shift of DTQWs performs a particular type of entanglement, where the upper probability amplitude, $|\psi^+\rangle_p \equiv_c \langle +|\Psi\rangle$, is shifted by one space step in a given direction, while the lower, $|\psi^-\rangle_p \equiv_c \langle -|\Psi\rangle$, is shifted in the other direction.

The coin operation, \hat{C}_j^s , superposes the upper and lower spin components of the entangled state, namely $\hat{S}^s |\Psi_j\rangle$. This coin operation can be viewed as (case 1) one of the two following possibilities (i) and (ii), as well as (case 2) the result of a combination of these two possibilities: (i) a (non-destructive) rotation of the spin, and (ii) a measurement in a different basis (destructive rotation), thus corresponding to the operation $M_j^{\pm'} = M_j^{\pm} \hat{K}_j^s$, where \hat{K}_j^s is either (case 1) \hat{C}_j^s itself or (case 2) a part of \hat{C}_j^s (imagine we decompose \hat{C}_j^s into two spin rotations, one corresponding to (i) and the other to (ii)).

3. A measurement of the spin, which desuperposes the spin state in some direction, i.e. determines the value of the spin along this direction, either plus or minus, which at the same time disentangles the quantum state, i.e. makes the spin state independent of the position (this is a possible way to view disentanglement). The operation \hat{M}_j^{\pm} thus corresponds to two possible operations, as indicated by the superscript \pm ,

$$\hat{M}_j^{\pm} = \frac{c\langle \pm |}{\mathcal{N}_j^{\pm}}. \quad (\text{D.7})$$

The probabilities of the spin-measurement outcomes are given by the squared position-Hilbert-space norms,

$$P_j^{\pm} = (\mathcal{N}_j^{\pm})^2 \equiv \|_c \langle \pm | \hat{W}_j^a | \Psi_j \rangle \|^2_p = \left({}_c \langle \pm | \hat{W}_j^a | \Psi_j \rangle \right)^{\dagger} {}_c \langle \pm | \hat{W}_j^a | \Psi_j \rangle, \quad (\text{D.8})$$

with

$$P_j^+ = 1 - P_j^- = P_j. \quad (\text{D.9})$$

Again, the subscript 'p' indicates that the norm is that of the position Hilbert space. The indicated time dependence of this operation is that associated to the norm, i.e. to the product $W_j^a T_j$, and has nothing to do with the (quantum) randomness of the measurement outcome. As said above, this operation disentangles the state previously entangled by the spin-dependent shift operation, and selects only an external ket. We could define the measurement operation as usual, i.e. with a projector instead of a bra, but then the scheme anyways only keeps the external part of the state (and reinitializes the spin state), so we would have to introduce an operator for this selection, which would precisely be a bra that, applied on the corresponding projector, would deliver the same bra; we then simply define the measurement by the action of a bra and not a projector.

D.1.2 Compact expressions for the one-step scheme

Now that we have defined each of the three substeps of the one-step scheme, let us describe this one-step scheme compactly. A more explicit expression of the action of the walk operator is

$$\hat{W}_j^s |\Psi_j\rangle = e^{i\omega_j} \begin{pmatrix} \alpha_j e^{-i\hat{P}} |\psi_j^+\rangle_{\text{p}} + \beta_j e^{i\hat{P}} |\psi_j^-\rangle_{\text{p}} \\ -\beta_j^* e^{-i\hat{P}} |\psi_j^+\rangle_{\text{p}} + \alpha_j^* e^{i\hat{P}} |\psi_j^-\rangle_{\text{p}} \end{pmatrix} \equiv \begin{pmatrix} {}_{\text{c}}\langle + | \hat{W}_j^s | \Psi_j \rangle \\ {}_{\text{c}}\langle - | \hat{W}_j^s | \Psi_j \rangle \end{pmatrix}, \quad (\text{D.10})$$

with

$$|\Psi_j\rangle \equiv \begin{pmatrix} {}_{\text{c}}\langle + | \Psi_j \rangle = |\psi_j^+\rangle_{\text{p}} \\ {}_{\text{c}}\langle - | \Psi_j \rangle = |\psi_j^-\rangle_{\text{p}} \end{pmatrix}. \quad (\text{D.11})$$

The $+$ and $-$ probabilities, (D.8), are respectively given by

$$\begin{aligned} P_j^+ &= \| {}_{\text{c}}\langle + | \hat{W}_j^s | \Psi_j \rangle \|^2 = |\alpha_j|^2 \| \psi_j^+ \|^2_{\text{p}} + |\beta_j|^2 \| \psi_j^- \|^2_{\text{p}} + 2 \operatorname{Re} \left\{ \alpha_j \beta_j^* {}_{\text{p}}\langle \psi_j^- | e^{-2i\hat{P}} | \psi_j^+ \rangle_{\text{p}} \right\} \\ P_j^- &= \| {}_{\text{c}}\langle - | \hat{W}_j^s | \Psi_j \rangle \|^2 = |\beta_j|^2 \| \psi_j^+ \|^2_{\text{p}} + |\alpha_j|^2 \| \psi_j^- \|^2_{\text{p}} - 2 \operatorname{Re} \left\{ \alpha_j \beta_j^* {}_{\text{p}}\langle \psi_j^- | e^{-2i\hat{P}} | \psi_j^+ \rangle_{\text{p}} \right\}, \end{aligned} \quad (\text{D.12})$$

both quantities being positive by construction (they are norms). Now, even if we start at $j = 0$ with an entangled state $|\Psi_{j=0}\rangle$, instead of a factorized one of the form $\hat{T}_{j=0} |\psi_{j=0}\rangle_{\text{p}}$, the scheme runs with an external ket, namely $|\psi_j\rangle_{\text{p}} \equiv {}_{\text{c}}\langle \pm | \hat{W}_{j-1}^s | \Psi_{j-1} \rangle / \sqrt{P_{j-1}^\pm}$, and the Aharonov operators, that act on this external ket, read

$$\begin{aligned} \hat{A}_j^+ &= e^{i\omega_j} \left(\alpha_j c_j^+ e^{-i\hat{P}} + \beta_j c_j^- e^{i\hat{P}} \right) / \sqrt{P_j^+} \\ \hat{A}_j^- &= e^{i\omega_j} \left(-\beta_j^* c_j^+ e^{-i\hat{P}} + \alpha_j^* c_j^- e^{i\hat{P}} \right) / \sqrt{P_j^-}. \end{aligned} \quad (\text{D.13})$$

The expressions of the $+$ and $-$ probabilities given above simplify into

$$\begin{aligned} P_j^+ &= |\alpha_j|^2 |c_j^+|^2 + |\beta_j|^2 |c_j^-|^2 + 2 \operatorname{Re} \left\{ \alpha_j \beta_j^* c_j^+ c_j^{-*} {}_{\text{p}}\langle \psi_j | e^{-2i\hat{P}} | \psi_j \rangle_{\text{p}} \right\} \\ P_j^- &= |\beta_j|^2 |c_j^+|^2 + |\alpha_j|^2 |c_j^-|^2 - 2 \operatorname{Re} \left\{ \alpha_j \beta_j^* c_j^+ c_j^{-*} {}_{\text{p}}\langle \psi_j | e^{-2i\hat{P}} | \psi_j \rangle_{\text{p}} \right\}. \end{aligned} \quad (\text{D.14})$$

D.1.3 Explicit expression for the N -step outcome

After N time steps, the resulting state is

$$|\psi_N^{a_i^k}\rangle_{\text{p}} = \underbrace{\hat{A}_N^+ \hat{A}_{N-1}^+ \hat{A}_{N-2}^- \hat{A}_{N-3}^+ \dots \hat{A}_{j+2}^- \hat{A}_{j+1}^- \hat{A}_j^+ \hat{A}_{j-1}^+ \hat{A}_{j-2}^- \hat{A}_{j-3}^+ \dots \hat{A}_2^- \hat{A}_1^+ \hat{A}_0^+}_{N \text{ elements in the product}} |\psi_0\rangle_{\text{p}}, \quad (\text{D.15})$$

where a_i^k , $i = 1, \dots, \mathcal{A}_N^k$, is one of the $\mathcal{A}_N^k = k! \binom{N}{k}$ possible arrangements of k operators \hat{A}^+ among the N possible locations in an ordered product (which is combinatorially equivalent to a list) of N elements, the other locations being occupied by \hat{A}^- operators.

This state has the following probability to happen:

$$\mathcal{P}(\psi_N^{a_i^k}) = \prod_{m=1}^k P_{j=\tau^+(m)}^+ \prod_{n=1}^{N-k} P_{j=\tau^-(n)}^-, \quad (\text{D.16})$$

where $\tau^+(m)$ (resp. $\tau^-(n)$) is the time at which the m -th \hat{A}^+ (resp. n -th \hat{A}^-) happens. The couple of sequences (τ^+, τ^-) is mapped one to one with one of the a_i^k 's. This probability of a given sequence of outcomes, Eq. (D.16), results from the combination of two effects:

1. The quantum interferences between the left- and right-going walkers, realised by DTQW part of the Aharonov operators, and which manifest themselves in the one-step probabilities, the P_j^+ 's and P_j^- 's.
2. An effectively-classical randomness effect, realised by the measurement part of the Aharonov operator, which is reflected by the product of all the P_j^+ 's and P_j^- 's. To be completely explicit: the probability of obtaining a given sequence of Aharonov operators is that of a given sequence of outcomes in successive Bernouilli experiments, with possibly time-dependent probabilities. In the next subsection, we will show that this connection with effectively-classical randomness effect goes further, and grows with the amount of averaging over several realizations of Aharonov's scheme.

In the case where the walk operator \hat{W}^s and the spin preparation \hat{T} do not depend on time, the Aharonov operators \hat{A}^\pm do not depend on time either, and each a_i^k state has the same probability to happen (thus independent of i):

$$\mathcal{P}(\psi_N^{a_i^k}) = P^k(1 - P)^{N-k}. \quad (\text{D.17})$$

With no further assumptions, Aharonov's scheme has no simpler formal expression than (D.15), with the Aharonov plus and minus operators given by Eqs. (D.13).

D.1.4 Spatial probability distributions

D.1.4.1 Probability distribution of a given outcome: possibly high quantum-interferences effects

The probability of being at time j on site p having obtained the arrangement a_i^k after j successive spin measurements, is given by

$$\mathcal{P}(j, p | \psi_j^{a_i^k}) \equiv |\psi_{j,p}^{a_i^k}|^2. \quad (\text{D.18})$$

As manifest by looking at Eqs. (D.15) and (D.13), this spatial probability distribution will be in part the result of quantum interferences between the left- and right-going walkers.

D.1.4.2 Averaging over all possible outcomes suppresses quantum interferences

Averaging over all possible outcomes yields

$$P_{j,p} = \sum_{\psi_j} \mathcal{P}(j, p | \psi_j) \mathcal{P}(\psi_j) = \sum_{k=1}^j \sum_{i=1}^{\mathcal{A}_j^k} \mathcal{P}(j, p | \psi_j^{a_i^k}) \mathcal{P}(\psi_j^{a_i^k}), \quad (\text{D.19})$$

where we have used the abbreviation $\psi_j \equiv \psi_j^{a_i^k}$ in the first equality.

One can also perform this average on the before-last outcomes:

$$P_{j+1,p} = \sum_{\psi_j} \mathcal{P}(j+1, p | \psi_j) \mathcal{P}(\psi_j), \quad (\text{D.20})$$

where the probability of being at time $j+1$ on site p having obtained the arrangement a_i^k after $j-1$ successive spin measurements, is given by

$$\mathcal{P}(j+1, p | \psi_j) = P_j^+ |{}_p \langle p | A_j^+ | \psi_j \rangle_p|^2 + P_j^- |{}_p \langle p | A_j^- | \psi_j \rangle_p|^2. \quad (\text{D.21})$$

Now, because

$$\begin{aligned}
 |{}_p\langle p|A_j^+|\psi_j\rangle_p|^2 &= \frac{1}{P_j^+} \left[|\alpha_j|^2 |c_j^+|^2 |\psi_{j,p-1}|^2 + |\beta_j|^2 |c_j^-|^2 |\psi_{j,p+1}|^2 \right. \\
 &\quad \left. + 2 \operatorname{Re} \left\{ \alpha_j \beta_j^* c_j^+ c_j^{-*} \psi_{j,p-1} \psi_{j,p+1}^* \right\} \right] \\
 |{}_p\langle p|A_j^-|\psi_j\rangle_p|^2 &= \frac{1}{P_j^-} \left[|\beta_j|^2 |c_j^+|^2 |\psi_{j,p-1}|^2 + |\alpha_j|^2 |c_j^-|^2 |\psi_{j,p+1}|^2 \right. \\
 &\quad \left. - 2 \operatorname{Re} \left\{ \alpha_j \beta_j^* c_j^+ c_j^{-*} \psi_{j,p-1} \psi_{j,p+1}^* \right\} \right], \tag{D.22}
 \end{aligned}$$

the interference terms between the left- and right-going walkers cancel each other in Eq. (D.21), which yields

$$\mathcal{P}(j+1, p|\psi_j) = |c_j^+|^2 |\psi_{j,p-1}|^2 + |c_j^-|^2 |\psi_{j,p+1}|^2. \tag{D.23}$$

Plugging this expression in the average over the before-last outcomes, Eq. (D.20), delivers

$$P_{j+1,p} = |c_{j-1}^+|^2 P_{j-1,p-1} + |c_{j-1}^-|^2 P_{j-1,p+1}. \tag{D.24}$$

The averaged probability distribution $P_{j,p}$ thus follows a classical random walk with probabilities of going right and left, from time j to time $j+1$, respectively given by $\pi_j = \pi_j^+ = |c_j^+|^2$ and $\pi_j^- = |c_j^-|^2 = 1 - \pi_j^+$. After averaging over all possible outcomes, the quantumness of the system is removed. The average displacement (resp. variance) of $P_{N,p}$ is the sum of the average displacements (resp. variances) between two consecutive time steps, $\sum_{j=0}^N (\pi_j^+ - \pi_j^-)$ (resp. $\sum_{j=0}^N \pi_j^+ \pi_j^-$), which results in $N(\pi^+ - \pi^-)$ (resp. $N\pi^+ \pi^-$) when π_j do not depend on the time j .

In the continuous-spacetime limit, and in the case where the probability π_j does not depend on time, the probability distribution $P(t, x)$ follows a diffusion equation with a bias drift speed $c = \lim\{(\pi^+ - \pi^-)l/\Delta t\}$ and a diffusion coefficient $D = \lim\{\pi^+ \pi^- l^2/(2\Delta t)\}$, where the limit corresponds to a space step $l \rightarrow 0$ and a time step $\Delta t \rightarrow 0$. Note that $l^2/(2\Delta t)$ must have a finite limit for this continuum limit to exist, and thus that $\pi^+ - \pi^-$ must scale as the length step l , which makes sense since $P(t, x)l\Delta t$ is the probability to be between time t and $t + \Delta t$ and position x and $x + l$. In the case where π_j does depend on time, one can still define a bias drift speed and a diffusion coefficient, but locally in time.

D.2 Coinless scheme: no more quantum interferences on given realizations of the scheme

In this case $\beta_j = 0$, $|\alpha_j|^2 = 1$, and the outcomes of the measurement operation yield no superposition between left- and right-going states. As a consequence, not only the probability distribution averaged over all possible outcomes follows a (possibly time-dependent) classical random walk, which is the case even in the coined scheme, as shown previously, but also the mean position of a given realization of the quantum random walk, and even more: at each time step, the initial probability distribution of the quantum walker is actually simply shifted right or left by one space step, with probabilities π_j^+ and π_j^- , and without deformation.

The quantumness of the scheme still shows up on three aspects:

1. The scheme transports the initial external ket $|\psi_{j=0}\rangle_p$ up to time $j = N$ without

destroying it (along some classical random path determined by the successive outcomes of spin measurement). One can thus use this quantum state at any time and make it interfere with another quantum state.

2. The scheme generically adds a phase information, since at each time step, the walker $|\psi_j\rangle_{\text{p}}$ catches, while being shifted right (resp. left) with probability π_j^+ (resp. π_j^-), a phase $c_j^\pm/|c_j^\pm|$.
3. The classicality of a given realisation of the coinless quantum random walk is only effective, since what produces this is the intrinsic randomness of quantum measurement, which has nothing to do¹ with classical randomness, that models a lack of information of the system under study.

For the sake of completeness, let us give the Aharonov operators in this coinless case:

$$\hat{A}^\pm = e^{i\phi_j^\pm} e^{\mp i\hat{P}l}, \quad (\text{D.25})$$

where

$$e^{i\phi_j^\pm} \equiv \frac{c_j^\pm}{|c_j^\pm|}, \quad (\text{D.26})$$

so that the state at time N is given by

$$|\psi_{j=N}^{a_i^k}\rangle_{\text{p}} = \left[\prod_{m=1}^k \exp\left(i\phi_{j=\tau^+(m)}^+\right) \prod_{n=1}^{N-k} \exp\left(i\phi_{j=\tau^-(n)}^-\right) \right] |\psi_{j=0}(p_0 + (k - (N - k)))\rangle_{\text{p}}. \quad (\text{D.27})$$

where we have noted $\psi_j = \psi_j(p_0)$, p_0 being a reference position (typically, the center of a wavepacket), that is shifted left or right by the spin-dependent translation operators. In this coinless case, to each arrangement a_i^k of Aharonov operators, corresponds one of the \mathcal{A}_N^k possible classical zig-zag paths that the walker follows if we impose it to make k steps to the right and $N - k$ to the left.

D.3 An effect of the quantum interferences realized by the coined scheme: classical-path deformation

We refer the reader to both the original paper [32] and Kempe's review [116] for details on this example, which shows one of the possible effects of quantum interferences in the coined scheme. In this example, one considers a wavepacket whose width is kept large with respect to the space step during the time evolution. In this approximation, one can choose the angle of the coin operation in such a way that the one-step scheme is the following: the walker's wave function is either shifted to the left (resp. right) by far more (resp. less) than a lattice step, with a small (resp. high) probability. Because this is an approximation, the wave function is actually slightly deformed, on the contrary to the coinless scheme, but one sees that, apart from this small wave-function deformation, the effect of quantum interferences in this example is a deformation of the classical path: the step taken to the left (resp. right) is superclassical (resp. subclassical), and the corresponding probability is subclassical

¹At least this is the current dominant view, since, in particular, the experiments of Alain Aspect from 1980 to 1983, which impose to make a choice between locality and causality in the description of quantum mechanics; see his thesis at <https://tel.archives-ouvertes.fr/tel-00011844/document>.

(resp. superclassical²). As a pedagogical example, the authors choose the strictly-left-going walker, see Fig.1 of [32], whose mean position overcomes by far the distance reached by its classical counterpart. For the wave-function deformation to appear, the final outcome must be computed exactly (without the approximation used to explain the effect, which assumes no deformation); in the case of a strictly-left-going walker, one simply needs to apply, to the initial state, the N -th power of the minus Aharonov operator, in order to obtain the state at time N , which results in Eq. (4) of [32].

²By ‘superclassical (resp. subclassical) step’, I mean that the quantum-average displacement of the left-going (resp. right-going) walker is bigger (resp. smaller) than a lattice step. By ‘superclassical (resp. subclassical) probability’, I mean that the quantum walker goes right (resp. left), i.e. we measure a spin up (resp. down), with a probability which is higher (resp. lower) than that of its classical counterpart going right (resp. left).

On the momentum and the quasimomentum

Consider a continuous spacetime. To any classical, i.e. point particle having momentum \mathbf{P} , one can associate a wave having a so-called de Broglie wavevector $\mathbf{K} = \mathbf{P}/\hbar$, where \hbar is the reduced Planck's constant. It is one of the two components of the correspondence principle of quantum mechanics, the complementary component being the relation between energy and frequency. In this thesis I use dimensionless variables, which is equivalent to work in so-called natural units, with $\hbar = 1$, so that the classical momentum and the wavevector have the same value.

Now, the DTQWs are defined on a graph which is often eventually mapped to a spacetime lattice. On a lattice, the choice of the region – i.e., in the one-dimensional case, of the interval – to which the wavevectors belong is not unique¹. Hence, referring to k as ‘the momentum’, in the sense this word is used in standard quantum mechanics, can be misleading. Instead, k will be referred to, in a continuous-spacetime perspective, as our preferred *quasimomentum*, and it will be called ‘the’ quasimomentum, although it is only defined modulo the interval length L , in the sense that any wavevector equal to a given one modulo L delivers exactly the same results. In the continuum limit considered in this work, this quasimomentum k will be replaced by a certain continuum-limit momentum K , i.e. a certain value of *the* quantum-mechanical variable which is canonically conjugate to the position. More precisely, a certain continuum-limit momentum K is typically, roughly speaking, a certain limit of the ratio between the quasimomentum and the step of the spacetime lattice, ϵ . Indeed, both quantities k and ϵ must typically go to zero in the continuum limit, and their ratio can have an arbitrary finite limit, so that one actually maps a certain continuum-limit momentum K to a particular *family of quasimomenta which is indexed by ϵ* , of the form $k = f_\epsilon(K)$, where the function f_ϵ depends on the interval chosen for the quasimomenta. The sign of a given quasimomentum is typically preserved, when taking the continuum limit, if this interval is *partitioned into a (strictly) positive and a (strictly) negative subset*. We choose the symmetric interval $[-\pi; \pi[$ to facilitate the use of intuition; with such a symmetric interval, one can in particular merely set $k = K\epsilon$.

Note that, the word ‘momentum’ being simply non-used in a lattice situation, it could actually be appropriate to use it instead of the word ‘quasimomentum’, typically if (i) this quasimomentum has a standard-momentum counterpart in a certain continuum spacetime, which is the case in the present work, and (ii) as long as our main intuition of the quasimomentum is not in conflict with that of the continuum-limit standard momentum, which to me is the case with the symmetric-interval choice. To me, indeed, the relation $k = K\epsilon$ makes it rather natural to extend the use of the word ‘momentum’ to the lattice,

¹Only the volume of this region is imposed, but its location in (the unbounded) \mathbf{k} -space is arbitrary. This volume is the length of the interval in the one-dimensional case, and the wavevector is a real number, k .

because of the following reason: to satisfy condition (ii), one could (ii.a) require that the quasimomenta interval contain 0, and (ii.b) that it contain $-k$ if it contains k , which selects the *unique* symmetric interval. Instead of (ii.b), one could also require that all quasimomenta are positive, which induces a mapping with the standard-momentum norm instead of its component on the momentum axis, and also selects a unique interval.

In solid-state physics, the terminology ‘quasimomentum’ is widely used, and is interchangeable with the terminology ‘crystal momentum’. In the present work, there is, obviously, a priori no crystal, and the terminology ‘quasimomentum’ is a priori only related to a common mathematical feature of the present work and solid-state physics, that is, the presence of a lattice. While this common mathematical description obviously translates into common effective mathematical features shared by solid-state systems and DTQWs, note that, in the continuum-limit applications of the present work, the spacetime lattice on which the DTQWs are defined have, not only a priori, but indeed nothing to do with the crystal lattice of solid state physics. One could envisage making physical connections between DTQWs and solid-state physics. To make a physical connection between the ‘quasimomentum’ of this thesis and the ‘crystal momentum’ of solid-state physics, one would have typically to find a proper mapping between the overlap integrals of solid-state physics and the parameters that define our DTQWs. The effective mass of solid-state physics, which is a measure of the resistance to transport, increases when the overlap, i.e. the ‘connectivity’ between nodes diminishes, so that I would expect the overlap to be a decreasing function of the mixing angle θ , if a proper mapping to solid-state physics can be found. The solid-state picture could in particular help to develop an intuition on the ‘phenomenology’ of the connections between nodes in DTQWs.

Unitary group

F.1 Dimension N

The unitary group of dimension N , $U(N)$, is the group of $N \times N$ unitary matrices, i.e. $U(N) = \{U \in M_N(\mathbb{C}) / U^\dagger U = \mathbf{1}_N\}$. It is a compact and (not simply) connected Lie group, so that the exponential map generates the whole group¹. Consider an arbitrary element $U \in U(N)$. Its determinant $\det U = e^{i\omega}$, $\omega \in [0, 2\pi[$, which follows directly from $U^\dagger U = \mathbf{1}$. We define $\bar{U} = U/\delta$, where $\delta^N = \det U$. The matrix \bar{U} is unitary and has unit determinant, i.e. it is an element of $SU(N)$. Any element of $U(N)$ can thus be factorized into the product of an element of $U(1)$ by an element of $SU(N)$. This factorization is not unique because δ is not uniquely defined by the equation $\delta^N = \det U$. Indeed, this equation has the N distinct solutions $\delta_k = \exp[i(\omega + 2k\pi)/N]$, $k = 0, \dots, N-1$, and each solution defines a different factorization. We choose $k = 0$, which defines unambiguously a unique factorisation.

F.2 Dimension 2

F.2.1 A possible parametrization of $U(2)$

According to the above explanation, we can factorize uniquely any $U \in U(2)$ as the product of $e^{i\alpha}$, $\alpha = \omega/2 \in [0, \pi[$, by $\bar{U} \in SU(2)$. Writing $\bar{U}^\dagger \bar{U} = \mathbf{1}_2$ with

$$\bar{U} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad (\text{F.1})$$

yields the following equations,

$$|a|^2 + |c|^2 = 1 \quad (\text{F.2a})$$

$$|b|^2 + |d|^2 = 1 \quad (\text{F.2b})$$

$$a^*b + c^*d = 0, \quad (\text{F.2c})$$

and $\det \bar{U} = 1$ reads

$$ad - bc = 1. \quad (\text{F.3})$$

If $b = 0$, then $ad = 1$ and $c^*d = 0$, so that $c = 0$ and then $a = d^*$. If $b \neq 0$, then plugging $a = -cd^*/b^*$ into (F.2a) and using (F.2b) yields $|b| = |c|$. We thus have $|a|^2 + |b|^2 = 1$, so that there exist $\theta \in [-\pi/2, 0[$ such that $|a| = \cos \theta$ and $|b| = -\sin \theta$, and we can actually use $\theta = 0$ to parametrize the case $b = 0$ described previously, so that $\theta \in [-\pi/2, 0]$. Hence,

¹See Appendix P for a glimpse on topology, in particular on the notions of compactness and connectedness.

there exist $(\xi, \zeta) \in]-2\pi, 0] \times [0, 2\pi[$ such that

$$a = e^{i\xi} \cos \theta \quad (\text{F.4a})$$

$$b = e^{i\zeta} \sin \theta. \quad (\text{F.4b})$$

From Eq. (F.2b), there also exist $\rho \in [0, 2\pi[$ such that

$$d = e^{i\rho} \cos \theta, \quad (\text{F.5})$$

and then plugging (F.4a), (F.4b), and (F.5) in (F.2c) yields $c = -e^{i(\xi-\zeta+\rho)} \sin \theta$. Writing then $ad - bc = 1$, one deduces that $\xi = -\rho$. Any $\bar{U} \in \text{SU}(2)$ has thus a unique writing of the following form,

$$\begin{aligned} \bar{U} &= \begin{bmatrix} e^{i\xi} \cos \theta & e^{i\zeta} \sin \theta \\ -e^{-i\zeta} \sin \theta & e^{-i\xi} \cos \theta \end{bmatrix} \\ &= e^{i\frac{\xi+\zeta}{2}\sigma_3} e^{i\theta\sigma_2} e^{i\frac{\xi-\zeta}{2}\sigma_3}, \end{aligned} \quad (\text{F.6a})$$

as recalled in Eq. (8), with the parameter ranges specified by the set (7).

F.2.2 Link with the Euler angles of $\text{SO}(3)$ for an active rotation

We define

$$\begin{aligned} \psi &= \zeta - \xi \\ \Theta &= -2\theta \end{aligned} \quad (\text{F.7})$$

$$\phi = -\zeta - \xi, \quad (\text{F.8})$$

so that $\psi \in [0, 4\pi[$ and $\phi \in]-2\pi, 2\pi[$. It is actually enough to restrict ϕ to $[0, 2\pi[$ to map the whole $\text{SU}(2)$ group². The $\text{SU}(2)$ matrix \bar{U} thus reads

$$\bar{U} = e^{-i\phi(\sigma_3/2)} e^{-i\Theta(\sigma_2/2)} e^{-i\psi(\sigma_3/2)}, \quad (\text{F.9})$$

and the mapping of $\text{SU}(2)$ is one to one (if $ab \neq 0$) with the following ranges:

$$(\psi, \Theta, \phi) \in [0, 4\pi[\times [0, \pi] \times [0, 2\pi[. \quad (\text{F.10})$$

Now, the angles ψ , Θ and ϕ are the Euler angles of an active rotation of $\text{SO}(3)$: ψ is the so called *rotation* angle, Θ the *nutation* angle, and ϕ the *precession* angle. To map $\text{SO}(3)$ one to one with these Euler angles, one has to restrict ψ to $[0, 2\pi[$ ($\text{SU}(2)$ covers $\text{SO}(3)$ twice). Any matrix of $\text{SO}(3)$ can be parametrized with these Euler angles: indeed, to define any rotation, one can first perform a rotation of *arbitrary* angle $\psi \in [0, 2\pi[$ around \mathbf{e}_z , and then change the rotation unit vector from \mathbf{e}_z to an *arbitrary* direction \mathbf{e}'_z obtained by reorienting \mathbf{e}_z (unchanged after the rotation above itself by ψ) in the direction specified by the arbitrary spherical-coordinates angles $(\Theta, \phi) \in [0, \pi] \times [0, 2\pi[$, above \mathbf{e}_y and ‘the original’ \mathbf{e}_z , respectively³. To a matrix of $\text{SO}(3)$ having some $\psi_0 \in [0, 2\pi[$ corresponds 2 matrices of

²If $\phi \in]-2\pi, 0[$, then either (i) $\psi \in [0, 2\pi[$, in which case choosing $\phi + 2\pi \in [0, 2\pi[$ and $\psi + 2\pi \in [0, 4\pi[$ yields the same matrix, or (ii) $\psi \in [2\pi, 4\pi[$, in which case choosing $\phi + 2\pi \in [0, 2\pi[$ and $\psi - 2\pi \in [0, 4\pi[$ also yields the same matrix.

³A good way for me to see this is the following. Let J_1, J_2, J_3 be the generators of $\text{SO}(3)$. The coordinates of the rotated vector in the original basis are $v' = e^{-i\phi J_3} e^{-i\Theta J_2} e^{-i\psi J_3} v$. We know that its coordinates in the basis of spherical coordinates (Θ, ϕ) are given by $e^{i\Theta J_2} e^{i\phi J_3} v'$, which is equal to $e^{-i\psi J_3} v$: in this new basis, we have thus indeed just performed a rotation of angle ψ above the vertical direction, which is \mathbf{e}'_z .

SU(2): that with ψ_0 and that with $\psi_0 + 2\pi$, which is the opposite of the first⁴. When $\Theta = 0$ we are at the north pole of the Bloch sphere, and when $\Theta = \pi$, we are at the south pole (spin flipping). For more details, see the following links⁵:

1. <http://www.hep.caltech.edu/~fcp/physics/quantumMechanics/angularMomentum/angularMomentum.pdf>,
2. http://www.phys.nthu.edu.tw/~class/Group_theory/Chap%207.pdf,
3. <http://www.mat.univie.ac.at/~westra/so3su2.pdf>,
4. https://www.google.es/url?sa=t&rct=j&q=&esrc=s&source=web&cd=1&ved=0ahUKEwjSlMXSr9fVAhXJhrQKHc9RAWIQFggrMAA&url=https%3A%2F%2Fwww.math.ens.fr%2Fenseignement%2Ftelecharger_fichier.php%3Ffichier%3D588&usq=AFQjCNH-G8XJeMZdqmhzTg4mazqc19Hvjw.

⁴For extensive details and proofs on this SU(2)/SO(3) mapping, see, e.g., Ref. <http://www.hep.caltech.edu/~fcp/physics/quantumMechanics/angularMomentum/angularMomentum.pdf>, in particular Eqs. (52) to (54) and pages 11 to 14.

⁵The convention for the Euler angles may change from one document to the other.

Connecting two conventions for the DTQW on the line

In our definition of the walk, we choose to apply first the shift \hat{S} and then the coin operation \hat{U} for practical reasons: in the sections concerning non-homogeneous walks, the Taylor expansion is simpler with this order in the operations because the values of the spacetime-dependent angles defining the coin operation are not shifted from the running spacetime-lattice point, so that we don't have to Taylor expand them. The most-used convention is, however, the inverse one, namely applying first the coin operation \hat{U}^s and then the shift \hat{S}^s , yielding a walk operator $\hat{W}^s = \hat{S}^s \hat{U}^s$, the superscript 's' being for 'standard'. We are going to show that both conventions map one to one through a time-reversal operation.

Let us first consider an arbitrary DTQW with the convention used in this thesis, i.e. let us consider the evolution given by Eq. (2) for time $j \in \llbracket 0, j_{\max} \rrbracket$. The state of the walker at time j_{\max} is given by

$$|\Psi_{j_{\max}}\rangle = \hat{E}_{j_{\max}} |\Psi_0\rangle, \quad (\text{G.1})$$

where the j_{\max} -step evolution operator reads

$$\hat{E}_{j_{\max}} = \prod_{j=0}^{j_{\max}-1} \hat{U}_j \hat{S}, \quad (\text{G.2})$$

the product being growingly time ordered from right to left. One can rewrite Eq. (G.1) as

$$|\Psi_0\rangle = \hat{E}_{j_{\max}}^{-1} |\Psi_{j_{\max}}\rangle, \quad (\text{G.3})$$

where the inverse j_{\max} -step evolution operator reads

$$\hat{E}_{j_{\max}}^{-1} = \prod_{j=1}^{j_{\max}} \hat{S}^{-1} (\hat{U}_{j_{\max}-j})^{-1}. \quad (\text{G.4})$$

Let us now consider the one-step evolution of a generic standard-convention DTQW:

$$|\Phi_{r+1}\rangle = \hat{W}_r^s |\Phi_r\rangle. \quad (\text{G.5})$$

The label $r \in \llbracket 0, j_{\max} \rrbracket$ indicates discrete time on another timeline. The state of the walker at time $r = j_{\max}$ is thus given by

$$|\Phi_{r=j_{\max}}\rangle = \hat{E}_{r=j_{\max}}^s |\Phi_{r=0}\rangle, \quad (\text{G.6})$$

where the j_{\max} -step evolution operator reads, in this standard convention,

$$\hat{E}_{r=j_{\max}}^s = \prod_{r=0}^{j_{\max}-1} \hat{S}^s \hat{U}_r^s. \quad (\text{G.7})$$

Hence, if we choose

$$\begin{aligned}\hat{S}^s &\equiv \hat{S}^{-1} \\ \hat{U}_r^s &\equiv (\hat{U}_{j_{\max}-j})^{-1} = (\hat{U}_{j_{\max}-j})^\dagger,\end{aligned}\tag{G.8}$$

that is to say,

$$\hat{E}_{r=j_{\max}}^s \equiv \hat{E}_{j_{\max}}^{-1},\tag{G.9}$$

then Eq. (G.6) is the same as Eq. (G.3), provided that we also choose

$$|\Phi_{r=0}\rangle = |\Psi_{j=j_{\max}}\rangle,\tag{G.10}$$

which imposes

$$|\Phi_{r=j_{\max}}\rangle = |\Psi_{j=0}\rangle.\tag{G.11}$$

Any evolution operator written in our convention, $\hat{E}_{j_{\max}}$, taking an initial state $|\Psi_{j=0}\rangle$ to a final state $|\Psi_{j=j_{\max}}\rangle$, thus always coincides with an inverse, i.e. time-reversed evolution operator of the standard convention, namely $(\hat{E}_{r=j_{\max}}^s)^{-1} \equiv \hat{E}_{j_{\max}}$, and we can write $r = j_{\max} - j$.

The converse result obviously also holds. In particular, the PDE obtained in the continuum limit of a standard-convention DTQW having an evolution operator $\hat{E}_{r_{\max}}^s$, satisfying appropriate zeroth-order constraints but otherwise *arbitrary*, is the same as that obtained for the DTQW of our convention which is defined by the evolution operator $\hat{E}_{j=r_{\max}} \equiv (\hat{E}_{r_{\max}}^s)^{-1}$.

Actually, if the aim is simply to determine the continuum limit of some DTQW written in the standard convention, regardless of any initial and final states, i.e. regardless of connecting the two different timelines, it is enough to work on the one-step evolution equation: take the inverse of some $S^s U_j^s$ originally defined, i.e. simply compute $(U_j^s)^\dagger$, apply any continuum limit results to the DTQW written in our convention with coin operation $U_j = (U_j^s)^\dagger$, and then perform the substitution $\partial_t \rightarrow -\partial_t$ in the final PDE to obtain the desired result¹.

Note that the standard-convention shift operation makes the upper spin component go right in time, and the lower go left, whereas this is reversed in our protocol.

¹The continuous variable t corresponds to the discrete time of our (resp. the standard) convention before (resp. after) the substitution.

Geometry of field theories

H.1 Fiber bundles

H.1.1 Definition

To each element x of a so-called base space B , we attach a copy of a so-called fiber space F , which is then noted F_x , the fiber at x . The collection of all the fibers, $E_F \equiv \bigcup_{x \in B} F_x$, is called the total space. We also introduce a surjection $\pi : E_F \rightarrow B$, called projection on the base, such that $\pi^{-1}(x) = F_x$. Now, for the total space to be a so-called fiber bundle, it must be locally (topologically) trivial, i.e. locally (homeomorphically mappable to) the simplest space one can build out of two spaces F and B , which is their cartesian product. Formally, this means that for any $x \in B$, there exist a neighborhood U of x such that the inverse projection of U is homeomorphic to $U \times F$. This homeomorphism ϕ is like a chart (function) of the subset $\pi^{-1}(U)$ of E_F (and thus a *local* chart of E_F), $\phi : U \times F \rightarrow \pi^{-1}(U)$, called local trivialization of E_F (it is a trivialization of $\pi^{-1}(U)$)¹. This means that the additional (topological) information on E_F , apart from the that of the fiber and the base, is contained in the global structure of E_F ; locally, E_F carries no more (topological) information than that contained in the fiber and the base.

This condition of local (topological) triviality thus defines fiber bundles. Now, how to describe the variety of these objects? The question is how to characterise a given fiber bundle, how to construct it, how to attach the fibers to the base in order to build a globally (topologically) non-trivial space out of the fiber and the base? The most common way of characterising/building the fiber bundle is by specifying how a so-called structure group G acts on the fiber.

Before explaining what the action of a group G is, and how such an action on the fiber is related to the topological structure of the fiber bundle E_F , we must introduce the standard object used to describe the topology of a space, that is, an atlas². Of course, it would not be

¹The notion of chart we use here is more general than the ‘standard’ one used for manifolds (that is why we rather say ‘trivialization’ than ‘chart’). Indeed, the codomain $U \times F$ cannot be homeomorphised to a Euclidean space \mathbb{R}^n if U and F are not themselves homeomorphic to some Euclidean space. Moreover, we are not, at this stage, interested in localising absolute positions (which would require a metric, while the notions we define here do not need any metric): the role of ϕ is simply to indicate that the local topology is trivial, i.e. is reduced to that of the objects we take as inputs, i.e. the base and the fiber, to build a new one, i.e. the fiber bundle; we will see below that this implies that we do not need to specify the trivializing functions out of the ‘reconnection domains’ (see below). As a sum-up: locally, there is no additional topological information in the object we build than that of the input objects. Note however that, if we introduce a metric, there can be additional metric information even locally, i.e. in $\pi^{-1}(U)$ with respect to that contained in U and F .

Note that ‘standard’ charts on manifolds are rather defined from the manifold domain to the Euclidean codomain. Here the word ‘trivialization’ should also rather be used for the inverse function ϕ^{-1} , but it is common, in this fiber-bundle context, to define ϕ from $U \times F$ to $\pi^{-1}(U)$, because it is practical to track the elements of the fiber F as arguments of the function we define, instead of images.

²Again, the notion of ‘atlas’ used here is more general than that used in the study of manifolds, because there is no metric for now, only topology, while there is metricity by definition in the study of manifolds, since we refer to Euclidean spaces.

very clever to introduce an atlas of E_F ignoring that it is a fiber bundle. Let us introduce a suitable atlas. Let $(U_i)_{i \in I}$ be an open cover of the base, and $\phi_i : U_i \times F \rightarrow \pi^{-1}(U_i)$ the trivialization of $\pi^{-1}(U_i)$. The particular suitable atlas of E_F I was announcing is thus simply $(\pi^{-1}(U_i), \phi_i)_{i \in I}$. Of course, we can end up with a ‘standard’ Euclidean atlas if we can provide Euclidean atlases for U and F . The global topology of the space E_F is encoded in the so-called transition functions defined by $t_{i,j}(x) = \phi_{i,x} \circ \phi_{x,j} : F \rightarrow F$, where $\phi_{i,x}(f) \equiv \phi_i(x, f)$, and the domain of definition of $t_{i,j}$ is the intersection $U_i \cap U_j$. Since we already know the local topology of E_F , it is (topologically) useless to specify the trivializing functions out of the intersections³, but we do need to specify the transition functions.

Let us now define the (left) action φ of some group G on some space S which is then called (left) G -set. Have in mind, as a broader motivation for such a definition, that we often find the situation where some family of internal transformations in some space S happen to form a group in the mathematical sense⁴. We thus define

$$\begin{aligned} \varphi : G \times S &\rightarrow S \\ (g, s) &\mapsto \varphi(g, s) \equiv g \cdot s, \end{aligned} \quad (\text{H.1})$$

which must satisfy the two following conditions, for all $x \in S$:

$$\begin{aligned} \text{identity condition:} \quad & e \cdot x = x \\ \text{compatibility condition:} \quad & (gh) \cdot x = g \cdot (h \cdot x), \end{aligned} \quad (\text{H.2})$$

where $(g, h) \in G^2$ and e is the neutral element of G .

Now, as announced, we require that some group G structure the fiber, which means the following: the (image of some $x \in U_i \cap U_j$ by the) transition function is constrained to be an element of G , i.e. $t_{i,j} : U_i \cap U_j \rightarrow G$. The fiber bundle is then called fiber G -bundle, and the atlas a G -atlas. The fiber bundle is said trivial when G is reduced to its neutral element.

H.1.2 Examples

H.1.2.1 Sphere bundles

The lines correspond to the base space, and the columns to the fiber.

$G = \{e\}$: trivial bundle			
	segment	circle	sphere
segment	filled rectangle	cylinder	filled cylinder + half sphere glued at its base to one of the two circular bases of the cylinder
circle	cylinder	torus	filled torus
sphere	annulus	annulus	annulus

$G = \{e, r\}$, r =reflexion			
	segment	circle	sphere
segment	filled rectangle	cylinder	
circle	Möbius strip	Klein bottle	
sphere			

³Again, this is why we use the word ‘trivialization’ rather than ‘chart’, which would imply that we want to localise an absolute position, which can only be done if we introduce a metric, while this is not necessary for our purpose right now.

⁴The minimal non-trivial internal transformation in some space S is the exchange between the (generically abstract) positions, i.e. the labels, of two elements of S , called a transposition. The set of such an exchange transformation and the identity is the simple example of group we can give.

$G = U(1)=\text{circle}$			
	G with right action (or S^1 embedded in S^3 (in a fibration view))		
S^3 (or S^2)	Hopf fibration		

H.1.2.2 Vector bundles

The fiber is a vectorial space V .

- **Tangent bundle**

The fiber at x is the tangent space $T_x M$ of some base manifold⁵ $B = M$ at x . The so-called tangent bundle is then denoted TM .

- **Cotangent bundle**

It is useful to define the cotangent space to do calculus on the manifold. Let us use Dirac notations, and let $|v_x\rangle$ be a vector of $T_x M$. The cotangent space at x is that generated by all the bras $\langle v_x|$. More generically, given a vector space $\{|v\rangle\}$, we define the co-space, or dual space $\{\langle v|\}$. The cotangent space at x is denoted $T_x^* M$.

- **Vector bundle of a representation-space generated by linear representations of groups**

I find Wikipedia's "Group representation" web page very good as a general (very) short presentation of this wide subject. Consider a given group G acting on several spaces S_α 's (say, from the left):

$$\begin{aligned}\varphi_\alpha : G \times S_\alpha &\rightarrow S_\alpha \\ (g, s) &\mapsto \varphi_\alpha(g, s).\end{aligned}\tag{H.3}$$

If S_α is a vectorial space $S_\alpha = V_\alpha$, it is natural to be interested in linear actions of G on the S_α 's, in which case one would use a notation such as $\varphi_\alpha(g, s) \equiv \rho_\alpha(g) \cdot s = \rho_\alpha(g)s$. The function ρ_α is called linear representation of G , $\rho_\alpha(G)$ is the representation image, and V_α the representation space. The main part (this is a euphemism) of the mathematical litterature on group representation theory deals with linear representations⁶.

H.1.2.3 Principal bundles

The fiber is the structure group G itself (endowed with right action). The fiber bundle is then called principal G -bundle.

⁵To obtain a manifold from a topological space, we must endow it with a differential structure, i.e. we must be able to do differential calculus on it, although this is not that easy when the manifold is not flat, and is best approached, e.g., with Cartan's exterior calculus.

⁶Some references on non-linear representations of groups are https://en.wikipedia.org/wiki/Nonlinear_realization, http://www.numdam.org/article/ASENS_1977_4_10_3_405_0.pdf, <http://www.ams.org/journals/bull/1984-11-02/S0273-0979-1984-15290-X/S0273-0979-1984-15290-X.pdf>, https://www.researchgate.net/profile/Daniel_Sternheimer/publication/225993353_Nonlinear_group_representations_and_evolution_equations/links/0deec52b064c7c2508000000/Nonlinear_group_representations_and_evolution_equations.pdf, https://www.researchgate.net/profile/Daniel_Sternheimer/publication/225993353_Nonlinear_group_representations_and_evolution_equations/links/0deec52b064c7c2508000000/Nonlinear_group_representations_and_evolution_equations.pdf. In the work of DAriano, there is also a non-linear representation [59].

Gauge-invariant generator of a symmetry of the electromagnetic field (Hamiltonian mechanics)

I.1 Introduction: electromagnetic field and potential

Consider a particle of charge q and mass m in an *electromagnetic field* $(\mathbf{E}(\mathbf{r},t), \mathbf{B}(\mathbf{r},t))$. To analyse this system in the framework of analytical (and hence quantum) mechanics, we must describe the electromagnetic field with an *electromagnetic potential* $(\phi_g(\mathbf{r},t), \mathbf{A}_g(\mathbf{r},t))$, satisfying

$$\mathbf{B} = \nabla \wedge \mathbf{A}_g , \quad (\text{I.1})$$

$$\mathbf{E} = -\nabla \phi_g - \frac{\partial \mathbf{A}_g}{\partial t} . \quad (\text{I.2})$$

The existence of such a potential is a consequence of the homogeneous Maxwell's equations. This potential is not unique, and the subscript g denotes the chosen *gauge*, which is at this stage arbitrary.

I.2 Symmetry of the electromagnetic field and associated conserved quantity (Lagrangian formalism)

A possible *Lagrangian* for the previous system is

$$L_g(\mathbf{r}, \mathbf{v}, t) = \frac{1}{2} m \mathbf{v}^2 - q [\phi_g(\mathbf{r}, t) - \mathbf{v} \cdot \mathbf{A}_g(\mathbf{r}, t)] . \quad (\text{I.3})$$

Suppose the electromagnetic field is invariant under some *continuous symmetry* \mathcal{S} . This implies that there exist a gauge g_o in which the electromagnetic potential $(\phi_{g_o}(\mathbf{r}, t), \mathbf{A}_{g_o}(\mathbf{r}, t))$, and hence the Lagrangian $L_{g_o}(\mathbf{r}, \mathbf{v}, t)$, are invariant under \mathcal{S} (otherwise the *action*, which is function only of the fields and not the potentials if one neglects the boundary terms, could not be invariant under \mathcal{S}). Noether's theorem then exhibits a *conserved quantity* $Q^{\mathcal{S}}(\mathbf{r}, \mathbf{v}, t)$ associated to this symmetry \mathcal{S} , in terms of a derivative of $L_{g_o}(\mathbf{r}, \mathbf{v}, t)$. The conservation equation reads:

$$\frac{d}{dt} Q^{\mathcal{S}}(\mathbf{r}(t), \mathbf{v}(t), t) = 0 . \quad (\text{I.4})$$

I.3 Generator of the symmetry (Hamiltonian formalism)

The *Hamiltonian* of the system reads

$$H_g(\mathbf{r}, \mathbf{p}_g, t) = \frac{(\mathbf{p}_g - q\mathbf{A}_g(\mathbf{r}, t))^2}{2m} + q\phi_g(\mathbf{r}, t) , \quad (\text{I.5})$$

where the *canonical momentum* is defined by

$$\mathbf{p}_g \equiv \frac{\partial L_g}{\partial \mathbf{v}} = m\mathbf{v} + q\mathbf{A}_g , \quad (\text{I.6})$$

and depends manifestly on the gauge g ¹. The invariance of $L_{g_o}(\mathbf{r}, \mathbf{v}, t)$ under \mathcal{S} implies the invariance of $H_{g_o}(\mathbf{r}, \mathbf{p}_{g_o}, t)$ under \mathcal{S} .

We rewrite the conserved quantity as a function of $(\mathbf{r}, \mathbf{p}_{g_o}, t)$, using (I.6) for $g = g_o$:

$$G_{g_o}^{\mathcal{S}}(\mathbf{r}, \mathbf{p}_{g_o}, t) \equiv Q^{\mathcal{S}} \left(\mathbf{r}, \frac{\mathbf{p}_{g_o} - q\mathbf{A}_{g_o}(\mathbf{r}, t)}{m}, t \right) . \quad (\text{I.7})$$

As a function of its variables, $G_{g_o}^{\mathcal{S}}$ is called *generator* of \mathcal{S} . This function $G_{g_o}^{\mathcal{S}}$ depends explicitly on g_o through \mathbf{A}_{g_o} (hence the subscript g_o in $G_{g_o}^{\mathcal{S}}$). This means that this function is not gauge invariant in the following sense: if we consider a generic gauge g , the quantity $G_{g_o}^{\mathcal{S}}(\mathbf{r}, \mathbf{p}_g, t)$ is not a conserved quantity, and this simply because the canonical momentum is not gauge invariant.

Recall that total time-derivative of some function $f(\mathbf{r}, \mathbf{p}_g, t)$ is given by:

$$\frac{df}{dt} = \{f, H_g\}_g + \frac{\partial f}{\partial t} , \quad (\text{I.8})$$

where the g - *Poisson brackets* of two functions A and B of the variables $(\mathbf{r}, \mathbf{p}_g, t)$ is defined by

$$\{A, B\}_g = \sum_{i=1}^3 \frac{\partial A}{\partial x^i} \frac{\partial B}{\partial p_g^i} - \frac{\partial B}{\partial x^i} \frac{\partial A}{\partial p_g^i} , \quad (\text{I.9})$$

so that the conservation equation, (I.4), reads:

$$\{G_{g_o}^{\mathcal{S}}, H_{g_o}\}_{g_o} + \frac{\partial G_{g_o}^{\mathcal{S}}}{\partial t} = 0 . \quad (\text{I.10})$$

When the generator does not depend explicitly on time, which is equivalent to state that the Hamiltonian $H_{g_o}(\mathbf{r}, \mathbf{p}_{g_o}, t)$ does not depend explicitly on time, its conservation is then simply expressed by its commutation (in the sense of Poisson brackets) with this Hamiltonian. Let us rephrase what we have seen in the former paragraph: if we write the Hamiltonian in an arbitrary gauge g , the function of $(\mathbf{r}, \mathbf{p}_g, t)$ associated to \mathcal{S} , *i.e.* that will commute with the Hamiltonian in the sense of (I.10), is not $G_{g_o}^{\mathcal{S}}$. We are looking for the expression of such a function, that we will call *gauge-invariant generator*, as a function of the usual generator $G_{g_o}^{\mathcal{S}}$.

¹Indeed, the speed of the particle, \mathbf{v} , does not depend on the gauge, since it is determined by Newton's law, where only the electromagnetic field plays a role (through the Lorentz force), and not the potential.

I.4 Gauge-invariant generator

Gauges g and g_o are generically linked by:

$$\phi_g(\mathbf{r}, t) = \phi_{g_o}(\mathbf{r}, t) - \frac{\partial}{\partial t} \chi_g(\mathbf{r}, t) , \quad (\text{I.11})$$

$$\mathbf{A}_g(\mathbf{r}, t) = \mathbf{A}_{g_o}(\mathbf{r}, t) + \nabla \chi_g(\mathbf{r}, t) , \quad (\text{I.12})$$

so that the canonical momenta in the two gauges are linked by

$$\mathbf{p}_g = \mathbf{p}_{g_o} + q \nabla \chi_g . \quad (\text{I.13})$$

We can then express $G_{g_o}^{\mathcal{S}}(\mathbf{r}, \mathbf{p}_{g_o}, t)$ as a function of the momentum in a generic gauge, namely \mathbf{p}_g :

$$\boxed{G_g^{\mathcal{S}}(\mathbf{r}, \mathbf{p}_g, t) \equiv G_{g_o}^{\mathcal{S}}(\mathbf{r}, \mathbf{p}_g - q \nabla \chi_g(\mathbf{r}, t), t)} . \quad (\text{I.14})$$

This expression is by construction a conserved quantity, and it is gauge invariant in the following sense: for any gauges g and g' , we have

$$G_g^{\mathcal{S}}(\mathbf{r}, \mathbf{p}_g, t) = G_{g'}^{\mathcal{S}}(\mathbf{r}, \mathbf{p}_{g'}, t) = Q^{\mathcal{S}}(\mathbf{r}, \mathbf{v}, t) . \quad (\text{I.15})$$

Thus, whatever gauge g we choose to write the Hamiltonian of the system, be it non invariant under \mathcal{S} , we can always, from the knowledge of the generator $G_{g_o}^{\mathcal{S}}$, find a function of \mathbf{p}_g , namely the gauge-invariant generator $G_g^{\mathcal{S}}$, which is conserved in time, that is:

$$\{G_g^{\mathcal{S}}, H_g\}_g + \frac{\partial G_g^{\mathcal{S}}}{\partial t} = 0 . \quad (\text{I.16})$$

On the isospin

The mass of the proton and that of the neutron differ approximately by 0.1% from each other. At sufficiently low energy¹, one can thus not detect the difference between both masses, so that the proton and neutron differ only in (i) their electric charge, e or 0 , and (ii) their so-called (nuclear) isospin (contraction of ‘isotopic spin’), $+1/2$ or $-1/2$.

The isospin internal degree of freedom (d.o.f.) is that associated to the nuclear force, as the electromagnetic internal d.o.f., i.e. the complex phase of the considered matter field, is associated to the electromagnetic force, which was found out by Weyl, Fock and London, and widespread by Pauli in 1941 [293].

The nuclear-isospin d.o.f. is however more complex than the electromagnetic phase. It is named that way because it is described by the spin-1/2 formalism: indeed, it belongs to a two-dimensional complex Hilbert space and transforms under its associated (global) gauge transformations as the spin transforms under spatial rotations. The projection of the isospin d.o.f. on some arbitrary axis is $+1/2$ for a proton, and $-1/2$ for a neutron. Note two things: (i) this has nothing to do with measurement or physical angular momentum, only the mathematics are the same, and (ii) a rotation of the isospin d.o.f. from projection $+1/2$ to $-1/2$ is enough to transform a proton into a neutron (or vice versa), *only* if one can neglect the electromagnetic interaction.

The idea of the isospin, i.e. that the neutron and the proton are two manifestations of the same nucleon, was introduced by Heisenberg in 1932 [294, 295, 296], but it was named that way only in 1937, by Wigner, who underlined the aforementioned link with the spin (see the introduction of [199] for historical details).

In 1954, Yang and Mills proposed, extending Weyl’s gauge principle for quantum electromagnetism to the nuclear interaction, to make the invariance of nuclear interactions under global isospin rotations, a local invariance. Since the $SU(2)$ group of isospin gauge transformations is non-Abelian, on the contrary to the $U(1)$ group of electromagnetic gauge transformations, the isospin gauge field is called a non-Abelian gauge field. Yang and Mills did not reach a conclusion regarding the mass of this nuclear non-Abelian gauge field, which mediates the nuclear force, as the electromagnetic field mediates the electromagnetic force. This mass had to be computed and compared with that of pions, the mesons that mediate the nuclear interaction, as described by Yukawa’s meson theory; in his paper introducing the now so-called Yukawa’s potential for the nuclear interaction [235], Yukawa gave a prediction for the mass of the mediator, which was later recognized to be the pi meson, i.e. the pion, discovered in 1947, see <https://www.nature.com/physics/looking-back/lattes/lattes.pdf> for the original paper and <http://fafnir.phyast.pitt.edu/particles/pion.html> for 1997 comments from the CERN Courier. This picture of the nuclear interaction between nucleons as mediated by pions was later understood as a residual effect of the strong interaction between quarks inside and between nucleons.

¹Typically, at or below nuclear energies.

Classical fields and spin

We can point out two notable differences between half-integer- and integer-spin (classical i.e. first-quantized) fields, in the way they couple to gauge fields: (i) the Noether current J (associated to the gauge-group charge conservation) of half-integer-spin fields must be written with gamma matrices (trace of the spinorial (i.e. half-integer-spin) nature of the field in the Noether current), and (ii), apart from (i), the coupling between the gauge field and the Noether current is the same for both field natures, in the sense that it takes the form (in the Lagrangian or the Hamiltonian) $J^\mu A_\mu$, with $J_\mu \sim \Psi \partial_\mu \Psi$ for a half-integer-spin field Ψ and $J \sim \Phi \partial_\mu \Phi$ for an integer-spin field Φ , *but* for integer-spin fields, there is an additional mass-like coupling $(\Phi A_\mu)^2$ (in the Lagrangian or the Hamiltonian), which is involved in pair creation; an application to the case of the Higgs mechanism is detailed on the following slides by Englert: <https://indico.lal.in2p3.fr/event/2187/contribution/0/material/slides/0.pdf>.

Apart from these differences regarding their coupling to gauge fields, half-integer- and integer-spin fields differ in their free dynamics: the matter free term in the Lagrangian takes the schematic form $\Psi \partial_\mu \Psi$ for a half-integer-spin field, and $(\partial_\mu \Phi)^2$ for an integer-spin field.

I wonder how (if) we can single out in a simple picture the phenomenal properties of the Noether quantum coupling between matter and gauge fields, i.e. that of the form JA_μ , which are independent of the matter-field spin.

In the non-relativistic limit, these phenomenal properties result, at least for unstructured particles (i.e., in a non-quantum framework, point particles) from the interplay between the usual features of quantum mechanics and classical electrodynamics, which are formally captured by the Hamiltonian of an unstructured particle coupled to a gauge field (consider minimal coupling), if we forget about the half-integer-spin additional term that couples to the magnetic field (in the case of an Abelian gauge field); in other words, in such a non-relativistic framework, the essence of (first-quantized) quantum electrodynamics is contained in the correspondance principle applied to the electrodynamical classical Hamiltonian. The following papers are interesting: https://www.lorentz.leidenuniv.nl/IL-publications/sources/Kramers_50.pdf, http://link.springer.com/chapter/10.1007%2F978-3-662-04360-8_42, <https://www.math.toronto.edu/sigal/publications/53.pdf>. There is also a book by Healey entitled *Non-relativistic Quantum Electrodynamics*. Here are some notes on the scattering theory of non-relativistic quantum electrodynamics: <http://iopscience.iop.org/article/10.1088/0305-4470/16/1/014/meta>.

In a relativistic context, the idea would be to determine the phenomenal role played by the trace of the spinorial nature of the field (i.e. the presence of gamma matrices) in the current J , and the relativistic phenomenal component which is independent from the spinorial nature: is this phenomenal component ‘merely’ contained in the relativistic dispersion relation, which is the same whether the field has half-integer or integer spin?

Effect of linear plane gravitational waves on a DTQW matter distribution located in the polarization plane of the wave

L.1 Discussion without equations

Suppose we are interested in how a GW influences an initial matter distribution (or density), located in some plane transverse to this GW, which is stationary in free space i.e. when there is no GW.

Since the free-space ($\xi = 0$) walk operator is local in the momentum, any initial state whose spatial part (as opposed to the spin part) is a single Fourier mode (this is of course an ideal, non-physical situation), is stationary in free space (its density is homogeneous at any time), i.e. the free-space walk operator can only change the polarization of this Fourier mode. Now, among these states, we choose plane waves, i.e. eigenstates of the free-space walk operator, whose polarization is not changed by the time evolution, in order to capture only the density change induced by the GW and get rid of that induced by the free-space polarization change; One could think of considering such a single free-space plane wave as initial state. However, the density of such a state will not be modified by the GW, because the walk operator is local in the momentum even in the presence of a GW ($\xi \neq 0$).

One must then consider a superposition of Fourier modes as initial state. The minimal superposition is that of two modes, with generic wavevectors \mathbf{k}^1 and \mathbf{k}^2 . As said above, we want this state to be a free-space eigenstate, so that these two Fourier modes must have the same free-space eigen-energy. Their respective wavevectors must then have the same norm; and both polarizations must correspond to same-sign, say positive energies. The initial condition used in Subsection VI B of the paper is constructed in that way. For simplicity purposes, the retained wavevectors \mathbf{k}^1 and \mathbf{k}^2 are chosen to be orthogonal, respectively along the X and the Y axis.

In addition to (i) its easy technical tractability and (ii) its pedagogical interest (minimal free-space eigenstate having a density modified by the GW), this situation is interesting because this initial double-peaked momentum distribution yields an interference pattern in the physical-space density of the walker (even in the absence of GW), and this interference pattern facilitates the detection of the deformation induced by the GW, because of at least two reasons: (i) the high contrast between low- and high-density regions, and (ii) the fact that a measurement on a sample displaying a pattern predicted periodic by theory is more precise than if the pattern is non-periodic, because one can make (spatial) statistics thanks to these replications.

L.2 Formal material

If $\lambda_{\pm}(\xi, G(T); q_X, q_Y)$ are the eigenvalues of the walk operator in Fourier space, namely, $W(\xi, G(T); q_X, q_Y)$, we define the eigen-energies by

$$\lambda_{\pm}(\xi, G(T); q_X, q_Y) = \exp[-iE_{\pm}(\xi, G(T); q_X, q_Y)]. \quad (\text{L.1})$$

In Section V of the paper, we have computed the walk operator in Fourier space at first order in ξ ; it reads

$$\begin{aligned} W(\xi, G(T); q_X, q_Y) \\ \simeq \mathcal{W}^{(1)}(\xi, G(T); q_X, q_Y) \\ = W^{(0)}(q_X, q_Y) + \xi G(T) W^{(1)}(q_X, q_Y), \end{aligned} \quad (\text{L.2})$$

where the superscript in $\mathcal{W}^{(1)}$ means a computation at first order in ξ , and $W^{(0)}$ and $W^{(1)}$ are given by Eqs. (28) and (29) of the paper, respectively. If we work at first order in ξ , it only makes sense to search for eigen-elements of the walk operator at first order in ξ . We thus look for eigen-energies and eigenvectors of the form

$$E_{\pm}(\xi, G(T); q_X, q_Y) \quad (\text{L.3a})$$

$$\begin{aligned} &\simeq \mathcal{E}_{\pm}^{(1)}(\xi, G(T); q_X, q_Y) \\ &= E_{\pm}^{(0)}(q_X, q_Y) + \xi G(T) E^{(1)}(q_X, q_Y), \\ V_{\pm}(\xi, G(T); q_X, q_Y) \\ &\simeq \mathcal{V}_{\pm}^{(1)}(\xi, G(T); q_X, q_Y) \\ &= V_{\pm}^{(0)}(q_X, q_Y) + \xi G(T) V_{\pm}^{(1)}(q_X, q_Y), \end{aligned} \quad (\text{L.3b})$$

assuming no degeneracy, and where $\mathcal{E}_{\pm}^{(r)}(\xi, G(T); q_X, q_Y)$ and $\mathcal{V}_{\pm}^{(r)}(\xi, G(T); q_X, q_Y)$ are respectively the eigen-energies and eigenvectors computed at order r in ξ . A small calculation (that of standard perturbation theory) would then give us the corrections as functions of the zeroth-order eigen-elements and of the walk perturbation $W^{(1)}$. In Subsection VI A, we have computed these eigen-elements, not only at first order in ξ , but also at first order in q_X and q_Y , i.e. only for large spatial scales, which are those relevant to the continuum limit.

We want to go beyond. We are interested in how a gravitational wave, described by the walk operator at first order in ξ , influences an initial matter distribution (in the transverse (X, Y) plane) which is stationary in free space (i.e. if there is no wave). Elementary stationary distributions are generated by free walkers of given energy, i.e. eigenvectors of the real-space version of $W^{(0)}(q_X, q_Y)$ ¹. As mentioned, we want to study not only large scales, i.e. not only the continuum-limit situation, which is that of a Dirac fermion in curved space, but also small scales comparable to the lattice spacing, where the DTQW evolution differs from that of a Dirac fermion in curved space; we will thus make *no* Taylor developments in q_X and q_Y .

In terms of perturbation theory, the term accounting for such a modification of the distribution is the walk perturbation $W^{(1)}$ applied to a zeroth-order eigenvector, namely, $\xi G(T) W^{(1)} V_{\pm}^{(0)}(q_X, q_Y)$. For the initial distribution to be stationary in the presence of the

¹As mentioned in the previous section, there are stationary distributions which are *not* eigenvectors of (the real-space version of) $W^{(0)}(q_X, q_Y)$: these correspond to Fourier modes whose polarization is *not* an eigenpolarization of the zeroth-order walk operator

wave, at first order in ξ , one would need to add the term $\xi G(T) W^{(0)} V_{\pm}^{(1)}(q_X, q_Y)$. We do not add this term, and thus the initial distribution is indeed modified by the wave.

Generically, any initial walker $\tilde{\Psi}_0(k_X, k_Y)$ can be decomposed as a superposition of the plus and minus eigenvectors, since these are a basis of the Hilbert space; such a decomposition can be written

$$\begin{aligned} \tilde{\Psi}_0(k_X, k_Y) &= \alpha_+(k_X, k_Y) \frac{V_+^{(0)}(q_X, q_Y)}{\|V_+^{(0)}(q_X, q_Y)\|_{\text{spin}}} \\ &\quad + \alpha_-(k_X, k_Y) \frac{V_-^{(0)}(q_X, q_Y)}{\|V_-^{(0)}(q_X, q_Y)\|_{\text{spin}}}, \end{aligned} \quad (\text{L.4})$$

where $\|\cdot\|_{\text{spin}}$ indicates the norm in spin space, i.e. the square-rooted density. This decomposition must be normalised, i.e.

$$\begin{aligned} &\iint \tilde{\Psi}_0^\dagger(k_X, k_Y) \tilde{\Psi}_0(k_X, k_Y) dk_X dk_Y \\ &= \iint (|\alpha_+(k_X, k_Y)|^2 + |\alpha_-(k_X, k_Y)|^2) dk_X dk_Y \\ &= 1, \end{aligned} \quad (\text{L.5})$$

where

$$\iint = \frac{1}{\sqrt{2\pi}^2} \int_{k_X=-\pi}^{\pi} \int_{k_Y=-\pi}^{\pi} . \quad (\text{L.6})$$

In order for the initial distribution to be stationary under $W^{(0)}(q_X, q_Y)$, it has to be an eigenvector of this operator (as already mentioned), say $V_+^{(0)}(q_X, q_Y)$, which means choosing $\alpha_- = 0$ and α_+ such that

$$\frac{1}{\sqrt{2\pi}^2} \int_{k_X=-\pi}^{\pi} \int_{k_Y=-\pi}^{\pi} |\alpha_+(k_x, k_Y)|^2 dk_X dk_Y = 1. \quad (\text{L.7})$$

One could consider $|\alpha_+(k_x, k_Y)|^2$ to be a Gaussian centered around some wavevector \mathbf{k}_0 , that is, classically, a walker going at some given average classical speed \mathbf{k}_0 . One would thus have, to go to physical space, to integrate the derivative of a Gaussian (product of V_+ , which contains terms proportional to the wavevector, by a Gaussian), which would yield a Gaussian. If the Gaussian in momentum space is very peaked, the Gaussian in physical space would have a very large spread, i.e. it would be almost a uniform distribution in some finite region centered around its maximum. If the Gaussian in momentum space has a large spread, this would yield a walker localised in physical space. One would then see how the uniform distribution or the localised one are deformed by the wave.

Another interesting situation to look at is that of a momentum distribution containing two peaks, one at some \mathbf{k}^1 and another at some \mathbf{k}^2 , because then this yields, in physical space, an interference pattern in the (X, Y) plane, on which the deformation induced by the wave could be more detectable because of high contrast between low- and high-density regions. These two wavevectors, \mathbf{k}^1 and \mathbf{k}^2 , must have the same norm if we want the distribution to be stationary under $W^{(0)}(q_X, q_Y)$ in physical space; indeed, the two exponentials containing the time dependency must coincide, so that we can factor this exponential out of the momentum-

space integral. This corresponds to choosing

$$|\alpha_+(k_x, k_Y)|^2 = c^1 G(\mathbf{k} - \mathbf{k}^1) + c^2 G(\mathbf{k} - \mathbf{k}^2), \quad (\text{L.8})$$

where $G(\mathbf{k} - \mathbf{k}_0)$ is a Gaussian centered around \mathbf{k}_0 . We choose to normalise $G(\mathbf{k})$ to $1/2$, so that giving the same weight to the two Gaussians imposes, for a proper normalisation, to choose $c^1 = c^2 = 1$. Now this implies we can choose

$$\begin{aligned} \alpha_+(k_x, k_Y) &= \sqrt{G(\mathbf{k} - \mathbf{k}^1) + G(\mathbf{k} - \mathbf{k}^2)} \\ &\simeq \sqrt{G(\mathbf{k} - \mathbf{k}^1)} + \sqrt{G(\mathbf{k} - \mathbf{k}^2)}, \end{aligned} \quad (\text{L.9})$$

where the approximated equality holds as long as the Gaussians are peaked enough.

Now, to simplify this exemplifying study, we will work in the limit where the square-rooted Gaussians tend to delta functions, i.e.

$$\alpha_+(k_x, k_Y) = \delta^{(2)}(\mathbf{k} - \mathbf{k}^1) + \delta^{(2)}(\mathbf{k} - \mathbf{k}^2), \quad (\text{L.10})$$

which yields in physical space the interference between two plane waves corresponding to the selected modes, \mathbf{k}^1 and \mathbf{k}^2 . Again, for the sake of simplicity, we choose $\mathbf{k}^1 = (k, 0)$ and $\mathbf{k}^2 = (0, k)$, where $k = q/2$, so that

$$\alpha_+(k_x, k_Y) = \delta(k_X - k)\delta(k_Y) + \delta(k_X)\delta(k_Y - k). \quad (\text{L.11})$$

The initial wave function then reads

$$\Psi_0(X, Y) = \Psi^1 e^{iqX} + \Psi^2 e^{iqY}, \quad (\text{L.12})$$

where Ψ^1 and Ψ^2 are given by Eqs. (36) of the paper. This initial state yields the density of Eq. (38).

Dirac equation in curved spacetime

In this Appendix, all physical quantities related to spin, such as the spinors Φ or Ψ , or the gamma matrices γ^μ or γ^a , are abstract quantities in the spin space, while in Appendix B of Publication 4, i.e. Ref [4], we have chosen to use respectively the ket and the hat notations to designate such an abstract nature, despite the clumsiness, in order to be coherent with the main matter of the paper, which already uses non-ket and non-hat notations for a *particular representation* of the Clifford algebra, i.e. for quantities written in a particular basis of the spin space.

M.1 The Dirac equation in a generic curved spacetime

The Dirac equation in an $(N = 1 + n)$ -dimensional curved spacetime with metric $g_{\mu\nu}$ reads

$$(i\gamma^\mu D_\mu - m) \Phi = 0 . \quad (\text{M.1})$$

The wavefunction Φ is a d -component spinor, where the smallest possible d is $d = 2^{N/2}$ if N is even and $d = 2^{(N-1)/2}$ if N is odd. The γ^μ (greek indices) satisfy the $g_{\mu\nu}$ -Clifford algebra, $\{\gamma^\mu, \gamma^\nu\} = g^{\mu\nu}$. Eventually, D is the spin-space covariant derivative, given by

$$D_\mu = \partial_\mu + \Gamma_\mu , \quad (\text{M.2})$$

where the spinorial connection Γ_μ is of the form

$$\Gamma_\mu = \frac{1}{2} \omega_{ab\mu} S^{ab} . \quad (\text{M.3})$$

In this expression, S^{ab} are the generators of the d -component spinorial representation of $\text{SO}(n,1)$, and one can prove that they are given by

$$S^{ab} = \frac{1}{4} [\gamma^a, \gamma^b] , \quad (\text{M.4})$$

where the γ^a (latin indices) satisfy the η_{ab} -Clifford algebra. The $\omega_{ab\mu}$ are the coefficients of the spinorial connection, and one can show that they are given, in the N -ads formalism, by

$$\omega_{ab\mu} = g_{\alpha\beta} e_a^\beta \nabla_\mu e_b^\alpha . \quad (\text{M.5})$$

In this expression, the e_a^μ is the inverse N -bein field, i.e. the contravariant components of the N -ads $(e_a)_{a=1,N}$ on the coordinate basis $(e_\mu)_{\mu=1,N}$. Eventually, ∇ is the physical-space covariant derivative, defined for any vector V by

$$\nabla_\mu V^\alpha = \partial_\mu V^\alpha + \Gamma_{\mu\nu}^\alpha V^\nu , \quad (\text{M.6})$$

where the $\Gamma_{\mu\nu}^\alpha$ are the coefficients of the vectorial connection. An N -ad is generically a basis of spacetime, but we often use this term to refer to a fixed (and hence generally non-coordinate) basis, which is in the present context chosen orthonormal, i.e. corresponding to a Minkowskian metric: $e_a \cdot e_b = \eta_{ab}$. We can go from the Minkowskian (or Lorentzian)

components V^a to the coordinate components V^μ , and inversely, by

$$V^\mu = e_a^\mu V^a, \quad V^a = e_\mu^a V^\mu, \quad (\text{M.7})$$

where e_μ^a is the N -bein field, i.e. the contravariant components of the coordinate-basis vectors on the N -ad. These relations can also be used for the γ matrices, just replace V by γ (don't forget however that γ is not a tensor by any means). Here is an important practical remark: to take the derivative of a spinor in curved spacetime with this N -ad formalism, we don't need to compute the $\Gamma_{\mu\nu}^\alpha$, as the following computation shows:

$$\Gamma_\mu = \frac{1}{2} \omega_{ab\mu} S^{ab} \quad (\text{M.8})$$

$$= \frac{1}{2} g_{\alpha\beta} e_a^\beta (\partial_\mu e_b^\alpha + \Gamma_{\mu\nu}^\alpha e_b^\nu) S^{ab} \quad (\text{M.9})$$

$$= \frac{1}{2} g_{\alpha\beta} e_a^\beta (\partial_\mu e_b^\alpha) S^{ab}, \quad (\text{M.10})$$

where, in going from the second to the third line, the second term of the sum vanishes because S^{ab} is antisymmetric while $\Gamma_{\mu\nu}^\alpha g_{\alpha\beta} e_a^\beta e_b^\nu$ is symmetric. A similar remark enables us to write this other equivalent expression for the spinorial connection:

$$\Gamma_\mu = \frac{1}{2} e_a^\alpha \partial_\mu (g_{\alpha\beta} e_b^\beta) S^{ab} = \frac{1}{2} e_a^\alpha. \quad (\text{M.11})$$

In the end, the Dirac equation in curved spacetime can be written more explicitly as

$$\left[i \gamma^a e_a^\mu \left\{ \partial_\mu + \frac{1}{2} e_a^\beta \partial_\mu (g_{\alpha\beta} e_b^\alpha) S^{ab} \right\} - m \right] \Phi = 0. \quad (\text{M.12})$$

Here come three final remarks. The first remark is that $e_a^\mu e_\nu^a = \delta_\nu^\mu$ and $e_\mu^a e_b^a = \delta_\mu^b$, so that $[e_a^\mu] = [e_\mu^a]^{-1}$, where the upper index always corresponds to rows and the lower index to columns; however, since we always choose a symmetric metric, we can always choose a symmetric N -bein, in which case rows and columns can be inverted. The second remark is that denoting the N -bein field and its inverse with the same letter e is justified by the fact that $g_{\mu\nu} e_a^\nu = \eta_{ab} e_\mu^b$, which can be noted either $e_{a\mu}$ or $e_{\mu a}$; however, we can use the letter E to refer to, say, the inverse N -bein, so as not to confuse, for example, E_1^1 with e_1^1 , or use round brackets around the latin indices. The third remark is that we have used the N -ad formalism because (i) it is the simplest way to obtain an expression for the coefficients of the spinorial connection (CSC), since it is easier to look for (and classify) the solutions to the Clifford algebra in *flat* spacetime, and (ii) in the end, we don't even need the CSC to covariantly derive a spinor in curved space, but only the N -bein field, see expression (M.11).

M.2 The Dirac equation in particular (1+2)D spacetimes

M.2.1 Choice of metric

We will from now on work in (1+2)D spacetime with dimensionless coordinates $X^0 = T, X^1 = X$ and $X^2 = Y$. The metric is noted $G_{\mu\nu}$, with a capital letter to remember that it is function of dimensionless coordinates. To simplify the problem, we assume that

1. $G_{00} = 1$
2. (ii) the length element dS^2 is invariant under $X^0 \rightarrow -X^0$, i.e. all the components G_{0i} , $i \neq 0$, vanish.

The metric then has the form

$$[G_{\mu\nu}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & G_{XX} & G_{XY} \\ 0 & G_{XY} & G_{YY} \end{bmatrix}, \quad (\text{M.13})$$

where G_{XX} , G_{YY} and G_{XY} are three arbitrary functions of (T, X, Y) . Such a metric is much simpler than a generic one, but still quite general, and it enables to treat many interesting physical situations.

M.2.2 Relation between the metric and the 3-bein

Consider now an orthonormal triad associated to the Minkowskian coordinates $(\tilde{T}, \tilde{X}, \tilde{Y})$. This triad generates a 3-bein field $e_\mu^a = \partial \tilde{X}^a / \partial X^\mu$ (its inverse is noted E_a^μ). At any point, the length element dS^2 can be expressed in terms of the global coordinates X^μ but also in terms of the Minkowskian coordinates \tilde{X}^a , because it is a local quantity:

$$\begin{aligned} dS^2 &= dT^2 + G_{XX}dX^2 + 2G_{XY}dXdY + G_{YY}dY^2 \\ &= d\tilde{T}^2 - d\tilde{X}^2 - d\tilde{Y}^2. \end{aligned} \quad (\text{M.14})$$

We choose $\tilde{T} = T$, so that $e_0^0 = 1$ and $e_i^0 = e_0^i = 0$ for $i \in \{X, Y\}$. Hence, we can write the following decomposition:

$$d\tilde{X} = \frac{\partial \tilde{X}}{\partial X} dX + \frac{\partial \tilde{X}}{\partial Y} dY, \quad d\tilde{Y} = \frac{\partial \tilde{Y}}{\partial X} dX + \frac{\partial \tilde{Y}}{\partial Y} dY. \quad (\text{M.15})$$

M.2.2.1 Case of a symmetric 3-bein

I wonder if the fact that the metric is symmetric implies that we can choose a symmetric 3-bein *without losing any generality*. Anyways, we can still look for a symmetric 3-bein, i.e. such that

$$e_2^1 = e_1^2, \quad \text{i.e.} \quad \frac{\partial \tilde{Y}}{\partial X} = \frac{\partial \tilde{X}}{\partial Y}. \quad (\text{M.16})$$

With these choices, Eq. (M.14) leads to the following set of equations:

$$-G_{XY} = e_2^1(e_1^1 + e_2^2), \quad -G_{XX} = (e_1^1)^2 + (e_2^1)^2, \quad -G_{YY} = (e_2^2)^2 + (e_1^2)^2. \quad (\text{M.17})$$

A solution to this system is given by

$$e_1^1 = \frac{-G_{XX} + \sqrt{G}}{\sqrt{2\sqrt{G} - \Sigma}}, \quad e_2^2 = \frac{-G_{YY} + \sqrt{G}}{\sqrt{2\sqrt{G} - \Sigma}}, \quad e_2^1 = \frac{-G_{XY}}{\sqrt{2\sqrt{G} - \Sigma}}, \quad (\text{M.18})$$

with $G = \det[G_{\mu\nu}] = G_{XX}G_{YY} - G_{XY}^2$ and $\Sigma = G_{XX} + G_{YY}$. This solution can straightforwardly be inverted into

$$\mathcal{E}_1 = E_1^1 = \frac{1}{\sqrt{G}} \frac{-G_{YY} + \sqrt{G}}{\sqrt{2\sqrt{G} - \Sigma}}, \quad \mathcal{E}_2 = E_2^2 = \frac{1}{\sqrt{G}} \frac{-G_{XX} + \sqrt{G}}{\sqrt{2\sqrt{G} - \Sigma}}, \quad \mathcal{B} = E_2^1 = \frac{1}{\sqrt{G}} \frac{G_{XY}}{\sqrt{2\sqrt{G} - \Sigma}}. \quad (\text{M.19})$$

M.2.2.2 ‘General’ case

M.2.3 Working out the Dirac equation in our particular spacetime

The Dirac equation in the (1+2)D spacetime considered previously can be expanded into

$$\partial_0 \Phi = (-L_1 \partial_1 - L_2 \partial_2 + K) \Phi , \quad (\text{M.20})$$

where the operators L_1 , L_2 and K are given by

$$\begin{aligned} L_1 &= \mathcal{E}_1 \gamma^0 \gamma^1 + \mathcal{B} \gamma^0 \gamma^2 \\ L_2 &= \mathcal{B} \gamma^0 \gamma^1 + \mathcal{E}_2 \gamma^0 \gamma^2 \\ K &= -\Gamma_0 - L_1 \Gamma_1 - L_2 \Gamma_2 - i \gamma^0 m . \end{aligned} \quad (\text{M.21})$$

In (1+2)D, the smallest dimension for the spin Hilbert space is $d = 2$. Let (b_-, b_+) be a basis of this two-dimensional Hilbert space, i.e. $\Phi = \phi^- b_- + \phi^+ b_+$. We can choose the following representation for the γ matrices,

$$[(\gamma^0)^u_v] = \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad [(\gamma^1)^u_v] = i\sigma_2 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad [(\gamma^2)^u_v] = i\sigma_3 = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \quad (\text{M.22})$$

with $(u, v) \in \{-, +\}^2$. In this representation, the Dirac equation reads:

$$\partial_T [\Phi^u] = \left\{ (\mathcal{E}_1 \sigma_3 - \mathcal{B} \sigma_2) \partial_X + (\mathcal{B} \sigma_3 - \mathcal{E}_2 \sigma_2) \partial_Y + [K^u_v] \right\} [\Phi^u] . \quad (\text{M.23})$$

If the metric is diagonal, then $\mathcal{B} = 0$, and the previous equation get simplified into:

$$\partial_T [\Phi^u] = \left\{ \mathcal{E}_1 \sigma_3 \partial_X - \mathcal{E}_2 \sigma_2 \partial_Y + [K^u_v] \right\} [\Phi^u] , \quad (\text{M.24})$$

where we can choose $\mathcal{E}_1 = 1/\sqrt{-G_{XX}}$ and $\mathcal{E}_2 = 1/\sqrt{-G_{YY}}$.

M.3 2D DTQWs as Dirac fermions in curved spacetime with diagonal metric

M.3.1 Recovering the Dirac dynamics from a DTQW

We want to find a walk $\Psi_{j+1} = W_j \Psi_j$ whose continuous-limit dynamics correspond to Eq. (M.24). We must first notice that the continuous-limit dynamics of such a walk will always take the generic form

$$\partial_T [\Psi^h] = (-M_1 \partial_X - M_2 \partial_Y + Q) [\Psi^h] , \quad (\text{M.25})$$

with $h \in \{L, R\}$, where (b_L, b_R) is some basis of the spin Hilbert space.

We set $P_1 = M_1/\mathcal{E}_1$ and $P_2 = M_2/\mathcal{E}_2$, so that the previous equation becomes

$$\partial_T [\Psi^h] = (-\mathcal{E}_1 P_1 \partial_X - \mathcal{E}_2 P_2 \partial_Y + Q) [\Psi^h] . \quad (\text{M.26})$$

Suppose we find a walk W such that the passage matrix \mathcal{P} from basis (b_L, b_R) to basis (b_-, b_+) , defined by $[\Psi^h] = \mathcal{P}[\Psi^u]$, satisfies:

$$\mathcal{P}^{-1} P_1 \mathcal{P} = -\sigma_3 \quad (\text{M.27})$$

$$\mathcal{P}^{-1} P_2 \mathcal{P} = \sigma_2 . \quad (\text{M.28})$$

In basis (b_-, b_+) , Eq. (M.26) will then read:

$$\partial_T[\Psi^u] = (\mathcal{E}_1\sigma_3\partial_X - \mathcal{E}_2\sigma_2\partial_Y + R) [\Psi^u] , \quad \text{with} \quad R = \mathcal{P}^{-1}(\partial_X + \partial_Y - \partial_T + Q)\mathcal{P} . \quad (\text{M.29})$$

Now, to link (M.29) to (M.24), we have to match the normalization conditions. On the one hand, Φ in Eq. (M.24) is normalized with respect to the covariant volume element $dV = \sqrt{\det G} dXdY$, with $\sqrt{\det G} = (\mathcal{E}_1\mathcal{E}_2)^{-1}$:

$$\int dV (|\phi^-|^2 + |\phi^+|^2) = 1 . \quad (\text{M.30})$$

On the other hand, Ψ in (M.29) is normalized with respect to $dXdY$:

$$\int dXdY (|\psi^-|^2 + |\psi^+|^2) = 1 . \quad (\text{M.31})$$

Hence, if, starting from (M.29), we set

$$\Phi \equiv (\det G)^{-1/4} \Psi \quad (\text{M.32})$$

$$= (\mathcal{E}_1\mathcal{E}_2)^{1/2} \Psi , \quad (\text{M.33})$$

then (M.29) can be put in the form of Eq. (M.24), provided that

$$[K^u_v] = (R + \mathcal{E}_1\sigma_3\partial_X - \mathcal{E}_2\sigma_2\partial_Y - \partial_T) (\mathcal{E}_1\mathcal{E}_2)^{-1/2} . \quad (\text{M.34})$$

M.3.2 Constraints on P_1 and the passage matrix \mathcal{P}

Let us now examine the constraints on P_1 and \mathcal{P} which are imposed by Eq. (M.27). Generically, P_1 is a 2×2 matrix with complex entries:

$$P_1 = \begin{bmatrix} a & b \\ c & d \end{bmatrix} , \quad (a, b, c, d) \in \mathbb{C}^4 . \quad (\text{M.35})$$

Now, condition (M.27) imposes:

$$P_1 = \begin{bmatrix} a & b \\ \frac{1-a^2}{b} & -a \end{bmatrix} , \quad (\text{M.36})$$

together with the following form for the passage matrix:

$$\mathcal{P} = \begin{bmatrix} x_- & x_+ \\ y_- & y_+ \end{bmatrix} , \quad (\text{M.37})$$

with

$$\begin{aligned} by_- &= (-1 - a) x_- \\ by_+ &= (1 - a) x_+ . \end{aligned} \quad (\text{M.38})$$

General ideas on (perturbative) renormalization

Reading that I am far from being an expert – which is more than a euphemism – on perturbative renormalization, is obviously unnecessary for any reader that will go through the following lines. I thus ask for his indulgence and suggestions to improve this appendix. I am longing to work, not only on this particular subject, but also many others, and eventually connect them to quantum walks.

Perturbative renormalization is a computational procedure, i.e. a series of computational rules, which, to first speak in epistemological terms – with no need to elaborate on either the technical details or the physical nature of such a procedure –, eventually enabled to ‘extract’ predictive results out of the ‘first’ computations carried out in the history of QFT, which are still standard and useful precisely when perturbative renormalization works. These standard computations are grounded on a perturbation series whose convergence radius actually vanishes in general, which makes them a priori unable to predict any physical result¹.

Indeed, while one is allowed to add an arbitrary (but finite!) number of terms, one a priori expects that the numerical result provided by such a sum will simply be of *no* predictive value if the predictive hope of this sum relies on viewing it as the truncation of a series which does not converge. While this is in general true, i.e. these finite sums give wrong numerical predictions, it is actually possible to produce correct numerical predictions by, as we say, *renormalizing*, or *resuming* this sum, i.e. by modifying it according to some rules. It is at this point necessary to give more technical details. The aforementioned sum, as we said, contains a finite number of terms; however, for these terms, which are integrals, to be finite themselves, i.e. for the integrals to converge, one first has to introduce a so-called ultraviolet *regulator*, i.e. an upper-bound, or cutoff, for the accessible energies².

Now, the guiding idea underlying the perturbative renormalization ‘recipe’, is the following: while the regulator makes the integrals involved in the sum be well-defined, i.e. convergent, this sum gives wrong predictions ‘because’ the regulation modifies the

¹This series, which does generally not converge, is essentially the exponential of the interaction term of the considered model. Note that, (i) in a Hilbert-space framework, this simply means that the evolution operator is actually a mathematically ill-defined object, i.e. that one cannot define the exponential of the Hamiltonian operator – indeed, there is no reason that the free part of the Hamiltonian compensate the interaction part, because these two terms are completely different by nature –, while (ii) in a path-integral framework, this means the path integral is a divergent object.

²This is how perturbative renormalization was historically developed: the ultraviolet divergences of most of the lowest-order Feynman diagrams have an ultraviolet divergence, so that the ultraviolet cutoff was introduced. Actually, one realizes after developing the renormalization method, that there are also infrared divergences in the theory, which was quickly pointed out by Landau, in the 50’s.

physical theory (which is anyways mathematically ill-defined); to recover the ‘good physical theory’ (although mathematically ill-defined), one must figure out how to modify these finite integrals so that their limit with infinitely-big regulator, i.e. in the original pre-regularization situation, is finite.

Eventually, the physics behind these mathematics holds in the following lines. The coupling constant of an interaction, formally introduced as a constant often denoted by g in the interaction Lagrangian, is of no physical significance, and must be, as we say, renormalized, i.e. made function of the typical energy scale μ at which the interaction occurs; this is achieved by the computational procedure detailed above, i.e. it is the physical way of viewing such computations. This renormalized coupling constant $g_R(\mu)$ is that which is measured in experiments. The energy scale is simply the input energy if the system can be considered isolated. In particle physics, μ is thus given by the kinetic energy communicated to the particles before making them collide.

The regulator can be viewed as a mere intermediate tool which is in the end replaced by a renormalization-flow picture, which defines $g_R(\mu)$ by relating the couples (g_R^i, μ^i) labeled by i , which simply indicates that g_R^i is the good numerical value of the measured coupling constant if we are at energy scale μ^i . This connects with the non-perturbative methods based on the renormalization group, see further down.

Let us stress that, while such a perturbative renormalization happens to produce accurate predictions, it still does not solve the mathematical problem of ill-definition of the theory, in the sense that the mathematical idea underlying the addition of the terms in the *renormalized* sum is that this sum should *still* be the truncation of some series which, as the first ‘bare’ series, is standardly seen as not converging either. This is not surprising since perturbative renormalization ‘simply’ modifies the value of the coupling constant, which will never be enough to make a series with radius *zero* be defined, since the litteral model in such a picture is viewed as unchanged^{3,4}.

The branch of mathematical physics aiming at solving the problem of ill mathematical definition of QFT is generically called *axiomatic QFT*. In an epistemological picture, the so-called *constructive QFT* program, born in the 60’s, can be viewed as a desire to connect, as much as possible, the mathematical developments of a given axiomatic QFT with the succesful predictions of renormalization theory; this is done by lowering the standard mathematical ‘desire of generality’ and constructing a series of concrete examples of reference, i.e., a series of Lagrangians, in which one can precisely define (*rather meta-mathematical*) *translation rules* to relate the mathematically ill-defined, but physically predictive original Lagrangian-based QFT, to such a mathematically well-defined axiomatic QFT.

For more details, see the following introductory review written by Jaffe in

³Perturbative renormalization should thus be regarded as a series of computational rules which, although developed upon a mathematically ill-defined framework, produce predictive results. This subject illustrates particularly beautifully, I believe, that physics need, if not often, at least sometimes, not be proper from the mathematical point of view, but that mathematics are rather used as either (i) a practical tool, namely mathematical *computations*, or (ii) an inspirational tool, thanks to their formal, i.e. *symbolization power*. Indeed, formalism can help to conceptualize useful *physical* concepts, regardless of the mathematical well-definition of the formal objects one introduces; the only thing that physics requires from some formalism is that the *numerical* computations this formalism suggest make predictive results.

⁴I need to investigate more about this matter: it may be that some constructive approaches (see below) are actually able to view the renormalized sum as the truncation of a series which, this time, does converge, which would make sense.

2000, <http://www.arthurjaffe.com/Assets/pdf/CQFT.pdf>, the following mathematical-physics Master's thesis of 2013, by Sheikh, <https://esc.fnwi.uva.nl/thesis/centraal/files/f1519507583.pdf>, and the following epistemological work by Li <http://jamesowenweatherall.com/wp-content/uploads/2015/10/irvine-draft.pdf>, which provides a rough diagram of the links between the different axiomatic and constructive QFT approaches existing in current literature. Rivasseau is one of the leading figures in these rigorous approaches to QFT, and his books are standards.

In a path-integral framework, axiomatic QFT is grounded on a spacetime-lattice formulation of QFT, the so-called *lattice gauge theories (LGTs)*. While, in a constructivist perspective, LGTs can, on the one hand, sometimes provide a way to derive the perturbative renormalization rules from the lattice situation, e.g., to express the perturbatively-grounded finite sums, and in particular the counterterms added to the regularized finite sums⁵, as functions of the quantities defined on the lattice, LGTs can, on the other hand, be used without explicitly referring to the resuming, through so-called non-perturbative methods, which are all based, in LGTs, on the *renormalization group*, which is a non-perturbative way of viewing the perturbative renormalization of the coupling constant according to typical energies involved in the interaction. The renormalization-group picture provides, in particular, a criterion for the predictive power of QFT, which, since non-perturbatively grounded, does not require the perturbative renormalizability of the theory, i.e. the possibility to resum the regularized sums, which would be too strong of a criterion; such a predictive, although non perturbatively-renormalizable theory is said to be *asymptotically safe*, see the following FAQs (frequently asked questions), <http://www.percacci.it/roberto/physics/as/faq.html>. Several other non-perturbative methods exist.

⁵Recall that these counterterms are added in order to make each of the terms of the sum, which is an integral, converge when the ultraviolet regulator goes to infinity.

Unitarity of time evolution in quantum mechanics and quantum field theory

O.1 Unitarity in standard lattice gauge theories

Unitarity is a priori not ensured by Wilson’s original lattice discretization [27]. Indeed, Wilson used the (Euclidean) path-integral quantization, which is directly mapped to the Lagrangian formalism through a Wick rotation. Within such a framework, proving unitarity essentially always demands to map this Lagrangian formalism to a Hamiltonian one¹. In the standard continuum-spacetime situation, methods are known to do this for relatively general Lagrangians, which essentially ensures unitarity in most practical situations². Hence, discretizing the Lagrangian, as originally done by Wilson, will a priori yield issues regarding unitarity, because then standard continuum-spacetime methods mapping this Lagrangian formalism to the Hamiltonian one have to be reconsidered.

Now, one month after Wilson’s original paper, Kogut and Susskind [259] developed a Hamiltonian formulation of lattice gauge theories, which uses the canonical formalism instead of the path-integral one. In this formulation, only the spatial lattice is discretized, i.e. time is kept continuous, and unitarity is ensured by defining an appropriate Hermitian Hamiltonian on the spatial lattice.

¹Regarding this matter, let me quote Weinberg, *The Quantum Theory of Fields I* [31], Chapter 9, 4th paragraph: “At this point the reader may be wondering why if the path-integral method is so convenient we bothered in Chapter 7 to introduce the canonical formalism. Indeed, Feynman seems at first to have thought of his path-integral approach as a substitute for the ordinary canonical formulation of quantum mechanics. There are two reasons for starting with the canonical formalism. The first is a point of principle: although the path-integral formalism provides us with manifestly Lorentz-invariant diagrammatic rules, it does not make clear why the S -matrix calculated in this way is unitary. As far as I know, the only way to show that the path-integral formalism yields a unitary S -matrix is to use it to reconstruct the canonical formalism, in which unitarity is obvious. There is a kind of conservation of trouble here; we can use the canonical approach, in which unitarity is obvious and Lorentz invariance obscure, or the path-integral approach, which is manifestly Lorentz-invariant but far from manifestly unitary. Since the path-integral approach is here derived from the canonical approach, we know that the two approaches yield the same S -matrix, so that the S -matrix must indeed be both Lorentz-invariant and unitary.”

²For example, in axiomatic, and thus rigorous formulations of QFTs, the time-evolution unitarity is ensured, starting from a Euclidean path-integral, by demanding that this Euclidean path-integral satisfy a property called *reflection positivity*, see <https://ncatlab.org/nlab/show/Osterwalder-Schrader+theorem>.

APPENDIX P

On topology

This appendix is aimed at giving some intuition of the elementary notions and tools used in this branch of mathematics that topology is. The style of the presentation is often informal.

P.1 Introduction

- A *space* is a *set* endowed with a *structure*. It is customary to distinguish between two main kinds of structures: *algebraic* and *analytic* structures.

- An algebraic structure is the given of one or several *binary operations*, which may be simply called *operations*, between *elements* of the set. A binary operation takes as input two *elements* of the set, and produces as output another element of the set. Examples of such operations are the addition or the multiplication. The algebraic structure tells us how the elements of the set are related between each other *in terms of equalities between these elements*. An algebraic structure is thus in particular able to generate, from a well-chosen starting subset, called a *generator set*, the original set, by producing all elements of the original set with inputs from the generator set¹.

- An analytic structure is the given of, again, one or several binary ‘operations’, but, this time, between *subsets* of the set (hence the quotation marks); these binary ‘operations’ are usually the *union* and the *intersection*. The analytic structure tells us how the elements of the set are related between each other *in terms of groupings of these elements*, through the notions of *neighborhood* and of *open set*. An analytic structure can thus not generate a set², but is aimed at analysing a preexisting set in terms of groupings of its elements. Endowing a set with an analytic structure is a first step to define, very generally, notions such as *connectedness*, *continuity* or *compactness*.

- On the one hand, examples of spaces endowed with an algebraic structure are *groups*, or *linear spaces*, also called *vector spaces*. A group is a set (i) left invariant, i.e. stable, under some binary operation between its elements, (ii) which contains a *neutral element*, and (iii) in which all elements have an *inverse*³. A vector space is, essentially, a set stable under linear combinations of its elements⁴.

¹A simple example of algebraic structure is \mathbb{N}^* endowed with the addition operation. The smallest generating set is $\{1\}$.

²It can however generate a set of subsets of this set, namely, the set of all possible groupings induced by the considered analytic structure.

³A simple example of (non-finite) group is \mathbb{Z} endowed with the addition operation. The smallest generating set is $\{1, -1\}$.

⁴A vector space is thus in particular a (non-finite) group with respect to the addition operation, and it has an additional homothety stability.

- On the other hand, *topological spaces* are a very general type of spaces endowed with an analytic structure.

P.2 Topological spaces and homeomorphisms

- A topological space can be defined as a couple (X, τ) of a set X and the following structure, which is of analytic kind: a collection of subsets τ satisfying the following axioms:

1. **axiom** ' \emptyset & X ': The empty set \emptyset and the total space X itself belong to τ .
2. **axiom** ' \cup & \cup_∞ ': Any *finite* or *infinite* union of members of τ belongs to τ .
3. **axiom** ' \cap ': Any *finite*⁵ intersection of members of τ belongs to τ .

The elements of τ are called *open sets* and the collection τ is called a *topology on X* ⁶. One may first look at elementary examples and non-examples on Wikipedia: https://en.wikipedia.org/wiki/Topological_space.

- A function $f : X \rightarrow Y$ is said *continuous* if:

$$\forall x \in X, \forall \text{ neighborhood } N \text{ of } f(x), \exists \text{ neighborhood } M \text{ of } x \text{ such that } f(M) \subseteq N. \quad (\text{P.1})$$

This definition generalizes that used in *real analysis*, where $f : \mathbb{R} \rightarrow \mathbb{R}$.

- A *homeomorphism* is a continuous bijection whose inverse is also continuous.

- Two topological spaces are said *homeomorphic* if they are related by a homeomorphism. Such two spaces are said to have the *same topology*, or to be *topologically equal*. Note that if the set X is endowed with nothing else than a topology, it can actually not be distinguished, *in terms of relations between its elements*⁷, from a homeomorphic partner, and both sets are strictly *equal up to a homeomorphism*.

P.3 Connectedness and homotopy equivalence

P.3.1 Connectedness and path-connectedness

- A space is said *connected* if it cannot be represented as the union of two or more disjoint non-empty open subsets.

⁵If we allow for infinite intersections, then we can exhibit examples where some elements of τ are *closed* from the metric point of view, while we want the present axioms to induce a definition of an open set, which eventually coincides with the metric definition of such objects, see the following discussion: <https://math.stackexchange.com/questions/284970/in-a-topological-space-why-the-intersection-only-has-to-be-finite>.

⁶There is an alternative way of defining a topological space, through the notion of neighborhood. This definition is formally more cumbersome, but the notion of neighborhood is very intuitive, and so is the notion of open set that ensues from it: a subset of some set is said open if it is a neighborhood of all the elements it contains. One may first consult Wikipedia on this subject: https://en.wikipedia.org/wiki/Topological_space.

⁷This precision can actually be omitted, since the nature of the elements regardless of any relations between these elements is actually not a mathematical question, unless this nature can itself be described by a mathematical sub-structure for each element of the set, which again will deal, by nature, with *relations between the sub-elements of which each element is made*.

- A *continuous path*, or simply *path* in X , is a continuous function $f : [0,1] \rightarrow X$. The terminology ‘path’ is sometimes used for $f([0,1])$ rather than f , since this matches with the intuition behind the word ‘path’. One should normally be able to determine, from the context, whether the word ‘path’ refers to f or to $f([0,1])$.

- A space X is said *path-connected* if any two points x and y in X can be connected by a continuous path, i.e. if:

$$\exists \text{ continuous } f : [0,1] \rightarrow X \text{ such that } \begin{cases} f(0) = x \\ f(1) = y \end{cases} . \quad (\text{P.2})$$

- For example, the Lorentz Lie group $O(1,3)$ is, as a manifold, disconnected, but has four path-connected components (which are subgroups): the proper (i.e. special) and orthochronous (denoted by $+$), $SO^+(1,3)$, the proper and non-orthochronous, the improper and orthochronous, and the improper and non-orthochronous.

P.3.2 Homotopy and homotopy equivalence

- In the definition of a homeomorphism, bijectivity is necessary for the topology of the *total* space to be preserved⁸. Relaxing (i) bijectivity while keeping (ii) continuity enables to track (i) *differences* between spaces which are (ii) strictly topological.

- Two continuous functions $f, g : X \rightarrow Y$ are said *homotopic* if:

$$\exists \text{ continuous } H : X \times [0,1] \rightarrow Y \text{ such that } x \in X \Rightarrow \begin{cases} H(x,0) = f(x) \\ H(x,1) = g(x) \end{cases} . \quad (\text{P.3})$$

H is called a *homotopy*, and the relation ‘ f homotopic to g ’ can be noted $f \sim g$.

- It is easy to prove that the relation of homotopy between paths *having fixed end points* is an *equivalence relation*, i.e. a relation which is *binary*, *reflexive*, *symmetric* and *transitive*⁹. It is called *relative homotopy equivalence*, where “relative” means ‘relative to chosen fixed end points’.

- A more general notion can be defined, which does not assume fixed end points, and is, this time, simply called *homotopy equivalence*: X and Y are said homotopically equivalent, or of the same homotopy type, if

$$\exists \text{ continuous } \begin{cases} f : X \rightarrow Y \\ g : Y \rightarrow X \end{cases} \text{ such that } \begin{cases} g \circ f \sim \text{Id}_X \\ f \circ g \sim \text{Id}_Y \end{cases} . \quad (\text{P.4})$$

Comparing this definition with that of a homeomorphism reveals the formal procedure to, e.g., relax bijectivity and ‘transform’ a homeomorphism into a the more general notion of homotopy equivalence.

⁸This is by definition of ‘topology preservation’, but this definition is obviously set to first match with (and then generalize) intuitive results.

⁹For a proof, see, e.g., <https://www.math.cornell.edu/~hatcher/AT/ATch1.pdf>, Proposition 1.2.

- In the following, we will be interested homotopy classes of paths, i.e. sets of paths which are all homotopic, since, from the topological point of view, two homotopic paths are not distinguishable. We will, in particular, be interested in a particular type of paths, that is, *closed paths*, also called *loops*, namely continuous functions of the form $f : S^1 \rightarrow X$. Also, we will consider homotopy classes of loops *having a common fixed point* – which is both the starting and the end point of the loop path – since this is necessary for a group structure to be defined, see below. A loop that is homotopic to a point is said *contractible*.

P.4 Fundamental group

P.4.1 Genus in one and two dimensions

- The most natural way of introducing the *fundamental group* of a topological space is, to me – as well as to many others – through the *genus* g of 1D or 2D real manifolds, which correspond, essentially, to the intuitive notion of curve and surface, respectively¹⁰. The genus is intuitively the numbers of *holes* of a manifold, or the number of *handles*.

- For a 1D (non-knotted) real manifold, the genus is the maximum number of cuttings without rendering the resultant manifold disconnected, i.e. non-path-connected.

- The circle, i.e. the 1D sphere, or 1-sphere, S^1 , has one hole, i.e. genus $g = 1$. Indeed, it can be cut at most once – at any of its points – without making it disconnected.

- For a 2D (non-knotted) orientable real manifold, the genus is the maximum number of cuttings along non-intersecting loops without rendering the resultant manifold disconnected^{11,12}.

- The standard, i.e. 2D sphere, or 2-sphere, S^2 , has no hole, i.e. genus $g = 0$. Indeed, it contains no loop along which one can cut it without making it disconnected. The standard, i.e. 2D torus, or 2-torus, T^2 , also called (empty¹³) donut, has one hole, i.e. genus $g = 1$. Indeed, consider the donut as a fiber bundle of fiber S^1 over the base S^1 . One can, without making it disconnected, cut it at most once along, e.g., either (i) any loop homotopic to the base, i.e. winding around the handle, which yields a cylinder¹⁴, or (ii) any loop homotopic to the fiber, i.e. winding around the hole, which yields a 2D annulus¹⁵, but not both – although the resulting manifold would still be connected (it would be a rectangle) – since loops of type (i) intersect those of type (ii).

¹⁰Don't forget however that these 1D or 2D real manifolds can be made of several disconnected components.

¹¹I have rewritten Wikipedia's definition, see [https://en.wikipedia.org/wiki/Genus_\(mathematics\)#Orientable_surface](https://en.wikipedia.org/wiki/Genus_(mathematics)#Orientable_surface).

¹²One can also define the genus of non-orientable 2D real manifolds, such as the Moebius strip or the Klein bottle, which are rather seen as less intuitive than orientable ones.

¹³We will omit this precision afterwards.

¹⁴Having as a base the *base* of the original donut fiber bundle.

¹⁵Which is actually, topologically, also a cylinder, but having as a base the *fiber* of the original donut fiber bundle.

• The genus g is related to χ and can thus also be defined through χ – the Euler characteristic χ . For an orientable surface, the relation reads

$$\begin{cases} \chi = 2 - 2g & \text{closed surface} \\ \chi = 2 - 2g - b & \text{surface with } b \text{ boundary components.} \end{cases} \quad (\text{P.5})$$

• Endowing these manifolds with more properties, such as, typically, differentiability or, even more, analyticity, may simplify the topological study. For example, the genus can be defined in a more computational manner for *algebraic curves*¹⁶ and *Riemman surfaces*¹⁷. If one can then show that the obtained results do not depend on these extra properties, i.e. that the latter have merely been used as tools but are not necessary assumptions, then one can extend the results to all homeomorphically equivalent spaces lacking those properties.

P.4.2 Homotopy classes of loops, fundamental group

• From the previous examples, the intuition that the reader may have of the mathematical notion of loop defined above may be that of a loop ‘that winds once’, be it around a hole (e.g. hole of a donut) or not (e.g. handle of the donut). Actually, as mathematically defined above, a loop can, in some cases, wind several times.

• Note that in dimension 1, if the loop f is, e.g., a loop winding twice around a circle, then $f([0,1])$ is necessarily strictly surjective, more precisely, we must ‘pass by’ *each* point of the circle twice, which does not prevent f from being continuous. In dimension 2, instead, it is possible to draw a closed curve $f([0,1])$ on the surface of the donut, that winds twice around the hole of the donut, but still with a bijective f . For loops that wind several times around the handle of the donut, f must be strictly surjective, but it can be – and is naturally – so only over a discrete set of points¹⁸.

• One can show that all loops that wind the same number of times around the same *topological barrier* – e.g., a hole, or a handle – belong to the same homotopy class, while this is not so otherwise. The homotopy class of loops that wind once say, clockwise, around some topological barrier, will be denoted by 1, that of loops winding twice anticlockwise will be denoted by -2 , etc.

• We denote by $\pi_1(X)$ the set of all homotopy classes of loops of the topological space X , relative to a given fixed point x_0 which is omitted from the notation. The subscript ‘1’ refers to the fact that the tools we are using to track the topology are loops, i.e. 1-dimensional closed manifolds.

• One can show that $\pi_1(X)$ has a *group structure* with respect to a certain composition operation between (homotopy classes of) loops, that we may call *loop product* (or *addition*). This operation corresponds to the more general *composition of paths*, also called *path*

¹⁶An algebraic curve is a set of points on the Euclidean plane whose coordinates are zeros of some polynomial in two variables.

¹⁷A Riemman surface is a *1D complex manifold*, i.e., essentially, a 2D real manifolds endowed with analyticity.

¹⁸In contrast with loops winding several times around the hole of a circle, for which f must be surjective over a *continuous interval*.

product, when applied to loops¹⁹. The path product enables to generate, from two paths belonging to two given classes, respectively, a new path belonging to another given class. The group $\pi_1(X)$ is called the fundamental group (FG) of X . The generators of this group are the (homotopy classes of) loops that wind only once around a given topological barrier, together with the respective inverses.

- The FG of the circle S^1 is isomorphic to \mathbb{Z} equipped with the addition operation, which we simply note $\pi_1(S^1) = \mathbb{Z}$, where the equality sign means ‘up to a group isomorphism’. The neutral element of $\pi_1(S^1)$ is the class of loops contractible into the fixed point, i.e. 0.

- The FG contains more information than the genus. A first example for this is that given above: the circle S^1 has genus 1, but its FG is $\pi_1(S^1) = \mathbb{Z}$ ²⁰. Another example is the donut T^2 , which also has genus 1, but whose FG is $\pi_1(T^2) = \mathbb{Z}^2$, which traces, in particular, the fact that the manifold is two-dimensional, through the power 2 in \mathbb{Z}^2 .

P.5 Simple connectedness, weaker and higher forms of connectedness, i.e., respectively, k -uple connectedness and n -connectedness

- A topological space X is said *simply connected* when its FG is trivial, i.e. equal to the neutral element, which we denote by $\pi_1(X) = 0$. For example, $\pi_1(S^N) = 0$ for $N \geq 2$. When the FG is not trivial, the space is not simply connected. The space is said *k -uply connected* if, roughly speaking, it has k holes, or equivalently, k handles.

- The FG does not contain all the topological information about a topological space. It only records, roughly speaking, information about the holes of a manifold, which are the coarser empty spaces around which, purposely vaguely speaking, the manifold ‘winds’ or ‘wraps’²¹.

- There are higher-order homotopy groups, which record information about the topology of the space at a more refined level. Let us give an intuitive picture of this. Consider the standard, i.e. 3D ball, or 3-sphere, also called 3D sphere, S^3 . One can pierce it entirely

¹⁹For a definition of the path product, see, e.g., <https://www.math.cornell.edu/~hatcher/AT/ATch1.pdf>, page 26.

²⁰I’m looking for an example in which a loop can only wind a finite number of times, i.e. in which it is not possible to find, as continuous path, a loop that winds more than a finite number of times.

²¹That being said, recall that the FG still records more than the number of holes, i.e. the genus, as we have seen above by comparing the FGs of two equal-genus but topologically different manifolds, namely the circle, with FG \mathbb{Z} , and the torus, with FG \mathbb{Z}^2 . The FG also records information about how the simply-connected sub-components glue together, i.e., in particular, information about the edges of the manifold, or its orientability – although not always, e.g. the Moebius strip, which is a non-orientable surface, has the same FG as the 2D annulus and the circle. The FG can record information about the structure group of a fiber bundle. For instance, consider the donut and the Klein bottle, which are two fiber bundles of S^1 over S^1 , but with different structure groups: the torus has a trivial structure group, i.e. reduced to a neutral element, while the Klein bottle has the structure group \mathbb{Z}^2 acting by reflection on $S^1 \subset \mathbb{R}^2$, see <https://books.google.fr/books?id=wuULBQAAQBAJ&pg=PA111&lpg=PA111&dq=klein+bottle+fiber+bundle+structure+group&source=bl&ots=LFjgy11NKm&sig=T60iDmPFUmjDUADczRVvTBqkhaM&hl=fr&sa=X&ved=0ahUKEwiUnvyotbfVAhUjK8AKHTO-Dv4Q6AEISjAD#v=onepage&q=klein%20bottle%20fiber%20bundle%20structure%20group&f=false>. Well, the FG of the Klein bottle is different from that of the donut.

with a cylinder, which creates a hole and makes it become, topologically, a full donut, $D^2 \times S^1$, where D^2 is the standard disk. But one can also imagine that the ball has some empty space inside, as if some nucleus was absent; such a space is called a 3D annulus, let us denote it by A^3 . Now, loops are not able to track this empty space, that is: from the point of view of loops, A^3 is trivial, since any loop inside it is contractible, i.e. $\pi_1(A^3) = 0$, i.e. A^3 is simply connected (with respect to loops²²). But one intuitively feels that A^3 is not homeomorphic to S^3 . Indeed, A^3 is not trivial if we track its topology with 2-spheres. From the point of view of such spheres, A^3 is doubly connected, i.e. it has one ‘spherical hole’: a sphere that wraps around the ‘spherical hole’ is not contractible. Moreover, one can show (annulus theorem) that A^3 is homeomorphic to $S^2 \times [0,1]$, so that its homotopy group with respect to spheres, that we note $\pi_2(A^3)$, satisfies $\pi_2(A^3) = \pi_2(S^2) = \mathbb{Z}$.

• More generally, the set $\pi_n(X)$ of all homotopy classes of continuous tracking functions of the form $f : S^n \rightarrow X$ (with common fixed point omitted from the notation), has a group structure with respect to the composition of n -spheres, and is called n -th homotopy group of X . The space X is said *n-connected* if its homotopy groups are all trivial up to order n ²³, i.e.

$$\forall j \in \llbracket 1, n \rrbracket, \pi_j(X) = 0. \quad (\text{P.6})$$

P.6 Examples: $SU(N)$, and $SO(N)$ and its *universal cover*, $Spin(N)$.

- The group $SU(N)$ is simply connected for all N , i.e. it has no hole.
- $SO(N)$ has a *double cover* called the spin group $Spin(N)$.
- $N = 1$: $SO(1) = 1$, and $Spin(1) = \{-1, 1\} = O(1) = \{\text{reflexion, identity}\}$, which is not connected.
- $N = 2$: $Spin(2) = U(1)$, which is homeomorphic to both $SO(2)$ itself and S^1 , i.e. the circle, and is thus manifestly (i.e. through its homeomorphism to S^1) connected, but doubly, and not simply, i.e. it has exactly one hole.
- $N \geq 3$:
 - ★ $SO(N)$ is doubly connected.
 - ★ Its double cover $Spin(N)$ is simply connected and thus coincides, by definition, with the universal covering group of $SO(N)$.

An extensive list of examples of homotopy groups useful in physics is available at <http://felix.physics.sunysb.edu/~abanov/Teaching/Spring2009/Notes/abanov-cpA1-upload.pdf>.

²²This precision is always omitted in the standard terminology.

²³*n*-connectedness must not be confused with *k*-uple connectedness, defined above, *k* being essentially the number of holes of the space. In particular, the first notion is stronger than simple connectedness, while the second is weaker.

P.7 Compactness

- Compactness is a notion that can be defined given an arbitrary topological space, that generalizes the notion of a subset of Euclidean space being both *closed* (that is, containing all its limit points) and *bounded* (that is, having all its points lie within some fixed distance of each other).

- A topological space X is said *compact* if each of its open covers has a finite subcover. That is, X is compact if for every collection C of open subsets of X such that

$$X = \bigcup_{x \in C} x, \quad (\text{P.7})$$

there is a finite subset F of C such that

$$X = \bigcup_{x \in F} x. \quad (\text{P.8})$$

- The fact that we are here indeed dealing with a generalization of the notion of close and bounded subset of an Euclidean space is indicated by two fact: first, this notion can be defined in non-metric spaces; second, the Borel-Lebesgue theorem states that any closed and bounded subset of \mathbb{R} is compact²⁴.

²⁴The theorem is the proof of the former implying the latter. The latter implying the former is straightforward to prove.

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