Aix*Marseille université
Socialement engagée

NNT/NL : 2022AIXM0281/014ED184

THÈSE DE DOCTORAT

Soutenue à Aix-Marseille Université
le 5 septembre 2022 par

Nathanaël EON

Gauge invariance in classical and quantum cellular automata

Invariance de jauge dans les automates cellulaires classiques et quantiques

Discipline
Informatique

École doctorale
ED 184 MATHÉMATIQUES ET INFORMATIQUE

Laboratoire/Partenaires de recherche
Laboratoire d'Informatique & Systèmes

Composition du jury

Mari Carmen Bañuls Max Planck Institute for Quantum Optics	Rapporteure	Sylvain Sené Aix-Marseille Université	Président du jury
Armando Pérez Universitat de València	Rapporteur	Pablo Arnault Inria Saclay	Examinateur
Pablo Arrighi Université Paris-Saclay	Directeur de thèse	Omar Fawzi École Normale Supérieure de Lyon	Examinateur
Giuseppe Di Molfetta Aix-Marseille Université	Codirecteur de thèse	Irène Marcovici Université de Lorraine	Examinatrice

Invités

Paolo Perinotti
Università di Pavia

Guillaume Theyssier
Aix-Marseille Université

LIS LABORATOIRE D'INFORMATIQUE & SYSTÈMES

Affidavit

I, undersigned Nathanaël Dominique Eon, hereby declare that the work presented in this manuscript is my own, carried out under the scientific direction of Pablo Arrighi and Giuseppe Di Molfetta, in accordance with the principles of honesty, integrity and responsibility inherent to the research mission. The research work and the writing of this manuscript have been carried out in compliance with both the french national charter for Research Integrity and the Aix-Marseille University charter on the fight against plagiarism.

This work has not been submitted previously either in this country or in another country in the same or in a similar version to any other examination body.

Marseille, the 15th of May 2022

Publications and Conferences

List of publications realized as part of the PhD thesis :

The results in Chapter 1 have led to four publications. The authors names are ordered alphabetically.

- Pablo ARRIGHI, Giuseppe DI MOLFETTA et Nathanaël EON. « A gauge invariant reversible cellular automaton ». In : *International Workshop on Cellular Automata and Discrete Complex Systems*. Springer. 2018, p. 1-12
- Pablo ARRIGHI, Giuseppe DI MOLFETTA et Nathanaël EON. « Non-abelian gauge-invariant cellular automata ». In : *International Conference on Theory and Practice of Natural Computing*. Springer. 2019, p. 211-221
- Pablo ARRIGHI, Marin COSTES et Nathanaël EON. « Universal gauge-invariant cellular automata ». In : *MFCS*. T. 202. 2021, 9 :1-9 :14
- Pablo ARRIGHI, Giuseppe Di MOLFETTA et Nathanael EON. « Gauge invariance in cellular automata ». In : *Natural Computing* (2022), p. 1-13

The content of Chapter 2 has been submitted for publication under the title "*A relativistic discrete spacetime formulation of 3+1 QED*", it is available on arXiv under the reference number 2205.03148, and is a joined work with Giuseppe DI MOLFETTA, Giuseppe MAGNIFICO and Pablo ARRIGHI.

Publication realized during thesis and not part of the manuscript :

- Quentin ARISTOTE, Nathanael EON et Giuseppe Di MOLFETTA. « Dynamical triangulation induced by quantum walk ». In : *Symmetry* 12 (2020), p. 128

Participation to conferences and summer schools throughout the duration of the thesis :

1. 8th International Conference on the Theory and Practice of Natural Computing, TPNC 2019, Kingston, Canada.
2. École de Jeunes Chercheurs en Informatique Mathématique, EJCIM 2020, visioconference.
3. École de Printemps d'Informatique Théorique sur l'Informatique Quantique EPIT 2021, visioconference.
4. Quantum Information and Quantum Technology, QIQT 2021, Cargèse, France.

Résumé

L'invariance de jauge est un concept fondamental en physique, servant de fondement mathématique à la dérivation des interactions fondamentales. Dans cette thèse, la notion d'invariance de jauge est formalisée dans le cadre des automates cellulaires (AC).

Cette formalisation offre un chemin simple et direct vers les concepts essentiels de la symétrie de jauge. Usuellement, une symétrie de jauge est tout d'abord motivée par l'existence d'une symétrie globale. La théorie est ensuite étendue de sorte que cette symétrie devienne locale. Les AC permettent de formaliser ce processus d'extension de jauge. Nous montrons dans cette thèse l'équivalence entre l'existence d'une symétrie globale et l'existence d'une extension de jauge dite "relative". L'universalité des AC invariants de jauge est ensuite démontrée de deux façons indépendantes : premièrement via une équivalence avec les AC globalement symétriques, qui sont eux-mêmes universels, et deuxièmement via une approche entièrement constructive.

Dans le cadre des automates cellulaires quantiques, nous utilisons ici l'invariance de jauge pour parvenir à une formulation en espace-temps discret de l'électrodynamique quantique (EDQ) en trois dimensions d'espace. Elle prend la forme d'un circuit quantique, se répétant à l'infini dans l'espace et le temps, paramétré par un pas de discrétisation relativiste $\Delta_t = \Delta_x$. La stricte causalité de cette théorie est assurée de façon manifeste, puisque les fils du circuit coïncident exactement avec le cône de lumière, ce qui d'un point de vue pratique permet aussi d'optimiser la durée de la simulation en présence de décohérence. De fait, cette construction suit la logique qui amène à la définition du Lagrangien pour l'EDQ. C'est-à-dire qu'elle démarre par une marche quantique de Dirac, dont la convergence vers des fermions relativistes libres est connue. Puis cette marche est étendue au cas multi-particules à travers un automate cellulaire quantique de telle sorte que les relations d'anti-commutation des fermions et l'invariance de jauge discrète soient respectées. Pour implémenter ces contraintes, il est nécessaire d'introduire un champ de jauge. Finalement, une dynamique électromagnétique est donnée au champ de jauge. Celle-ci peut être vue comme une marche quantique sur chaque plaquette.

Mots clés : systèmes dynamiques, automate cellulaire, invariance de jauge, électrodynamique quantique, simulation quantique

Abstract

Gauge invariance is a fundamental concept in Physics, known to provide mathematical justification for the fundamental forces. In this thesis, gauge invariance is brought to the realm of classical and quantum cellular automata (CA).

In a classical setting, it provides a simple yet rigorous route straight to the core concepts of gauge theories. Usually, gauge theories are built from a theory featuring a global symmetry, which is then extended to make the symmetry a local one (a.k.a. gauge-invariant). CA allows for this gauge extension process to be made formal. We show the equivalence between the pre-existence of a global symmetry and the ability to perform a "relative" gauge extension. Moreover, gauge invariant cellular automata are shown to be universal, through two independent proofs: first through the equivalence with globally symmetric CA which are themselves universal, and second through an entirely constructive approach.

In the framework of quantum cellular automata (QCA), we use gauge invariance to construct a discrete spacetime formulation of $3+1$ quantum electrodynamics (QED). It takes the form of a quantum circuit, infinitely repeating across space and time, parameterized by the relativistic discretization step $\Delta_t = \Delta_x$. Strict causality is manifest as circuit wires coincide with the lightlike worldlines of QED; it follows that simulation time under decoherence is optimized. The construction replays the logic that leads to the QED Lagrangian. Namely, it starts from the Dirac quantum walk, well-known to converge towards free relativistic fermions. It then extends the quantum walk into a multi-particle sector quantum cellular automata in a way which respects the fermionic anti-commutation relations and the discrete gauge invariance symmetry. Both requirements can only be achieved at cost of introducing the gauge field. Lastly the gauge field is given its own electromagnetic dynamics, which can be formulated as a quantum walk at each plaquette.

Keywords: dynamical systems, cellular automata, gauge invariance, quantum electrodynamics, quantum simulation

Acknowledgements

My gratitude goes first to my supervisors, professors Pablo Arrighi and Giuseppe Di Molfetta, who were always there to guide me and never failed their role. I also thank the CaNa team for the invigorating research environment and support. Many insightful discussions allowed a computer scientist as myself to delve into the realm of gauge theories, for this my thanks goes to Dr. Pablo Arnault, Prof. Terry Farrelly, Prof. Simone Montangero and Kevissen Sellapillay. I am also very grateful to my collaborators for our joint work: Marin Costes, Dr. Giuseppe Magnifico and Quentin Aristote.

Le soutien de mes amis durant cette thèse est inqualifiable, un immense merci à Anahita, Cyril, Nell, Ines, Shady, Shayan, Carmel, Adrien, Khalil, Killian et Alexandre ainsi qu'à toute la communauté bahá'íe de Marseille. Je remercie aussi les doctorants de Luminy, et en particulier François Hamonic, pour les nombreuses discussions, scientifiques ou non, qui ont animé et éclairé ces trois dernières années.

J'aimerai enfin remercier mes sœurs et leurs époux Alexandra et Boris Fischer, Marie et Brett Emmons, Johanna et Pierre De Rochefort, ainsi que mes parents Cécile et Jean-Pierre Eon, pour leur soutien et amour constant et indéfectible.

Contents

List of Figures

"How resplendent the luminaries of knowledge that shine in an atom, and how vast the oceans of wisdom that surge within a drop!"

— Bahá'u'lláh

Introduction

Overview

This thesis may be seen as Physics from a Computer Scientist point of view. Yet, a Physicist would probably point out that this remains a Computer Science manuscript. I hope that both would be right. The results presented here aim at lying at the interface between both disciplines, using vocabulary, concepts and theories from each side, with the prospect that genuine cross-disciplinarity will be of benefit both Computer Science (CS) and Physics.

On the one hand, Physics provides CS with novel ideas, symmetries and experiences which help discover new paradigms. Quantum information and computation is a clear example of that. On a different scale perhaps, my hope is that gauge invariance, which is a fundamental symmetry, will eventually yield interesting results and new paradigms when brought to Computer Science. In short, Physics contributes to Computer Science.

On the other hand, Computer Science provides a playground for the simulation of physical systems, which allows for a better understanding of the underlying laws of nature as well as drawing predictions from them. There are countless examples of this, from particle physics to astronomy, where simulations were used to predict or confirm experiments. Cellular automata could be considered as a sandbox in this playground, ideal for the simulation of problems that can be cast in discrete space and time. Additionally, Computer Science can also bring about a different viewpoint or pedagogical approach to the study of some problems. In short, Computer Science contributes to Physics.

Gauge invariance...

The aspect of Physics under study here are gauge symmetries. Let us introduce them in a more general context. Modern physics accounts for four fundamental interactions, namely the electromagnetic, weak, strong and gravitational interactions. Gauge symmetry provides mathematical justification for these interactions. It requires of the theory to be invariant under the action of a group of local operators, the keyword here being "local". Gauge theories can be defined in both the classical (e.g. for the gravitational force) and quantum setting. The latter can be found in quantum field theories (QFT) such as the Standard Model—a model for the electromagnetic, weak and strong interactions [7].

In the current state of the art, there are usually two ways to simulate gauge theories (i.e. theories respecting gauge invariance) [8]: (i) using analog simulation, whereby

a physical system mimics another, or, (ii) through digital simulation, whereby the evolution of a system is recast as a circuit. In the former, time is continuous and there is a direct relation between the simulated time (inside the simulation) and the duration of the simulation (outside the simulation). In the latter however, the evolution is a circuit, defined through a finite (or countable) number of gates. It thus introduces a time discretization step. The focus here will be put on the latter.

...in cellular automata

Cellular automata is a classical, discrete space, discrete time, intrinsically local evolution model. It constitutes a well established model of computation in euclidean space. This thesis will only consider a tiny portion of the vast research field of cellular automata. The curious reader is recommended one of the many comprehensive reviews [9, 10, 11]. Starting from a space configuration, that is to say the association of a state (a.k.a. symbol) in a set Σ to each position in space, it provides a dynamics through a local circuit applied at every position simultaneously. Locality ensures a form causality—that is to say no information travels faster than the speed of light—because the information speed is bound by the circuit speed. Moreover, cellular automata allow for a complex dynamics to emerge from a local (simple) evolution rule. Such an emergence is reminiscent of the way a complex physical phenomenon can be described using a small number of laws. Locality, discrete space and time, and the emerging complexity of the dynamics makes of cellular automata an ideal playground for the study of discrete gauge theories, and for their digital simulation. Cellular automata have a quantum counterpart, namely quantum cellular automata (QCA) [12, 13] which will also allow for the simulation of discrete quantum gauge theories.

The work presented here focuses on the definition of gauge invariance in cellular automata, the study of its properties in a classical setting, and, its use in quantum settings to simulate quantum electrodynamics (QED).

Scope and aims

Bringing gauge invariance to cellular automata offers many perspectives. In a classical setting, it contributes to the wealth of symmetries and properties studied for cellular automata, with the potential to further categorize, understand and use this computation model in a different context.

In a quantum setting, it provides a new way to define and digitally simulate gauge theories. This is particularly interesting when considering quantum cellular automata for the digital simulation of quantum field theories such as QED and quantum chromodynamics, two parts of the Standard Model.

Gauge invariance in cellular automata, classical setting.

Cellular automata is a computation model first introduce more than half a century ago, from the work of Von Neumann [14]. This model is fascinating in that from a simple definition and construction, it allows complex dynamics and properties to emerge, and, it retains the essential aspects of the phenomenon that is implemented. Hence, it provides a natural framework for the study of natural and social phenomena. There are countless examples of this, such as a model for freeway traffic [15], snow avalanche [16], or even hydrodynamics [17].

Symmetries and properties in cellular automata. Cellular automata are inherently homogeneous in that it applies the same local revolution rule everywhere. Considering this as a computation model, it means that it is intrinsically parallel. Algorithms were developed to tap into this potential [18, 19]. Global properties and symmetries, often rooted in physics and mathematics, have also been defined and studied in cellular automata, allowing for the model to be used in different contexts. For example, concepts such as energy, potential, flow and conservation laws [20, 21] have counterparts in cellular automata. So do other essential properties in physics such as reversibility [22, 23] and time-symmetry [24].

Global symmetry: color-blindness. Among these properties and symmetries, the one closest to gauge-invariance is G–blindness (or color-blindness). In [25] the authors study G–blind cellular automata, where G is a group of permutation acting on the space configuration. G–blind cellular automata are globally symmetric under G, i.e. the global evolution commutes with the application of the same $g \in G$ at once at every position. They showed the surprising result that any CA can be simulated by such a globally symmetric one, when G is the symbol permutations. Globally symmetric CA are therefore universal [26, 27]: any CA can be simulated by a globally symmetric one.

Local symmetry: Gauge invariance. The first objective here will be to define gauge invariance in cellular automata. Gauge invariance is similar to G-blindness in that it asks the evolution to commute with a set of transformations. However, in the case of gauge invariance the transformations are local: a different g^x can now be chosen for every position x. These transformations are called gauge transformations. Due to the locality, requiring gauge invariance is stronger than G-blindness. For some sets G such as the symbol permutation, it even seems impossible to enforce gauge invariance for nontrivial dynamics: intuitively, all information about the configuration would be lost in the gauge transformation.

In Physics, the way to do this is to introduce a gauge field, that is to say extend Σ so that more information can be encoded, either at the nodes (cells) or at the links between positions. The action of a gauge transformation, and the dependence of the evolution under the gauge field, are then chosen so that the evolution be gauge invariant. Asking of a cellular automaton to be extensible into a gauge invariant one is thus weaker than straight out gauge invariance. This raises a question, because it is unclear whether the existence of such a gauge extension should be stronger or weaker than G-blindness. An equivalence between G-blindness and the existence of a specific type of gauge extension is shown in this manuscript.

Universality and equivalence. Since G-blind CA are shown to be universal in one spatial dimension, and, G-blind is equivalent to the existence of a "relative" gauge extension into a gauge invariant CA: gauge invariant CA also are universal in one dimension. We give another proof of the universality, without restriction on spatial dimensions, using *absolute* gauge extensions. The term absolute refers to a gauge field being positioned on the lattice sites: the gauge field at position x is used to keep track of the gauge transformations applied at x, which allows the evolution to effectively cancel them, and thereby effectively ensure gauge invariance. Another concept, close to that of universality, is the idea of equivalence. A new symmetry introduces a new way to compare cellular automata: two distinct cellular automata may be equivalent up to gauge symmetry. In Physics this redundancy is well known, and the choice of a specific dynamics is called gauge fixing. These concepts of equivalence and gauge fixing are formalized, and a preliminary study is conducted here.

Discrete formulation of 3+1 quantum electrodynamics.

Digital simulation of quantum phenomena [28], if done classically, scales exponentially with the size of the system simulated. Hence, in order to scale in size, the use of quantum mechanics itself is necessary. It may be used for instance in order to find ground state of Hamiltonians that hold the key to certain molecular structures or condensed matter properties [29]. In the longer term, however, it may even be used to simulate the dynamics of these from first principles, based on their constituent fundamental particles' dynamics. This has motivated a strand of works on the quantum simulation of quantum field theories (QFT) [30, 31, 8]. All of them rely on a prior spatial discretization, but some are based on a spacetime discretization, allowing for a natively discrete account of both relativistic and gauge symmetries. The second objective of this thesis is to provide a quantum simulation scheme based on a discrete spacetime formulation of $3+1$–quantum electrodynamics (QED) using quantum cellular automata (QCA).

Lattice QFT. Some QFT have well-established discrete counterparts. Lattice gauge theories appear for instance in condensed matter with applications to quantum error correction theory (e.g. Kitaev's toric code [32, 33]). In particle physics, the quantum simulation of non-Abelian lattice gauge theories, such as chromodynamics, has been extensively studied [34, 35]. Lattice quantum chromodynamics [36] has been used in order to obtain numerical values, to then be compared against experimental values from particle accelerators. This procedure is paradigmatic of the way new physics is discovered, making simulation take a central role. However, these techniques are computationally heavy. Finding a way to simulate lattice QFT efficiently and accurately, using a non-perturbative approach, through a quantum device would be a game changer.

Continuous-time, analog simulation of QFT. The standard ways to quantum simulate QFT begin asymmetrically by discretizing space but not time, by means of a Kogut-Susskind Hamiltonian [37, 38]. Next the matter (fermions) and the gauge field (bosons) degrees of freedom are encoded as quantum systems on the simulating de-

vice, whose interactions will mimic those of the Hamiltonian. These interactions are sometimes implemented as discrete-time unitaries, but even then these are short-time approximations of the Hamiltonian, as obtained by the Trotter formula under the *non-relativistic* $\Delta_t \ll \Delta_x$ discretization. This approach was recently realized experimentally on different architectures, for instance using an ion trap architecture [39], or using Rydberg arrays [40]. Recent, classical but quantum-inspired tensor networks techniques, come to complement this standard approach [41, 42, 43]. These use compact, approximate description of quantum states [44] such as the multiscale entanglement renormalization ansatz (MERA) [45, 46], discarding hopefully unwanted information about the states as they evolve such that the description keeps a manageable size, whilst attempting to keep track of interesting ingredients, including entanglement. The tensor network approach, however, mainly focuses on finding low energy states and will inevitably hit a scalability and precision barrier when dealing with many-body states and their dynamics.

Relativistic, digital simulation of QFT. In order to quantum simulate QFT in a *relativistic* manner, we must place space and time on an equal footing, discretizing both simultaneously, with parameter $\Delta_t = \Delta_x$. *Relativistic* in this context means that space and time are considered on an equal basis. This leads to an infinitely repeating quantum circuit, across space and time, namely a quantum cellular automata (QCA). The speed of light in the simulated QFT, will then strictly correspond with the 'circuit speed', i.e. the maximal speed allowed by the wires. This contrasts with the earlier mentioned analog simulation paradigm, where the $\Delta_t \ll \Delta_x$ assumption yields a non-strict and much lower speed of light for the simulated QFT, which matches, when things go well, the Lieb-Robinson bound [47]—a fragile process however [48, 49]. Figure 1 illustrates the circuit and light speed under both simulation paradigms. From a theoretical standpoint, *relativistic*, digital quantum simulation is therefore advantageous: (i) strict causality is ensured as the circuit wires match the lightlike worldlines of the simulated QFT ; (ii) space and time are treated on an equal footing as demanded by special relativity. Those theoretical advantages are expected to transpose in practice, where a simulation device that suffers from a given typical decoherence time τ, could simulate the QFT over a period of logical time of the order of τ as well. Experimental implementation of QCA have already been realized in practice and show promising results [50, 51].

A natively discrete approach to QFT. In the continuous, relativistic settings, the standard way to express a QFT is by means of a Lagrangian, i.e. a 'local cost function', which integrated over a possible history provides the action, which is to be minimized. The use of a particular Lagrangian is justified by means of special relativity and gauge symmetries. Our aim is instead to express the QFT directly as a family of infinitely repeating circuits of local quantum gates, parameterized by the time step. In order to justify the use of a particular QCA we must then, just like in the Lagrangian approach, begin with a quantum walk (QW) accounting for free fermions and then extend it to the multi-particle sector QCA by imposing the fermionic anti-commutation relations as well as discrete gauge invariance, thereby deducing the need for a gauge field. We can then 'turn on' the interaction by providing the gauge field with a simple dynamics.

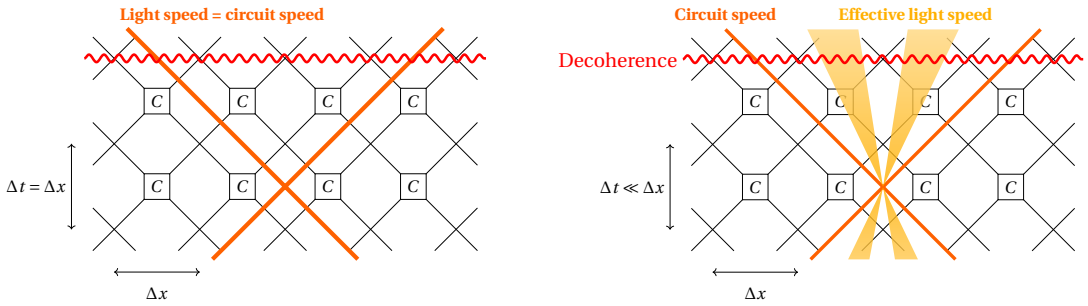


Figure 1.: (a) In *relativistic*, digital quantum simulation, the light-like worldlines of the simulated theory coincides with circuit wires, yielding strict causality. (b) In *non-relativistic*, Trotterized analog quantum simulation, light-like worldlines are approximately recovered through a Lieb-Robinson bound, and are slower. Thus, the simulation is running slower. As typical decoherence times match the depth of the circuit, the QFT is simulated over a shorter period.

That is, we must transpose the logics of construction that leads to a particular QFT in the Lagrangian approach, to a natively discrete setting, whose discretization parameter can then be made arbitrary small. This ought to provide a rigorous, natively discrete formulation of QFT.

Two essential advantages of this approach stand out when using it for quantum simulation of QED. First it is non-perturbative, allowing for the QFT to be simulated without restriction on the interaction between fields. Second, it offers up to an exponential a gain in complexity compared to classical methods. Indeed, simulating a space of size s with Δ_x space resolution over d dimensions classically would demand to have an exponential space $O(e^{s^d/\Delta_x^d})$ since it grows exponentially with the number of quantum systems to be simulated. Whereas it can be simulated on a quantum device in $O(s^d/\Delta_x^d)$.

Closest work. $1+1$ QED, also known as the Schwinger model [52], has been recovered under the *relativistic*, digital quantum simulation paradigm, by discretizing through $\Delta_t = \Delta_x$ and following gauge theoretical justifications in [53]. Next, this was generalized by [54, 55, 56] in order to allow for arbitrary $\Delta_t \leq \Delta_x$, so that both the continuous spacetime limits (which exists when the interaction is turned off) and the continuous time discrete space limits (which always exists) may be taken, the latter coinciding with the Kogut-Susskind Hamiltonian.

From one to three spatial dimensions. Going to higher dimensions poses three main difficulties, and a possible solution for each is given in this thesis. First, the implementation of the fermionic anti-commutation relation, e.g. through a Jordan-Wigner transformation, seems to break locality. Indeed, the phase added when two fermions (possibly very far apart) exchange positions, without one ever crossing the other, seems to be fundamentally global. However, with the help of the gauge field, this fermionic exchange phase can be fully implemented locally.

Second, in one spatial dimension there is no magnetic contribution to the evolution, only the fermionic dynamics and an electric contribution. However, going to higher dimension, a magnetic term (which corresponds to a gauge field dynamics) has to be defined.

Third, a difference in the fermionic internal degrees of freedom appears between two and three spatial dimensions. In one and two dimensions, the Dirac equation which defines the fermionic evolution, is a PDE on a wave function having two complex amplitudes at each position, corresponding to the internal degrees of freedom for the fermion. In three spatial dimensions, the Dirac equation is defined on a wave function having four complex amplitudes at each position. This has to be taken into account in the QCA formulation of 3+1 QED.

Outline

The first task we set to achieve is the definition of gauge invariance in cellular automata and the study of its properties. This is done throughout chapter 1.

- Section 1.1 defines cellular automata and its extension with a gauge field.
- Section 1.2 defines gauge invariance as a commutation relation between the cellular automata and a group of local (gauge) transformations.
- Section 1.3 shows that gauge invariant cellular automata are intrinsically universal and their connection to G–blindness.
- Section 1.4 defines the notion of equivalence in cellular automata and of gauge fixing to choose a specific dynamics amongst the equivalent ones.

The second task we set to achieve is the formulation of 3+1 QED in the context of QCA. This is done throughout chapter 2.

- Section 2.1 tackles the issue of anti-commutation while staying local. It also introduces gauge invariance in the specific context of QED.
- Section 2.2 presents a version of QED in two spatial dimensions, with a formulation of the free fermionic dynamics, to which are added the electric and magnetic terms.
- Section 2.3 extends the previous version to three dimensions, increasing the number of qubits per site from two to four.

These last two sections make use of appendix A which details the path from one particle QW to non-interacting QCA.

Finally, chapter 3 presents the conclusion of this thesis and how the results it presents may serve as starting point of further research.

Some work, done during the thesis, is not included in this manuscript. It deals with quantum walks that deform geometry in a semi-classical fashion, see [6].

1. Cellular automata and gauge invariance

Cellular automata and gauge invariance are two disjoint fields of study, our first goal is to define them in a unified framework. A cellular automaton is an evolution rule acting on space configurations. Gauge symmetry is the invariance of the evolution (here the cellular automaton) under a group of local transformations called gauge transformations. Hence, gauge invariance can be informally defined as a commutation relation between the cellular automaton and the group of gauge transformations. Section 1.1 formally defines cellular automata and how to extend them to add a gauge field. Section 1.2 formally defines gauge invariance in cellular automata and the way the extension can be used to ensure gauge invariance.

From a Physics perspective one usually motivates the demand for a certain gauge symmetry, from an already existing global symmetry. From a mathematical perspective, the gauge field that then gets introduced for such purpose is often seen as a connection between two gauge choices at neighboring points. This raises questions however, because there is no immediate reason why a gauge symmetry should necessarily arise from an already existing global symmetry (one could ask for a certain ad hoc gauge symmetry from scratch). Nor is there an immediate reason why a gauge field should necessarily be interpretable as a connection (a gauge field could be made to hold absolute instead of relative information about gauge choices). In subsection 1.3.1, we prove an original result relating these two folklore perspectives on gauge theories using purely combinatorial definitions. Namely, we prove that the CA that admit *relative* gauge extension are exactly those that have the corresponding global symmetry in the first place. The term relative refers to a specific type of gauge extension for which the gauge field is positioned on the links, i.e. it is interpretable as a connection. This result coupled with the universality of globally symmetric CA in one spatial dimension ensures the universality of one dimensional gauge invariant CA, proven in subsection 1.3.1. This universality result is then shown for any dimension in subsection 1.3.3 using *absolute* gauge extension, where absolute refers to the positioning of the gauge field on the sites instead of the links.

Gauge invariance, as any symmetry, introduces some degree of freedom. Two symmetric cellular automata, that is to say two cellular automata that have the same dynamics up to gauge transformations, are in a sense equivalent. This is made formal in section 1.4.

In this chapter, everything is set up in the classical setting, hence it should be accessible to anyone with a small background in computer science.

EXAMPLE: ILLLUSTRATION OF CORE CONCEPTS

Throughout this chapter, this box will provide illustration of the core concepts. It can be safely skipped.

1.1. Cellular automata

Notations. Here is a list of notations that will be used when considering cellular automata:

- $\mathbb{Z}^d$: underlying structure of space with dimension d,
- Π: the directions of space—a.k.a. the ports to the edges for a given position,
- $\mathcal{N} \subset \mathbb{Z}^d$: neighborhood,
- Σ, Δ: alphabets,
- $\mathscr{C}$: set of all configurations,
- c_x for $c \in \mathscr{C}$ and $x \in \mathbb{Z}^d$: shorthand for $c(x)$,
- $c_{x;\eta}$ for $c \in \mathscr{C}$, $x \in \mathbb{Z}^d$ and $\eta \in \Pi$: shorthand for $c(x:\eta)$,
- $c_{t,x}$ for $c \in \mathscr{C}$, $t \in \mathbb{N}$ and $x \in \mathbb{Z}^d$: shorthand for $\left(F^t(c)\right)_x$, where F is the CA considered,
- c_I for $c \in \mathscr{C}$ and $I \subset \mathbb{Z}^d$: shorthand for $c : I \longrightarrow \Sigma$ the configuration restricted to a set I of specific positions,

A cellular automaton (CA) is a dynamical system which operates on a discrete, uniform space and evolves in discrete time steps through the application—homogeneously across space—of a local operator. Let us make this formal.

1.1.1. Space and alphabet

The discrete, uniform space is the grid $\mathbb{Z}^d$ with d the spatial dimension. CA can be defined on more general spaces by replacing the grid by bounded degree graphs, typically Cayley graphs [57], however this is out of the scope of this manuscript.

The *alphabet* (a.k.a. state space) Σ is a countable—often finite—set. Each position in space is associated to a letter of this alphabet. This association is called a configuration.

Definition 1 (Classical configuration)**.** *A* classical configuration *c over an alphabet* Σ *is a function that associates a state to each point in* $\mathbb{Z}^d$*:*

$$c : \mathbb{Z}^d \longrightarrow \Sigma. \tag{1.1}$$

The set of all configurations will be denoted $\mathscr{C}$ *and for* $\mathcal{N} \subset \mathbb{Z}^d$ *a finite neighborhood,* $\mathscr{C}_{\mathcal{N}}$ *is the set of finite configurations restricted to the subspace* $\mathcal{N}$*.*

A configuration should be seen as a picture of the system at a given time. The following shorthand notation will be used: c_I for the configuration c restricted to the set I—i.e. $c : I \longrightarrow \Sigma$—for $I \subset \mathbb{Z}^d$, and, $c_x = c(x)$ with $x \in \mathbb{Z}^d$ for the letter written at position x. The association of a position and its state is called a *cell*.

For a neighborhood $\mathcal{N}$, it is useful to introduce its radius as being the highest coordinate of the elements of the neighborhood.

Definition 2 (Radius of a neighborhood)**.** *The* radius r *of a finite neighborhood* $\mathcal{N} \subset \mathbb{Z}^d$ *is defined as:*

$$r = \max_{x \in \mathcal{N}} \left\{ \max_{i=0,\dots,d-1} x_i \right\}. \tag{1.2}$$

1.1.2. Evolution

Having described the state of the system at a given time through a configuration, it is now possible to describe its dynamics. The evolution, in the framework of CA, is realized through a local rule f that takes as input a configuration restricted to the neighborhood $\mathcal{N}$ of a cell, and outputs the next value of the cell.

$$f : \Sigma^{\mathcal{N}} \longrightarrow \Sigma. \tag{1.3}$$

Applying this local rule at every position simultaneously defines the evolution of a configuration.

Definition 3 (Cellular Automaton)**.** *A cellular automaton with alphabet* Σ*, dimension* d *and neighborhood* $\mathcal{N}$ *is a function* $F : \mathscr{C} \longrightarrow \mathscr{C}$ *which takes a configuration to another configuration by applying a local rule* $f : \Sigma^{\mathcal{N}} \longrightarrow \Sigma$ *at every position synchronously through:*

$$F(c)_i = f(c_{i+\mathcal{N}}) \tag{1.4}$$

where $i \in \mathbb{Z}^d$*.*

The notation $c_{t,x}$ describes the value of a cell at position x and time t.

EXAMPLE: TRANSPORT CELLULAR AUTOMATON

An example of a simple cellular automaton is the transport CA. Two bits are stored at each position, i.e. $\Sigma = \{0,1\}^2$. The first bit is moved in the negative direction whereas the second is moved in the positive direction.

Throughout the manuscript, the examples will be given in a block circuit form often referred to as (Margolus-)Partitioned CA [58]. Using Partitioned CA for the examples allows for a unified framework throughout the manuscript. This formalism is intrinsically universal for both reversible CA [59, 60] and quantum CA [61].
In this formalism, the transport CA can be implemented by the successive application of two layers of swap, one layer acting as a transport which exchanges the second bit at position x with the first bit at position $x+1$, the other layer exchanging the two bits at each position. This is illustrated in Fig 1.1

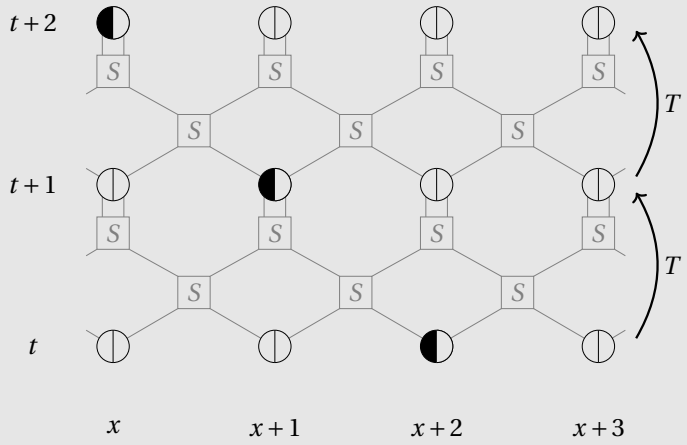


Figure 1.1.: Transport cellular automaton T in the partitioned formalism. The S gate correspond to the swap $S:(a,b)\mapsto(b,a)$. The black 'bit' at position $x+2$ is transported to position x at time $t+2$.

Using the partitioned formalism, each gate having as many inputs as outputs, it is easy to check the reversibility of the CA. This will also be useful in the quantum setting were the local gates will be unitaries.

1.1.3. Extension

In order to introduce gauge invariance in the framework of cellular automata, extending the previous definition of CA will be required. This extension consist in encoding information on the links, and not only on the vertices of the graph induced by $\mathbb{Z}^d$. To each vertex x is associated the outgoing edge ports $x:\eta$ where η denotes a direction (η and $-\eta$ are two opposite directions). Defined in this way, η can be considered as a port number for the vertex x. The set of directions is denoted by Π. Let Δ be a countable—often finite—set.

Definition 4 (Extended configuration)**.** *An* extended configuration *c over alphabet Σ and Δ is a function that associates an element of Σ and $|\Pi|$ elements (one for each*

outgoing edge) of Δ *to each point in* $\mathbb{Z}^d$*:*

$$c : \mathbb{Z}^d \longrightarrow \Sigma \times \Delta^{\Pi}. \tag{1.5}$$

Essentially, the extended configurations act both on every vertex (with alphabet Σ) and on each end of every edge (with alphabet Δ). Hence, for a configuration c, position x and direction η, $c_x \in \Sigma$ and $c_{x:\eta} \in \Delta$. In Physics, the edge configuration is called *gauge field*.

We denote by c^v the vertex configuration and c^e the edge configuration such that c is fully describe by (c^v, c^e) and

$$c^v : \mathbb{Z}^d \longrightarrow \Sigma \tag{1.6}$$

$$c^e : (\mathbb{Z}^d, \Pi) \longrightarrow \Delta. \tag{1.7}$$

Similarly, let $\mathscr{C} = \mathscr{C}^v \times \mathscr{C}^e$ where $\mathscr{C}^v = \Sigma^{\mathbb{Z}^d}$ are the vertex configurations and $\mathscr{C}^e = \Delta^{\mathbb{Z}^d \times \Pi}$ the edge configurations.

Remark 1. *In most instances, a single value for each edge would be sufficient. In those cases one can add the requirement that* $c_{x,\eta} = c_{x+\eta:-\eta}$ *and consider that the value indeed lives on the edge between vertices* x *and* $x+\eta$*.*

Although one can directly define an extended CA, one will often start from a simple dynamics and want to extend it, to obtain a symmetry such as gauge invariance or allow for more complex dynamics to emerge. In that case, the initial dynamics should still be seen in the extended CA, for instance when the edge configuration is empty, where empty means that it is uniformly equal to a specific state ϵ in Δ.

Definition 5 (Extended cellular automaton)**.** *Let* Δ *be a countable set and* F *a CA over alphabet* Σ*. An extension* F' *of* F *is a CA over alphabet* $\Sigma \times \Delta^{\Pi}$ *such that there exists* $\epsilon \in \Delta$ *for which the evolution* F' *applied on an extended configuration* c*, with* $c_{x:\eta} = \epsilon$ *for every position* x *and direction* η*, gives* $F'(c)^v = F(c^v)$*.*

Notice that when the edge configuration does not evolve in time, the condition holds for any time step. In such case, F is a sub-automaton of F' [62].

EXAMPLE: EXTENSION OF THE TRANSPORT CA

In order to illustrate the concept, let us extend the transport CA. It has alphabet $\Sigma = \{0,1\}^2$. First the configuration is extended so that it stores information on the port. For the sake of simplicity and clarity, we choose Δ to be the smallest unit of information, that is to say a bit: $\Delta = \{0,1\}$.
Then the dynamics has to be extended. One possibility consists in adding up the port value to the bit being transported. That is to say, the first bit at position $x+1$ will be summed to the bit on port $x+1:-1$ and the result is stored in the first bit at position x. The same goes for the second bit in the other direction.

The port bits are left unchanged. This is done by changing the first layer of gates with a new operator S' which acts as follows:

$$S' : (c_x, c_{x:+1}, c_{x+1:-1}, c_{x+1}) \mapsto (c_{x+1} + c_{x+1:-1}, c_{x:+1}, c_{x+1:-1}, c_x + c_{x:+1}) \tag{1.8}$$

where $a : +1$ and $b : -1$ denote the bit values stored on the ports. It is indeed an extension because the port configuration where all bits are at 0 plays the role of the empty configuration of definition 5 for which the dynamics is simply the usual transport. This dynamics is illustrated in figure 1.2.

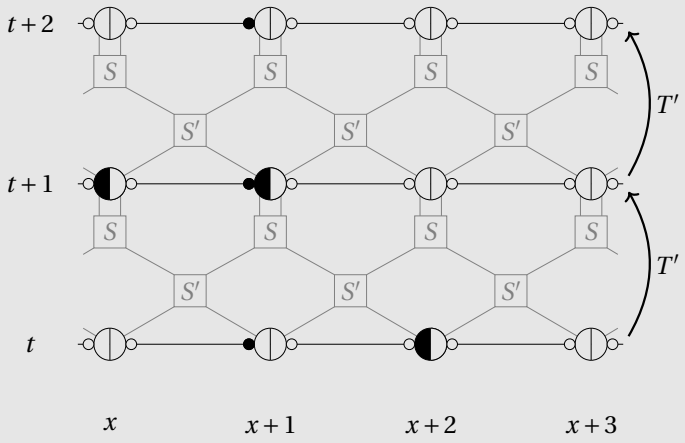


Figure 1.2.: Extension T' of the transport CA.

In this figure, the first bit at position $x+2$ is first transported to position $x+1$ but is then cancelled by the port bit at position $x+1 : -1$ and is not transported to position x at time $t+2$. However, the port bit at position $x+1 : -1$ is also summed with the first value at position x which explains the black 'bit' at position x and time $t+1$. This illustrates that new dynamics are possible through the use of extension.

1.2. Gauge invariance

1.2.1. Global symmetry

A CA is said to be globally symmetric whenever its global evolution is invariant under the application of an alphabet permutation—i.e. the application of the same permutation on every cell. Globally symmetric CA are also known as G-blind CA [25] with G a group of permutations over Σ. For a permutation $g \in G$, let $\overline{g}$ denote its application at every position simultaneously: $\overline{g}(c)_i = g(c_i)$.

Definition 6 (Globally symmetric)**.** *Let $F : \mathscr{C}^{\nu} \to \mathscr{C}^{\nu}$ be a CA and G a group of permutations over Σ. F is said globally G-symmetric if, for any g in G, F commutes with*

g—*i.e.* $F \circ \bar{g} = \bar{g} \circ F$.

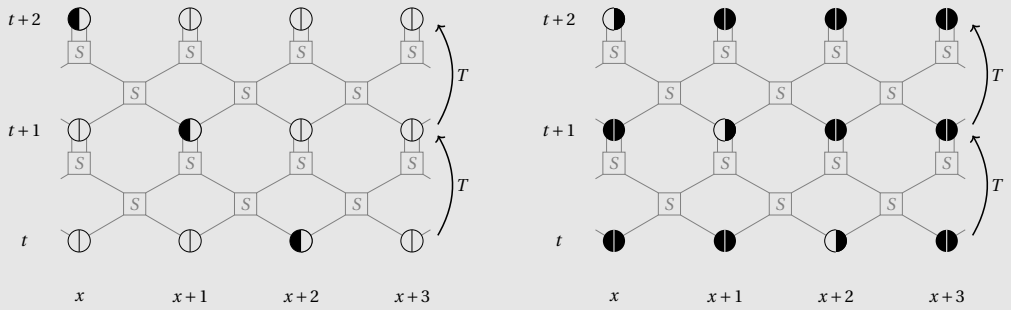
An intuition on globally G-symmetric CA can be given through the designation color-blind CA. If Σ encodes for a color, then a globally symmetric CA is impervious to a change in color for G the color permutations.

EXAMPLE: GLOBALLY SYMMETRIC TRANSPORT

Let g be the permutation which flips both bits of a state:

$$g : (a, b) \mapsto (\bar{a}, \bar{b}) \tag{1.9}$$

where $\bar{0} = 1$ and $\bar{1} = 0$. Then the transport CA is globally G-symmetric, for $G = \{Id, g\}$, because it does not depend on the color: it only moves the bits. Figure 1.3 illustrates this global symmetry.



(a) Without global transformation (b) With global transformation

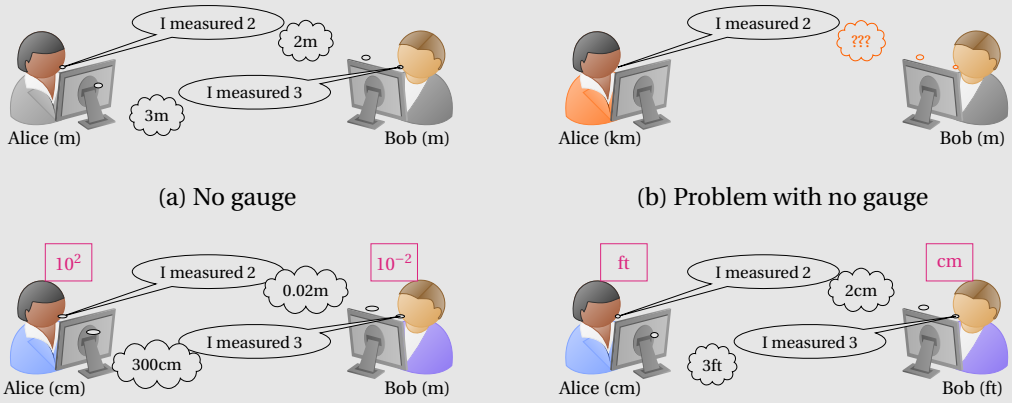
Figure 1.3.: The transport CA globally symmetric, both figures show the same dynamics (a bit moving to the left) with opposite colors.

1.2.2. Local symmetry

EXAMPLE: ANALOGY

The intuition behind gauge invariance may be better explained with an analogy. Say Alice wants to measure a distance. She can choose any unit she likes, be it the meter, the kilometer, the mile, or any other distance unit. What matters is that she knows the *gauge* used for her measurement. Then take Bob who also wants to measure a distance. He, too, has many units available. When Alice and Bob want to share their respective measurements, the first solution that comes to mind is for them to fix a specific gauge (a.k.a. unit) and require they both use the same (see figure 1.4a). However, this is not stable since a change of gauge for Alice would mean that Bob will either have to also change unit, or worse, he

may misinterpret the data he receives from Alice (see figure 1.4b). The simplest solution is for Alice and Bob to store the conversion rate between their units. When one changes its unit, it shares the information with the other so that both can update their conversion rate. Such model can be called gauge invariant, that is to say, impervious to a change in gauge locally, be it for Alice or Bob. This is illustrated in figure 1.4c.



(a) No gauge

(b) Problem with no gauge

(c) Relative gauge

(d) Absolute gauge

Figure 1.4.: Illustration of the analogy. The unit of measurement is given beside the name of each party, the gauge field when there is one is in the box above their head.

At this point, one may wonder why not just send the unit at the same time as the measurement, this should also give the required gauge invariance as illustrated in figure 1.4d. The reason for that is that it requires a fixed reference, and it may not be possible to define such fixed reference. For instance, in quantum electrodynamics (which we will come to in the next chapter), the difference of gauge is only a phase which cannot be measured in the absolute but only relative to another phase. In such cases, one can only store a *relative* information—i.e. the ratio between the gauges of Alice and Bob—and not an *absolute* information—i.e. the unit itself.

Coming back to cellular automata, what is measured is the configuration at a given position in space, that is to say an element of the alphabet Σ. A gauge is the way such element is measured. For instance if Σ has two elements, the first may be mapped to 0 and the second to 1, or the other way around, changing the 'meaning' of the measurement. In our case Alice at position x may measure using a specific permutation of Σ as gauge, while Bob at position $x+\eta$ measures using another permutation. Gauge information, be it absolute or relative, is then stored using the alphabet Δ on the edge they share, at $x:\eta$ for Alice and $x+\eta:-\eta$ for Bob. In order for a CA to be gauge invariant, its evolution must not depend on the specific choice of gauge of Alice

of Bob. That is to say, the CA has to commute with gauge transformations. Let us make this formal.

Local transformation. A CA is said locally symmetric whenever its global evolution is invariant under the application of a local function at every position. The first difference with globally symmetric CA is that the function is now allowed to differ from one position to the next. The second difference is that it can also act on the surrounding cells.

Definition 7 (Local transformation group)**.** *Let $\mathcal{N} \subset \mathbb{Z}^d$ be a finite neighborhood and g be a permutation over $\mathcal{C}_\mathcal{N}$. $g^x : \mathcal{C} \longrightarrow \mathcal{C}$ will denote the function that acts as g on the cells at $\{x+y, y \in \mathcal{N}\}$, and trivially everywhere else. A* local transformation group *G is a group of bijections over $\mathcal{C}_\mathcal{N}$, such that for any $g, h \in G$ and any $x \neq y \in \mathbb{Z}^d$, $g^x \circ h^y = h^y \circ g^x$.*

This permutation condition makes it irrelevant to consider which local transformation gets applied first, so that the product $g^x h^y$ be commutative. Verifying this condition can be done by checking over a hypercube with length twice the diameter of the neighborhood.

Definition 8 (Gauge transformation)**.** *Consider G a group of local transformations. A* gauge transformation *is a function $\gamma : \mathbb{Z}^d \longrightarrow G$. It is interpreted as acting over $c \in \mathcal{C}$ as follows:*

$$\gamma(c) = (\prod_{x \in \mathbb{Z}^d} \gamma^x)(c), \tag{1.10}$$

where γ^x is short for $\gamma(x)^x$, the local transformation $\gamma(x) \in G$ applied at position x. Γ will denote the set of gauge transformations.

Notice how an element $\gamma \in \Gamma$ may be thought of as a configuration over the alphabet G. Thus, γ_x is an element of G which can be applied on a finite configuration, while γ^x is its natural extension which can be applied onto a full configuration.

EXAMPLE: GAUGE TRANSFORMATION

In the transport CA, the alphabet is $\Sigma = \{0,1\}^2$. Let the transformation g flips both of the bits simultaneously. Hence, for $G = \{Id, g\}$, a gauge transformation is the application of either g or the identity at every position. This is illustrated in figure 1.5.

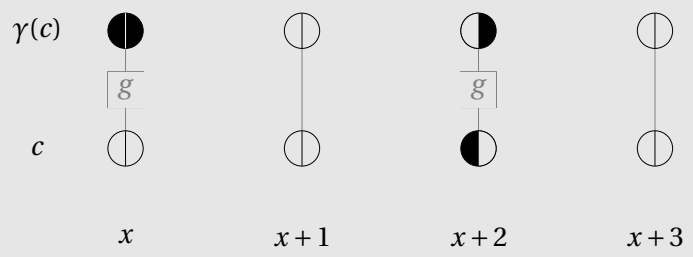


Figure 1.5.: Gauge transformation

Gauge invariance. Global symmetry in CA amounts to being 'insensitive' to a set of global transformations. A locally symmetric CA, which is referred to as gauge invariant cellular automata (GICA) is a CA 'insensitive' to gauge transformations: performing γ before F amounts to performing some γ' after F.

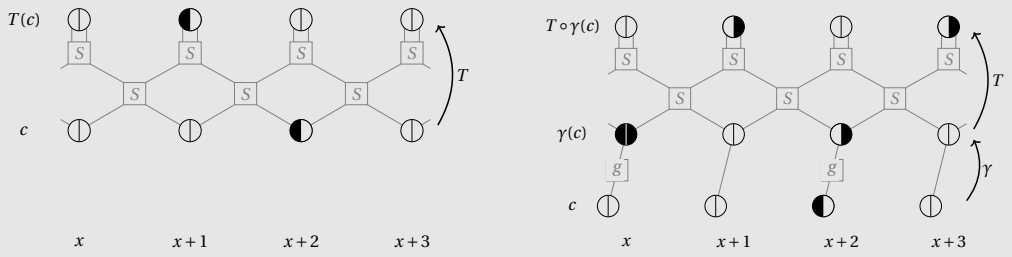
Definition 9 (Gauge invariant cellular automaton)**.** *Let F be a CA, G be a local gauge transformation group, and Γ be the corresponding set of gauge transformations. F is Γ-gauge invariant if and only if there exists a CA Z over the alphabet G, such that for all $\gamma \in \Gamma$:*

$$Z(\gamma) \circ F = F \circ \gamma. \tag{1.11}$$

The reason why γ' must result from a CA Z, instead of being left fully arbitrary, is because F is deterministic, shift-invariant and causal, from which it follows that γ', if it exists, can be computed deterministically, homogeneously and causally from the γ applied before. Thus, the above is demanding a weakened commutation relation between the evolution F and the set of gauge transformations Γ. In practice, in Physics in particular, Z is often taken to be the identity making gauge invariance a commutation relation. This will be the case in our examples.

EXAMPLE: TRANSPORT NOT GAUGE INVARIANT

Under the gauge transformations spanned by the local transformation group G previously defined, the transport CA is not gauge invariant. This is illustrated in figure 1.6 where the two configurations after the evolution are not related by a gauge transformation. That is to say, for any γ', the following holds: $\gamma' \circ T \neq T \circ \gamma$.



(a) Without gauge transformation (b) With a gauge transformation

Figure 1.6.: Transport CA not gauge invariant

1.2.3. Gauge extension

In Physics, one usually begins with a theory that explains how matter freely propagates in the absence of forces and which is not gauge invariant. For instance, in the case of electrons this theory is the Dirac equation, the group of gauge transformation considered is the group $U(1)$ of rotations, and the Dirac equation is not $U(1)$–gauge invariant. Next, one enriches the initial theory with an additional information, known as the gauge field, to make the resulting theory gauge invariant. In the case of the electron, the $U(1)$–gauge invariance is obtained thanks to the addition of the electromagnetic field. The resulting theory can still account for the free propagation of the matter field, but the presence of the gauge field also allows for richer behaviors, e.g. electromagnetism.

In CA, the initial theory is solely concerned with the dynamics on a discrete space and gauge invariance is not ensured. The theory thus has to be extended, using a gauge field, so as to recover gauge invariance. But when is it the case that a theory is a gauge extension of another, exactly? A rigorous definition of the notion of gauge extension, and of its relative subcase, is provided here in the discrete context of CA.

To gauge extend a CA, one has to meet three requirements: (i) the CA itself has to be extended; (ii) the gauge transformations should take into account the newly defined gauge field, and thus need be extended; (iii) the extended CA has to be gauge invariant relatively to the extended gauge transformations.

Definition 10 (Gauge extension)**.** *Let $F : \mathscr{C}^{\upsilon} \longrightarrow \mathscr{C}^{\upsilon}$ be a CA. Let Γ be a gauge transformation group with neighborhood $\mathcal{N}$ and defined through a local transformation group G over $\Sigma^{\mathcal{N}}$.*

A gauge extension of (F,Γ) is a tuple (F',Γ') with F' an extension of F and Γ' a gauge transformation group over $\mathscr{C}_{\mathcal{N}}$, such that:

- (Extension) *there exists a bijection $B : \Gamma' \longrightarrow \Gamma$ such that for any gauge transformation $\gamma' \in \Gamma'$:*

$$\gamma'(c)^{\upsilon} = \gamma(c^{\upsilon}) \tag{1.12}$$

where $\gamma = B(\gamma')$. In short, the action of the gauge transformation on the vertices has an equivalent in the non-extended case that can be separated from the transformation on the edges (a.k.a. the gauge field).

- (Gauge invariance) *F' is Γ'-gauge invariant.*

Intuitively, the gauge field's role is to keep track of which gauge transformation got applied where, so that enough information is stored to ensure gauge invariance. There are different ways to do this; for instance one could store the 'gauge' at each point, i.e. which gauge transformation has happened at the specific point. Such choice corresponds to the *absolute* information from the previous analogy. Another choice could be more parsimonious and only store the 'relative gauge', i.e. the gauge difference between two neighboring points, which is the *relative* information in the analogy.

The standard choice in the Physics literature is to place the gauge field between the matter cells only—i.e. on the links between two cells. The mathematical justification for this choice, is precisely that the gauge field may be interpreted as relative information between neighboring matter cells. Geometrically speaking, it may be understood as a 'connection' relating two close by 'tangent spaces' on a manifold.

A relative extension of a CA is such that there is an equality (or opposition) relation for the two values stored at the end of each edge. This can be enforced through a condition which goes as follows: for any configuration c, any position x and any direction η, ask that $c_{x;\eta} = c_{x+\eta;-\eta}$. This is the standard convention, which has the drawback of fixing a space direction: going back to the analogy, the conversion rate would be stored for Alice, and, Bob would have to know that he should compute the inverse opposite rate.

We would like here to argue that another convention is possible: $c_{x;\eta} = c^{-1}_{x+\eta;-\eta}$. In that case, the gauge field associated to a site corresponds to the transformation that needs to be applied in order to communicate with the neighbor—i.e. it is the conversion rate in the analogy. This avoids the drawback of the first convention since there is now a symmetry instead of an antisymmetry in the definition—i.e. there is no privileged space direction. Moreover, such convention allows for an easier generalization to graphs where a direction of space may not be simple to define.

Using this convention, it is clear that both ends of one link should *transform* inversely to one-another. But why should one *be* the inverse of the other? In other words, why should their product be the neutral element? This is quite natural if one think of them as conversion rates. Still, it is not a necessity for gauge invariance. However, lifting this restriction introduces an unnecessary degree of freedom. Hence, this restriction is a necessity if one demands 'minimal' gauge invariance. Another reproach that could be made is that this convention forces every element in Δ to have an inverse. While for a gauge extension in general this may be a restriction, we shall see that $\Delta = G$ (the local gauge transformation group) for relative gauge extensions. Hence, Δ is a group and having an inverse for each of its elements is not a constraint.

In the following, the convention where both ends have inverted values is used.

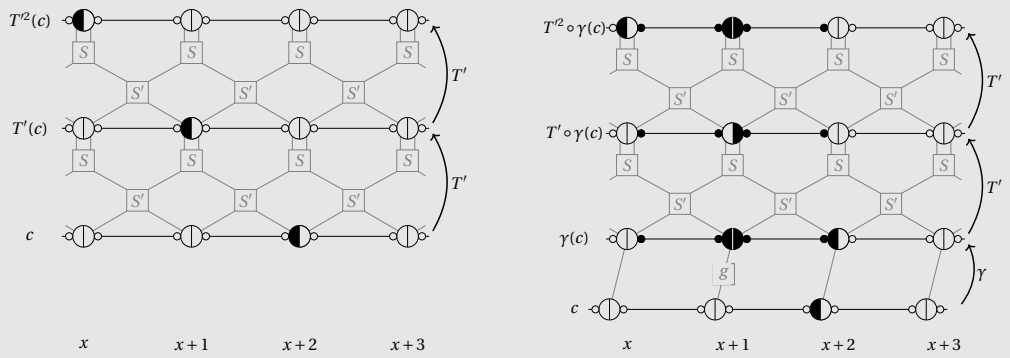
Definition 11 (Relative gauge extension)**.** *Given a CA F and a local gauge transformation group Γ of neighborhood 0, we say that a gauge extension (F',Γ') of (F,Γ) is* relative *when:*

1. *F' and Γ' act on the restricted space of configurations such that for any $c \in \mathscr{C}$, $x \in \mathbb{Z}^d$ and direction η,*
$$c_{x:\eta} = c^{-1}_{x+\eta:-\eta}, \tag{1.13}$$
2. *$\Delta = G$ and $\epsilon = Id$—i.e. the alphabet for the vertex configuration is G, and the neutral element ϵ (from definition 5) is the identity,*
3. *for every position $x:\eta$, a gauge transformation $\gamma \in \Gamma'$ acts on the edge as follows:*
$$\gamma(c)_{x:\eta} = \gamma_{x+\eta} \circ c_{x:\eta} \circ \gamma_x^{-1} \tag{1.14}$$

Thus, relative extension keeps track of the difference of gauge between two neighboring cells, using the gauge field alphabet. Note that the conventions in equations (1.13) and (1.14) are coherent—i.e. taking the inverse of the gauge transformation of one end does indeed give the gauge transformation stored at the other end of an edge.

EXAMPLE: RELATIVE GAUGE EXTENSION OF THE TRANSPORT CA

In the relative gauge extension, the set Δ is the same as the group of local transformations. In the case of our running example, G has only two elements: the identity and g. Those can be represented by a single bit, just like in the extended case represented in figure 1.2. There is however the additional constraint that both port bits pertaining to the same link be equal since $g = g^{-1}$.
Figure 1.7 illustrates how gauge invariance is recovered when gauge extending the transport CA. The left part shows the extended CA where the gauge field is set to the identity everywhere, hence leading to the transport dynamics. The right of the figure shows that the dynamics is resilient under gauge transformation since both final configurations ($T(c)$ and $T \circ \gamma(c)$) are the same up to a gauge transformation.



(a) Without gauge transformation

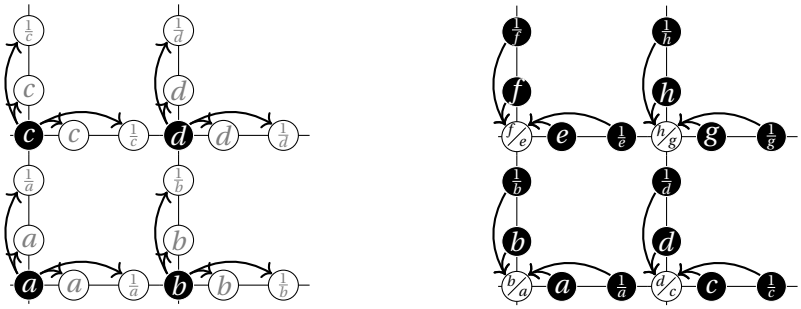
(b) With a gauge transformation

Figure 1.7.: Relative gauge extension of the transport CA

Here S' applies the operator stored in the gauge field to its input bits. It yields the same result as in figure 1.2 since the gauge field simply stores whether to do a bit flip.

From absolute to relative extension and vice versa. As mentioned before, there are two intuitive ways to extend CA: an 'absolute' extension where the gauge field is stored on the nodes of the graph (i.e. for any position x and directions η, ζ: $c_{x,\eta} = c_{x,\zeta}$), and, a 'relative' extension where the gauge field is stored on the links between nodes (i.e. for any position x and direction η, $c_{x,\eta} = c^{-1}_{x+\eta,-\eta}$). In the absolute case, let c^e_x denote the single gauge field per position.

If only considering relative and absolute extensions as different storage mechanism, both extensions are equivalent. To go from absolute to relative extension, one possibility is to copy c^e_x on half of the edges associated with x. An example in a two-dimensional space is given in figure 1.8a, with $c_{x,\mu} = c_{x,\nu} = c^e_x$. From relative to absolute, the gauge field values carried by the edges may instead be gathered on close by nodes. Figure 1.8b illustrates one possible choice with $c^e_x = (c_{x,\mu}, c_{x,\nu})$.



(a) Absolute to relative

(b) Relative to absolute

Figure 1.8.: Possible mapping between relative and absolute extensions. The middle circle corresponds to an absolute positioning while the circles on the edges are for relative positioning.

However, relative gauge extension may be considered as more than just a storage mechanism, as developed in definition 11. In that case, gauge transformations of the gauge field are further constrained through equation (1.14) which is not verified by every gauge extension. In that context, absolute extension becomes a weaker requirement than relative extension, since it only constrains the positioning of the gauge field and not how gauge transformations act on it. Any relative extension can still be made absolute. However, whether any absolute extension can be made relative, that is to say verify equation (1.14), is left open here.

1.2.4. About Abelian and non-Abelian gauge symmetry.

In Physics, gauge theories are often referred to as Abelian or non-Abelian, which in fact refers to the commutativity of the local transformation group G. Here, the definitions were given in the general case, and work in both the Abelian and non-Abelian cases.

EXAMPLE: NON-ABELIAN GAUGE SYMMETRY FOR THE TRANSPORT CA

First, let us extend the alphabet as follows: $\Sigma = \{0,1,2\}^3$, i.e. there are two trits per site instead of two bits. Figure 1.9 illustrates the transport using this alphabet.

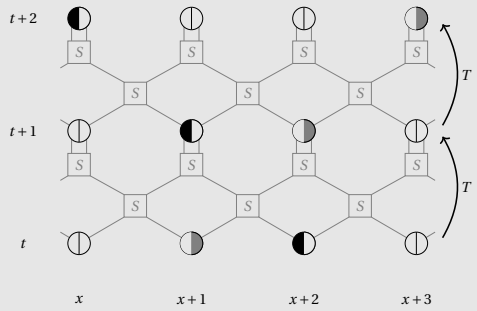


Figure 1.9.: Transport over a bigger alphabet

Let $S(3)$ be the (non-Abelian) group of permutations over 3 elements. We define the non-Abelian gauge transformation group G as the operators which apply the same permutation simultaneously on both trits:

$$G = \{ s \otimes s \mid s \in S(3) \}. \tag{1.15}$$

Through a relative gauge extension of the transport CA, the gauge field stores the permutation "difference" between a state and its neighbors and changes under a gauge transformation as in equation (1.14). Figure 1.10 illustrates how gauge invariance is ensured thanks to this gauge field.

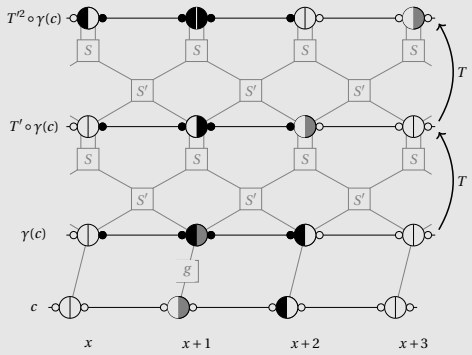


Figure 1.10.: Non-Abelian gauge symmetry for transport CA

The gauge transformation $g = g^{-1}$ swaps black and white colors, leaving the gray untouched. Hence, there are only two gauge field states in the example: empty for the identity and full for g. Gauge invariance is ensured through S' which applies the operator stored in the gauge field to its input trits (same process as in figure 1.2). It yields the same dynamics as in figure 1.9 with an additional color swaps, consistent with g, at $x+1$. Why such model is gauge invariant is formally developed in the next section where a construction is given to extend any globally invariant CA (which is the case of the transport) into a relative gauge extended one.

1.3. Universality

What is the relationship between globally and locally (a.k.a. gauge) invariant cellular automata? Does a CA have to be globally invariant to have a gauge invariant extension? These two questions relating different symmetries are most relevant in Physics, where one may wonder if a local symmetry is always a generalization of an already existing global symmetry. It is also an interesting question in itself for the construction of GICA. As it happens, there is a close relation between relative gauge extension and global symmetry which is explored in subsection 1.3.1.

Other questions regarding gauge symmetry also come into play when considering it under the light of cellular automata. Are there universal GICA? Given a CA and a gauge transformation group, can one always extend it into a GICA? If so, is there a minimal way to do so? This series of questions find answer in subsections 1.3.2 and 1.3.3.

1.3.1. Globally symmetric CA admits a relative gauge extension

From a Physics perspective, the gauge symmetry comes from an already existing global symmetry. We show here that there is an equivalence between being globally G-symmetric and having a relative gauge extension with respect to G.

Theorem 1 (Global symmetry and relative gauge extension)**.** *Let F be a CA over alphabet Σ, G a subgroup of the permutations of Σ, and Γ the set of gauge transformations defined using G as the group of local transformations. Then the following two properties are equivalent:*

1. *F is globally G-symmetric*
2. *(F,Γ) admits a relative gauge extension (F',Γ') with the identity for the gauge field evolution, such that F' commutes with any element of Γ' (stronger than gauge invariance because it does not require a Z-map).*

Proof.
(1 $\Rightarrow$ 2) Let f be the local rule of F with neighborhood $\mathcal{N}$. Let F' be a CA with neighborhood $\mathcal{N}$ over the extended configurations constrained as given by equation (1.13). Let the gauge field evolution be the identity. The trick will be for the local rule on the vertices to encode every element of the neighborhood into the same 'gauge basis'.

For y an element in the neighborhood of a position x, we define a path p from x to y as the sequence of vertices and the directions between these:

$$p = \left[(x,\eta_0), (x+\eta_0,\eta_1), \ldots, \left(x + \sum_{j=0}^{k-1} \eta_j, \eta_k \right) \right] \tag{1.16}$$

where $y = x + \sum_{j=0}^{k} \eta_j$.

The local rule will use the following scheme, starting by an encoding E, followed by the local rule f applied on the vertex configuration:

$$c \xrightarrow{E} c'^{v} \xrightarrow{f} c''^{v} \tag{1.17}$$

For every position y in the neighborhood $\mathcal{N}$, we define p_y a path from 0 to y. The encoding of c_y goes as follows:

$$E(c_{\mathcal{N}})_y = \prod_{(x,\eta)\in p_y} c_{x;\eta}^{-1}(c_y) \tag{1.18}$$

where the product order is $\prod_{i=0}^{k} \alpha_i = \alpha_0 \circ \ldots \circ \alpha_k$.

The encoding applies every gauge transformation in the path to the element at position y. This, in a sense allows to put every element in the same 'gauge basis': the one at position 0.

Note that we took an arbitrary path, what matters is that this path stays the same throughout the construction.

One small remark, if $\mathcal{N}$ is not connected—i.e. it contains an element such that there is no path in the neighborhood from 0 to this element—then the encoding would require taking as input part of the gauge field outside the neighborhood to create this path. This has no incidence on the logic of the proof itself, it simply requires an extension of $\mathcal{N}$.

Having defined the encoding, let us define the local rule f' such that the edge configuration stays unchanged, and the vertex configuration follows equation (1.18):

$$\begin{cases} f'(c_{\mathcal{N}})^{v} & = f \circ E(c_{\mathcal{N}}) \\ f'(c_{\mathcal{N}})^{e}_{0,\eta} & = c^{e}_{0,\eta} \end{cases} \tag{1.19}$$

with η being any direction.

We shall now prove that (F', Γ')—with Γ' defined through Eq. (1.14)—is a relative gauge extension of (F, Γ).

The fact that this is indeed an *extension* (definition 5) comes directly from the fact that f' acts exactly like f for an empty gauge field because the encoding would then act like the identity.

This extension was defined as *relative*. What is left to check is that this extension has the 2 required properties of a gauge extension from definition 10.

- *(Extension)* Because Γ' is defined through definition 11, it is immediate that it verifies the extension property.
- *(Gauge invariance)* For any $\gamma' \in \Gamma'$ we will check that $\gamma' \circ F' = F' \circ \gamma'$.

  Let γ' be a gauge transformation, then it will transform the vertices and edges as

follows—using equation (1.14) and $\gamma = B(\gamma')$ through definition 10:

$$c_x \longrightarrow \gamma_x(c_x) \tag{1.20}$$
$$c_{x:\eta} \longrightarrow \gamma_{x+\eta} \circ c_{x:\eta} \circ \gamma_x^{-1} \tag{1.21}$$

with x a position and η a direction.

For y an element of the neighborhood and p_y the path from 0 to y, one obtains:

$$E\left(\gamma(c)_{\mathcal{N}}\right)_y = \prod_{(x,\eta)\in p_y} \left[\gamma_{x+\eta} \circ c_{x:\eta} \circ \gamma_x^{-1}\right]^{-1} \gamma_y(c_y) \tag{1.22}$$
$$= \gamma_0 \left[\prod_{(x,\eta)\in p_y} c_{x:\eta}^{-1}(c_y)\right] \tag{1.23}$$
$$= \gamma_0 \circ E(c_{\mathcal{N}})_y. \tag{1.24}$$

It is apparent here that only γ_0 remains. Every other gauge transformation has been cancelled out, and this is true for every position y in the neighborhood. Therefore:

$$\left(F' \circ \gamma'(c)\right)_0 = f \circ \overline{\gamma_0} \circ E(c_{\mathcal{N}}) \tag{1.25}$$

where $\overline{\gamma_0}$ is the global transformation for which γ_0 is applied at every position—here constrained to the neighborhood.

Since F is globally G-symmetric, we have that $f \circ \overline{\gamma_0} = \gamma_0 \circ f$ and therefore

$$\left(F' \circ \gamma'(c)\right)_0 = \left(\gamma' \circ F'(c)\right)_0. \tag{1.26}$$

Through translation invariance of the CA, this finishes the proof.

(2 ⇒ 1) Suppose that (F', Γ') is a relative gauge extension of (F, Γ), such that F' commutes with any element of Γ', we shall prove that F is globally G-symmetric (with Γ the gauge transformation group based on G). Let c^v be a vertex configuration and e denote the empty edge configuration—i.e. identity everywhere. For any local gauge transformation g, we write $\bar{g}$ the global gauge transformation applying g everywhere—g denotes both the element of G and G' depending on the context:

$$\bar{g} \circ F'(c^v, e) = \bar{g}(F(c^v), a) \qquad \text{(Extension 5)}$$
$$= (\bar{g} \circ F(c^v), a') \qquad \text{(Extension 10)}$$

where a and a' are two edge configuration which depend on F' and $\bar{\gamma}$, their detail does

not matter here. And

$$\begin{aligned} F' \circ \bar{g}(c^\nu, e) &= F'(\bar{g}(c^\nu), \bar{g} \circ e \circ \bar{g}^{-1}) && \text{(Extension 11)} \\ &= F'(\bar{g}(c^\nu), e) && (1.27) \\ &= (F \circ \bar{g}(c^\nu), b) && \text{(Extension 5)} \end{aligned}$$

where b is a gauge field configuration which depends on F' and g. The G'-gauge invariance of F' gives $\bar{g} \circ F'(c^\nu, e) = F' \circ \bar{g}(c^\nu, e)$ and thus

$$\bar{g} \circ F(c) = F \circ \bar{g}(c). \tag{1.28}$$

Therefore, F is globally G-symmetric. □

This theorem gives a guideline when looking for relative gauge extensions which is: first search for a global symmetry. The construction will now be used to prove that relative gauge extensions of CA are universal in one spatial dimension.

1.3.2. Universality through relative gauge extension

Results in this subsection are only given for dimension 1. A prerequisite is the notion of intrinsic simulation and intrinsic universality for CA. The idea behind intrinsic simulation is that a CA A can reproduce the "same behavior" as the simulated CA B. Intrinsic universality means that A intrinsically simulates any other CA B. More formal definitions are given in [63, 64].

Remark 2 (Extensions are intrinsic simulations)**.** *An extension as defined through definition 5, with the identity as the gauge field evolution, is an intrinsic simulation.*

Indeed, taking the empty configuration for the edges, and having the gauge field evolve as the identity, means that the extension evolve exactly as the non-extended CA, hence it is an intrinsic simulation. However, note that using the non-empty edge configuration, one can get completely different evolutions.

In [25], Salo and Törmä prove that for any alphabet Σ, there exists an intrinsically universal globally G-symmetric cellular automaton on $\Sigma^{\mathbb{Z}}$ (note that this is a one dimensional CA), where G is the group of all permutations of σ. They provide a construction through which any CA can be encoded into a globally symmetric one—i.e. any single CA can be simulated by a globally symmetric one. The construction is built through an encoding of the information in the structure of the configuration rather than the states. A global transformation which preserve the structure will also preserve the information encoded inside it. Combining this result and theorem 1 gives a universality result for relative GICA:

Corollary 1 (One-dimensional gauge invariant universal cellular automata)**.** *For any alphabet Σ and subgroup G of the permutations of Σ, there exists an intrinsically universal one-dimensional G'-gauge invariant CA F' where G' is an extension of G using definition 10.*

Proof. It is enough to show that any single globally symmetric CA can be simulated by a relative gauge invariant one, as there exists an intrinsically universal globally symmetric CA [25, Theorem 1] and simulations are composable.

Let F be a globally G-symmetric CA on $\Sigma^{\mathbb{Z}}$. From theorem 1, (F,G) admits a relative gauge extension (F',G') with the evolution of the gauge field being the identity. Thus, F' is a G'-gauge invariant CA intrinsically simulates F. □

Such result is interesting on two accounts: (i) it shows that universality only requires relative gauge information and does not need any absolute information; (ii) it shows that relative gauge extensions, which are the ones usually appearing in Physics, are universal.

This construction is nevertheless limited to one dimension and gauge transformation of radius 0. It is unknown, to the best of our knowledge, whether this conditions can be lifted when restricting to relative gauge extensions. However, when not restricted, one can always extend a CA into a gauge invariant one as we will now show.

1.3.3. Universality through absolute gauge extension

We now prove that any CA can be intrinsically simulated by a gauge invariant one, with respect to any gauge transformation group, acting on any neighborhood. The construction of this section uses non-relative gauge extensions which allows getting rid of the prior requirements that there be a global symmetry or that the gauge transformations be of radius 0. The cost of this construction is a 5-fold increase in the radius of the local rule of the CA.

Intuitively, the gauge field will be used to keep track of every gauge transformation applied at a specific point in space, allowing for the evolution to counteract any gauge transformation.

Theorem 2 (Every CA admits a gauge extension)**.** *Any CA F and gauge transformation group Γ admits a gauge extension (F',Γ'). Furthermore, the local rule of F' acts as the identity over the gauge field.*

Proof. The proof given here is constructive for any CA over $\mathbb{Z}^d$.

Let G be a local gauge transformation group of neighborhood $\mathcal{N}$ with radius s and F be a CA of neighborhood $\mathcal{N}'$ which has radius s'. We denote r the highest radius between s and s'. In the following we will consider neighborhoods $R_x^k = [x-k\cdot r, x+k\cdot r]^d$ of each point $x\in\mathbb{Z}^d$, with $[a,b]=\{n\in\mathbb{Z} \mid a\leq n\leq b\}$.

First we use a vertex-centered gauge field, meaning that for any directions η,ν and position x, $c_{x:\eta}=c_{x:\nu}$ but the two end of an edge can have different gauge field values—i.e. there is exactly one gauge field value per position. Therefore, c_x^e will denote the only gauge field value for position x and directions are omitted.

Then we choose G as gauge field alphabet and define the effect of a gauge transformation γ^x as

$$\gamma^x(c^e)_x = \gamma_x \circ c_x^e \tag{1.29}$$

such that the gauge field simply keeps track of every gauge transformation applied around x. For any other gauge field value, γ^x has no impact. This condition along with the extension property of definition 10 fully defines the new gauge transformation group Γ'.

Next we define a new local rule f' over the neighborhood R_x^5. The definition below just states that the local rule applies $\prod_{i\in R_x^2} c_i^{e-1}$ to undo all previous gauge transformations, it then computes the evolution of f, and finally reapplies all the gauge transformations:

$$\begin{cases} f'\left(c_{R_x^5}\right)^v &= \prod_{i\in R_x^1} c_i^e \circ f_{R_x^2}\left(\prod_{i\in R_x^4} c_i^{e-1}(c^v_{R_x^5})_{R_x^3}\right) \\ f'\left(c_{R_x^5}\right)^e &= c_x^e \end{cases} \tag{1.30}$$

where $f_{R_x^2}$ denotes the function from R_x^3 to R_x^2 which computes the temporal evolution of our automaton.

This local rule can be rewritten globally, using the notation c^e to denote both the gauge field and the gauge transformation which applies c_x^e at each position x:

$$F'(c)_x = \left(c^e \circ F \circ c^{e-1}(c^v), c^e\right)_x \tag{1.31}$$

Let us check that (F', Γ') is a gauge extension:

- *(Extended CA 5)* When the edge configuration is empty F' acts the same as F over the vertex configuration, and as the identity over the edge configuration.
- *(Extension 10)* This property was used to define G'.
- *(Gauge invariance 9)* For any $\gamma' \in \Gamma'$—where Γ' is built from G' through definition 8—the condition $\gamma' \circ F' = F' \circ \gamma'$ has to be checked. The reasoning is done globally to simplify notations and $\gamma = B(\gamma')$ from definition 10:

$$\begin{aligned}
\left(F' \circ \gamma'(c)\right)^e &= \left(\gamma' \circ F'(c)\right)^e && \text{(Equation 1.31)} \\
& && (1.32) \\
\left(F' \circ \gamma'(c)\right)^v &= F'(\gamma(c^v), \gamma(c^e))^v && \text{(Extension 10)} \\
&= \gamma(c^e) \circ F \circ \gamma(c^e)^{-1}(\gamma(c^v)) && \text{(Definition of } F') \\
&= \gamma \circ c^e \circ F \circ c^{e-1} \circ \gamma^{-1} \circ \gamma\left(c^v\right) && \text{(Equation 1.29)} \\
&= \gamma \circ c^e \circ F \circ c^{e-1}\left(c^v\right) && (1.33) \\
&= \gamma\left(F'\left(c\right)^v\right) && \text{(Definition of } F') \\
&= \left(\gamma' \circ F'\left(c\right)\right)^v && \text{(Extension 10)}
\end{aligned}$$

□

This theorem allows for any CA to be gauge extended. Hence, there exists an intrinsically universal GICA.

Corollary 2 (Gauge invariant universal cellular automata)**.** *For any alphabet* Σ *and local transformation group* G*, there exists an intrinsically universal one-dimensional* G'*-gauge invariant CA* F *where* G' *is an extension of* G *using definition 10.*

Proof. Let F be an intrinsically universal CA and a local transformation group G. Through theorem 2, there exists F', G' such that F' is a G'-gauge invariant CA that intrinsically simulates F. Through composition of the simulation, F' is a gauge invariant intrinsically universal CA. □

1.4. Degrees of freedom

Any symmetry leaves a degree of freedom when it is enforced. For instance, globally symmetric CA can be defined up to a global transformation without changing the dynamics itself. In the case of gauge invariance, the degrees of freedom are local, and this section aims at understanding the degree of freedom it provides through two notions of equivalence. First, two cellular automata may be equivalent up to a gauge transformation, i.e. the evolution of one is the composition of the evolution of the other with a gauge transformation. This equivalence characterizes the degree of freedom with regard to the evolution. Second, two configurations may be equivalent up to gauge transformation—i.e. one is the gauge transformed of the other—which characterizes the degree of freedom with regard to the description of a configuration.

1.4.1. Equivalence of cellular automata and gauge fixing

Given a set of gauge transformations Γ, multiple CA may lead to equivalent dynamics up to Γ, such CA will be said Γ-equivalent. To define the equivalence, the CA Z from definition 9 will be specified when stating that a CA is gauge invariant.

Definition 12 (Equivalence of gauge invariant CA)**.** *Let* F *be a gauge invariant CA with respect to a given* Γ *and* Z*.* F *is simulated by a CA* F' *if and only if for each element* $c \in \mathscr{C}$ *there exists* $\gamma, \gamma' \in \Gamma$ *such that*

$$(\gamma \circ F)(c) = (F' \circ \gamma')(c). \tag{1.34}$$

They are equivalent if both simulate each other.

A short version can be stated as follows: F is simulated by F' if and only if

$$\forall c \in \mathscr{C}, \exists \gamma, \gamma' \in \Gamma \text{ such that } (\gamma \circ F)(c) = (F' \circ \gamma')(c). \tag{1.35}$$

In practice, F' is also gauge invariant with respect to a specific Γ and Z. Adding a constraint on Z, one may characterize the equivalence of two CA using different quantifiers and constraints which may be useful for some specific problems.

Theorem 3 (Equivalence of evolutions)**.** *Let F be a gauge invariant CA with respect to Γ and Z. Let F' be another CA over the same alphabet as F. If Z is reversible and F' is gauge invariant with respect to Γ and Z, then these three statements are equivalent:*

1. *F is simulated by F'.*
2. *$\forall c, \exists \gamma \in \Gamma$ such that $F(c) = F' \circ \gamma(c)$.*
3. *$\forall c, \forall \gamma' \in \Gamma, \exists \gamma \in \Gamma$ such that $\gamma \circ F(c) = F' \circ \gamma'(c)$.*

Proof. We shall prove the equivalence through three implications.

- Suppose (1), then for c a configuration, we have $\gamma, \gamma' \in \Gamma$ such that $(\gamma \circ F)(c) = (F' \circ \gamma')(c)$. But since Γ is a group, it implies that $F(c) = (\gamma^{-1} \circ F' \circ \gamma')(c)$. Since Z is reversible and F is gauge invariant $F(c) = (F' \circ Z^{-1}(\gamma^{-1}) \circ \gamma')(c)$. However, $Z^{-1}(\gamma^{-1}) \circ \gamma'$ is an element of Γ therefore we have proven that (1) implies (2).
- Suppose (2), let c be a configuration and take $\gamma \in \Gamma$ such that $F(c) = F' \circ \gamma(c)$. Since Γ is a group, for any $\gamma_1 \in \Gamma$ there exists $\gamma_3 \in \Gamma$ such that $\gamma = \gamma_3 \circ \gamma_1$. Therefore, from gauge invariance of F', $F(c) = Z(\gamma_3) \circ F' \circ \gamma_1(c)$ which is equivalent to $Z(\gamma_3)^{-1} \circ F(c) = F' \circ \gamma_1(c)$ because G is a group. And writing $\gamma_2 = Z(\gamma_3)^{-1}$ which is in Γ, we conclude that (2) implies (3).
- The fact that (3) implies (1) is immediate because (3) is a generalization of (1): both statements differ only by the quantifier before γ. If for any γ the property is true, then it is also true for one specific γ.

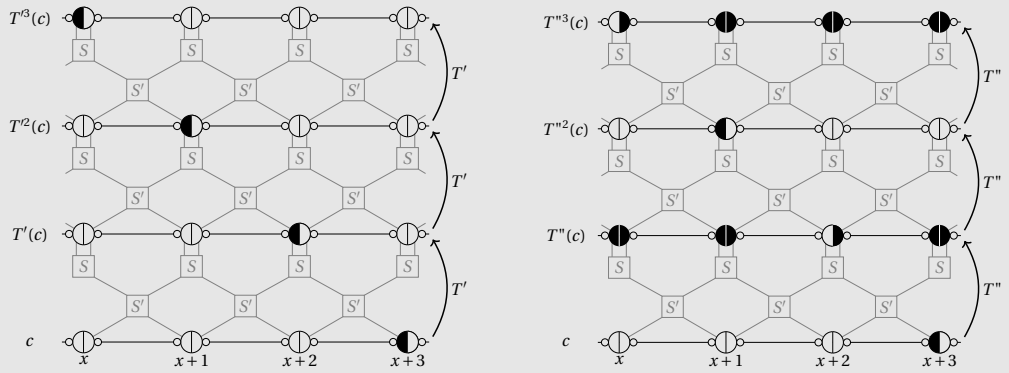
□

Gauge fixing. With equivalence of CA, one can use many representations for the same evolution model: two equivalent CA will model the same dynamics up to a gauge transformation. Therefore, there is a degree of freedom in choosing a specific CA as a model for a specific dynamics. Choosing this degree of freedom is called gauge fixing.

In other words, the explicit evolution scheme is undetermined because of the gauge invariance: if a configuration c at times t evolves into a configuration c', it is the same as if it evolved into $\gamma(c')$ for γ a gauge transformation. Gauge fixing is the choice of an explicit evolution scheme.

EXAMPLE: TWO EQUIVALENT TRANSPORT CA

Instead of the usual gauge invariant transport T', one could define the dynamics T" where the bits are flipped each time they are transported. One can intuitively see that it is almost the same, except that it completely flips the configuration with regard to the usual transport CA. In fact, these two automata are equivalent. This is represented in figure 1.11.



(a) Transport

(b) Transport with bit flip

Figure 1.11.: Equivalent dynamics

The two diagrams both show a bit moving to the left, starting with the same configuration. However on the right, at each odd time, it looks like a global transformation has been applied (which corresponds to a gauge transformation where the same operator γ has been applied everywhere). That illustrates the possibility to have two equivalent CA. Gauge fixing would be the specific choice of a dynamics.

1.4.2. Equivalence of configurations

Two configuration may be equivalent up to a gauge transformation.

Definition 13 (Equivalence of configurations)**.** *Let c and c' be two configurations. They are said equivalent if there exists a gauge transformation γ such that $c' = \gamma(c)$.*

This equivalence implies that there is a redundancy in the state representation. A simple way to remove this redundancy is to act directly on the equivalence classes of the gauge transformations, if they exist. Indeed, a GICA maps two equivalent configurations into two equivalent configuration, by definition of gauge invariance: for $c' = \gamma(c)$, one has that $F(c') = F \circ \gamma(c) = \gamma' \circ F(c)$.

However, when going quantum, such solution does not work any more because of the superposition of configurations: the superposition of two equivalent configurations that would not interfere normally may do so when considering their equivalence class. Hence, another approach will be required in that case. It is described in section 2.1.4.2.

In this chapter, gauge invariance was introduced in cellular automata as a commutation relation (1.11) of the evolution with a group of gauge transformations (definition 8). A notion of (gauge) extended cellular automata was also formalized in definitions 5 and 10. Two types of gauge extension were defined: relative and absolute. The former

puts a gauge field on the links between sites whereas the latter position it at each site. Using this distinction, global invariance (definition 6) in a cellular automaton was shown to be equivalent to having a relative gauge extension (theorem 1). Such result formalizes the link between global invariance and the possibility to extend the theory into a relative gauge invariant one. Coupling this equivalence with the universality of globally symmetric CA in one spatial dimension, the universality of one-dimensional gauge invariant CA was proven in corollary 1. This universality result was then generalized through a construction using an absolute gauge extension in theorem 2. Finally, the degrees of freedom left by gauge invariance were studied, and the equivalence between gauge invariant cellular automata was formalized in definition 12.

From classical to quantum

This chapter explored some classical properties of gauge invariance in cellular automata. The following chapter will focus on the quantum aspect, and how to use gauge invariance in quantum cellular automata for simulation purposes.

2. Quantum cellular and gauge invariance

The aim of the present chapter is to define the first natively relativistic discrete spacetime formulation of a 'real-life' QFT, namely 3+1 QED. There are three main challenges to this formulation: the implementation of the fermionic anti-commutation in a local manner, the definition of a magnetic term which did not appear in one dimension, the extension of the model to spin-dimension 4 when going from one or two spatial dimensions to the third.

Implementing the anti-commutation of fermions. Digital quantum simulation has been very successful at describing relativistic particles in different fields [65, 66, 67], but only a handful of works deal with interacting QFT with more than one particle [68, 69, 53, 56]. One of the difficulties is that in order to encode multiple fermions as qubits, one must enforce the anti-commutation of their creation/annihilation operators, e.g. through the Jordan-Wigner transformation. However, this method has all the looks of breaking locality, especially as soon as one considers more than one dimension of space. This was even formulated as a no-go result [70], stating that any QCA implementing the fermionic anti-commutation relations in two spatial dimensions would have very high internal space dimension, as in [71, 72]. But in the tensor network community, anti-commutation, locality and low internal space dimensions do coexist, at the cost of introducing a cut-off for the gauge field and two extra fermions per links, called rishons. And in lattice gauge theory, a solution where the fermionic degrees of freedom are replaced by bosonic ones at the cost of introducing two fermionic degrees of freedom, in addition to the bosonic ones, has been developed [73]. A similar idea, where just the parity of the gauge field is treated as a fermion, was hinted at in Farrelly's PhD thesis [74]. The first main contribution of this chapter is to combine these ideas and formalize them in the discrete spacetime setting. We introduce no extra field, but replicate the gauge field information once for each direction, as in the previous chapter. For each direction, its parity provides a rishon. Then the Jordan-Wigner transform needs only be implemented locally, at the level of each site. This does allow for a QCA of low internal space dimension, while enforcing fermionic anti-commutation. Ultimately, the reason why the no-go result [70] is circumvented is the presence of the gauge field, as well as our focus on expressing the *dynamics* in qubit-local manner—the creation/annihilation operators remain qubit non-local.

Fully discrete magnetic contribution. In QED's gauge invariant states, the fermions are the sources of the gauge field lines. In one spatial dimension there is no magnetic term, lines are confined to the unique dimension, and thus they have no dynamics

[53]. But in two and three spatial dimension, the Hamiltonian has an added magnetic term, a.k.a. the plaquette term. The second main contribution of this chapter is to introduce two possible discrete spacetime counterparts to the plaquette term. The first proposition works by simply integrating the plaquette term in the Fourier basis. But it requires a prior cut-off in the gauge field degrees of freedom, and allows for arbitrary changes in values within that cut-off, even in one time step. The second proposition takes the form of a local quantum walk (QW)-like evolution in the local gauge field degrees of freedom of each plaquette. It does not require a prior cut-off and ensures that gauge field values only change one step at a time. Both constructions agree in the continuum limit.

Further spin-dimensions. In one and two spatial dimensions, the Dirac equation is a PDE on a wave function having two complex amplitudes at each site, corresponding to internal degrees of freedom spin up and down. In the multi-particle settings, and because there can be no more than one particle in a given state and site, the four occupation numbers of a site are thus: no fermion, one spin up, one spin down, and, both a spin up and a spin down. This could be encoded as 2 qubits in the Dirac QCA. Going to three spatial dimensions, the Dirac equation now requires four complex amplitudes to encode the fermionic degrees of freedom. In the multi-particle settings, the number of qubits per site has then to be increased from 2 to 4 qubits, which makes the QCA a bit more involved. The third main contribution is to provide a construction of the $3+1$ QED QCA that matches the Dirac QW when restrained to the one particle sector, and implements the electric and magnetic contributions.

The chapter is organized as follows. In section 2.1 we set the conventions and show how to enforce the fermionic anti-commutation relations while allowing for a qubit-local definition of the gauge invariant operators that govern the dynamics of the theory. In section 2.2, we gradually derive the gauge invariant dynamics of the $2+1$ QED QCA starting from the Dirac QCA and adding the electric and magnetic contributions—the simpler, two spatial dimensional case makes the argument clearer. In section 2.3, we reach the $3+1$ QED QCA. Finally, we provide some perspectives.

2.1. Enforcing anti-commutation, locality and gauge invariance

In QFT, fermionic particles are represented by means of operators that annihilate them or create them at position x. These are denoted a_x and $a_x^\dagger$ respectively. Applying the annihilator on quantum states takes occupation number $|1\rangle^x$ to $|0\rangle^x$ and produces the null vector otherwise. The creator takes $|0\rangle^x$ to $|1\rangle^x$ and produces the null vector otherwise. Moreover, these operators are required to have the specific anti-commutation relations $\{a_x, a_y^\dagger\} = \delta_{x,y}$ where $\{\cdot,\cdot\}$ denotes the anti-commutator and δ the Kronecker delta.

In order to obtain a quantum numerical scheme for a QFT, to be run on a generic quantum computer or some specific-purpose quantum simulation device, we need to encode the QFT degrees of freedom as a lattice of qubits. The natural point of

departure is to interpret the occupation number degrees of freedom at each site (i.e. $|1\rangle^x$ vs $|0\rangle^x$), as qubits, thereby obtaining a lattice of qubits. But enforcing the fermionic anti-commutation whilst remaining qubit-local is non-trivial.

In subsection 2.1.2, the impact of the fermionic anti-commutation relations upon the qubit-local operators that are needed to express the discrete time dynamics, will be carefully worked out. In order to obtain them, however, we crucially rely on there being a gauge field, as demanded by gauge invariance.

2.1.1. Introducing the gauge field

The QED Lagrangian is built by considering the Dirac Lagrangian for free fermions, and then demanding that it be gauge invariant, under $U(1)$ gauge-transformations. This is impossible without introducing a new field, the gauge field, which in the case of QED turns out to be the electromagnetic field.

We will proceed in the same manner in the discrete. One reason for that is that in numerical analysis, the fact that a numerical scheme conserves the original symmetries is desirable and seen as a good sign of numerical stability. The other reason is more fundamental, as we aim to show that a natively discrete spacetime formulation of QED is just as legitimate at the Lagrangian formulation, in terms of its justification through symmetries.

Discrete gauge invariance in the context of classical cellular automata has been formalized in chapter 1. Together with the treatment of gauge invariance upon quantum walks [75, 76, 77, 78] and in lattice gauge theories in general [8], it inspired [53] to formulate discrete gauge invariance in the context of QCA in the following manner.

Discrete gauge transformations are again based on a group of local transformations, based upon the $U(1)$ group in the case of QED. Let $\varphi : \mathbb{Z} \to \mathbb{R}$, we denote by g_φ the discrete gauge transformation which associates, to each position, a local transformation parametrized by $\varphi(x)$. The local transformation at position x is denoted $g_{x,\varphi}$ and is defined as

$$g_{x,\varphi} : |l\rangle^x \mapsto e^{il\varphi(x)} |l\rangle^x \tag{2.1}$$

$$|l\rangle^y \mapsto |l\rangle^y \qquad \text{if } x \neq y. \tag{2.2}$$

Thus, a discrete gauge transformation g_φ is essentially a space-dependent phase, exempt of any regularity requirement, applied at every point of the lattice in accordance to the occupation number at that point. To be gauge invariant, the evolution of a QCA must commute with every possible gauge transformation.

The Dirac QCA, which solely describes moving fermions, is not gauge invariant unless we introduce the gauge field. The argument boils down to the elementary fact that, as a particle moves from position x to the adjacent position $x+\eta$,

$$|1\rangle^x \otimes |0\rangle^{x+\eta} \longmapsto |0\rangle^x \otimes |1\rangle^{x+\eta} \tag{2.3}$$

the discrete gauge transformation will trigger a phase $\varphi(x)$ applied beforehand, or

a phase $\varphi(x+\eta)$ applied afterwards. It follows that fermionic transport does not commute with gauge transformations.

In order to fix this, one needs to introduce a gauge field on the link between x and site $x+\eta$. A gauge field is much like a doorman/bouncer counter. It adds one whenever a particle crosses the link. Actually, in the present chapter, we will not place just one bouncer per link, but two. The bouncer at $x:\eta$ counts positively the number of fermions leaving x towards the link, and negatively those entering x from the link. The bouncer at $(x+\eta):-\eta$ counts negatively the number entering $x+\eta$ from the link, and positively those leaving $x+\eta$ towards the link. Now fermionic transport acts as

$$|1\rangle^{x}|l\rangle^{x:\eta}\otimes|-l\rangle^{(x+\eta):-\eta}|0\rangle^{x+\eta}\longmapsto|0\rangle^{x}|l+1\rangle^{x:\eta}\otimes|-l-1\rangle^{(x+\eta):-\eta}|1\rangle^{x+\eta} \tag{2.4}$$

and the discrete gauge transformation triggers a phase $(l+1)\varphi(x)-l\varphi(x+\eta)$ regardless of whether it is applied before of after the move.

The restriction that the two gauge fields of a link be opposite of signs, as in $|l\rangle^{x:\eta}$ and $|-l\rangle^{(x+\eta):-\eta}$, is quite natural if we think of them as holding the total number of fermions that went through the link, ever, and nothing else. Still, this restriction is not a necessity for gauge invariance. However, lifting the restriction is not a necessity for gauge invariance either, and in fact it would introduce an unnecessary degree of freedom: one that is not demanded by gauge invariance. So, this restriction is a necessity if we further demand 'minimal' gauge invariance, i.e. demand the gauge field to be obtained as a relative gauge extension (definition 11). We impose it across the grid, except of course at the boundaries, where it becomes vacuous.

Placing two gauge fields per link is non-standard but has several advantages: (i) each gauge field is well localized on a site, (ii) it gauge transforms in the same way as the fermions on that site, (iii) this is number conserving, (iv) it will help to implement the fermionic anti-commutation relations in a qubit-local manner as we will now see.

2.1.2. (Anti-)commuting annihilation and lowering operators

Consider the lattice generated by unit vectors describing the space directions. These vectors are denoted μ, ν and ρ, in two spatial dimensions, only μ and ν are used.

At each lattice site x lies a group of d qubits, each stating whether a fermion in mode $j\in 0\ldots(d-1)$ is present at the site. The possible modes correspond to the number of internal degrees of freedom (e.g. the spin) of the fermions. This encoding captures the Pauli exclusion principle as there cannot be two fermions in the same mode at the same site.

Each link (x,η) (where $\eta\in\{\pm\mu,\pm\nu,\pm\rho\}$) has a gauge field attached at both ends: one at $x:\eta$ and the other a $(x+\eta):-\eta$. Each gauge field lives in the Hilbert space of integers $\mathscr{H}_{\mathbb{Z}}$.

The electric counting operator, denoted $E_{x,\eta}$, is the observable corresponding to the gauge fields, i.e. is acts as $E_{x,\eta}|l\rangle^{x:\eta}=l|l\rangle^{x:\eta}$ and as the identity elsewhere. Following the restriction that the two gauge fields of a link be of opposite signs, one has $E_{x,\eta}=-E_{x+\eta,-\eta}$. The lowering operator of the gauge fields is $r_{x,\eta}$. It acts as $r_{x,\eta}|l\rangle^{x:\eta}=$

$|l-1\rangle^{x:\eta}$. Most often we need to act on both the gauge fields of a link with $U_{x,\eta} = r_{x,\eta} r^\dagger_{x+\eta,-\eta}$. One has $U_{x,\eta} = U^\dagger_{x+\eta,-\eta}$—i.e. lowering the gauge field value attached to one site corresponds to raising on the other site.

The operator Z denotes the parity observable. On a qubit, it acts like the Pauli Z, on a gauge field it acts as $Z|2l\rangle = |2l\rangle$ and $Z|2l+1\rangle = -|2l+1\rangle$.

All the operators described so far are qubit-local. We will now represent the fermionic annihilation $a_{x,j}$ and gauge lowering operators $V_{x,\eta}$ of the QFT as products of these qubit-local operators. These implementations will not be qubit-local, as we must meet the desired (anti-)commutation relations:

$$\{a_{x,j}, a^\dagger_{y,k}\} = \delta_{x,y}\delta_{j,k} \tag{2.5}$$

$$[V_{x,\eta}, V_{y,\zeta}] = 0 \tag{2.6}$$

$$[V_{x,\eta}, a_{y,j}] = 0 \tag{2.7}$$

with $\{\cdot,\cdot\}$ the anti-commutator, $[\cdot,\cdot]$ the commutator and $\delta_{x,y}$ corresponding to Kronecker delta.

These commutation relations are commonly implemented by means of the Jordan-Wigner (JW) transform. This will be the basis for the redefined version of the operators. However, in $2+1$ and $3+1$ dimensions, it leads to non-locality of the operators expressing dynamics if used as is [70]. In order to fix this we use the idea hinted in [74] and treat the parity of the gauge fields as a fermion. Moreover, we use two gauge fields per link, so that this parity plays the role of the rishons of lattice gauge theories.

Let $\prec$ denote a so-called JW order between all the registers, whether qubits or gauge fields. The sole requirement to make this work is that the registers at any given site be contiguous, i.e. they follow each other. In what follows, the examples will use, quite arbitrarily, that for a given site x, the gauge fields are ordered as $(x,0) \prec \ldots \prec (x,d-1) \prec x:-\mu \prec x:\mu \prec x:-\nu \prec x:\nu \prec x:-\rho \prec x:\rho$.

We define fermionic creation and gauge lowering operators based on this order. Let x be a position, j a mode and η a direction:

$$a^\dagger_{x,j} = |1\rangle^{x,j}\langle 0| \prod_{y\prec(x,j)} Z_y \tag{2.8}$$

$$s_{x,\eta} = r_{x,\eta} \prod_{y\prec x:\eta} Z_y \tag{2.9}$$

$$V_{x,\eta} = s_{x,\eta} s^\dagger_{x+\eta,-\eta} \tag{2.10}$$

$$= r_{x,\eta} \left(\prod_{y\in\left[x:\eta, x+\eta:-\eta\right[} Z_y \right) r^\dagger_{x+\eta,-\eta} \tag{2.11}$$

where $\left[a,b\right[$ is short for $\left[\min\{a,b\},\max\{a,b\}\right[$. When $x:\eta \prec x+\eta:-\eta$, this interval

does not contain $x+\eta:-\eta$ and $r_{x+\eta,-\eta}$ commutes the Z_ys leading to the simplification:

$$V_{x,\eta} = U_{x,\eta} \prod_{y\in\left[x:\eta,x+\eta:-\eta\right[} Z_y \tag{2.12}$$

The following fermionic anti-commutation relations are ensured by the JW transform:

$$\{a_{x,j}, a^\dagger_{y,k}\} = \delta_{x,y}\delta_{j,k} \tag{2.13}$$
$$\{s_{x,\eta}, s^\dagger_{y,\zeta}\} = \delta_{x,y}\delta_{\eta,\zeta} \tag{2.14}$$
$$\{a_{x,j}, s^\dagger_{y,\eta}\} = 0. \tag{2.15}$$

Since $V_{x,\eta}$ composed of two fermion-like operators, equations (2.14) and (2.15) yield:

$$[V_{x,\eta}, V_{y,\zeta}] = 0 \tag{2.16}$$
$$[V_{x,\eta}, a_y] = 0. \tag{2.17}$$

Hence, the (anti-)commutation of equations (2.5), (2.6) and (2.7) are ensured.

2.1.3. Local evolution operators

The annihilator operators $a^\dagger_{x,j}$ are not qubit-local since they have an infinite trail of Z operators. The lowering operators $V_{x,\eta}$ can also be non-local as soon as both ends of the link are far apart in the JW order. However, these operators are never required by themselves, except perhaps for some initial state preparation, but Physics does not demand that state preparation be a local process and $a^\dagger_{x,j}$ could then be understood as the result of a particle having come from infinity to its current position through local evolutions.

What matters physically is the evolution be local. One can then consider the operators allowing to express that: (i) the movement of fermions be that of free fermionic QCA, (ii) the gauge field induce an interaction between fermions—through the electric contribution, (iii) the gauge field vibrates—through the magnetic contribution. From these requirements, we can define the simplest qubit-local gauge invariant operators (checking for gauge invariance is postponed till subsection 2.1.4):

$$a^\dagger_{x,j} a_{x,k} \tag{2.18}$$
$$a^\dagger_{x+\eta,j} V^\dagger_{x,\eta} a_{x,k} \tag{2.19}$$
$$E^2_{x,\eta} \tag{2.20}$$
$$P_{x,\eta,\zeta} = V_{x,\eta} V_{x+\eta,\zeta} V^\dagger_{x+\zeta,\eta} V^\dagger_{x,\zeta} \tag{2.21}$$

with $\eta,\zeta \in \{\mu,\nu,\rho\}$ and $\eta \neq \zeta$. Eq. (2.18) represents a mass term (i.e. a fermionic only

operation, local to a site, changing the mode), Eq. (2.19) corresponds to a fermion hopping term (i.e. a transport), Eq. (2.20) is the squared electric operator defined previously, and Eq. (2.21) is a plaquette term (i.e. a local vibration of the gauge field). The QED QCA evolutions will be defined based upon those operators.

The mass term is qubit-local because it involves a pair of fermionic operators acting on the same site, cancelling out the trail of Z outside this site. The electric term is qubit-local by definition.

For the hopping term, developing the gauge field operators $V_{y,\gamma}$ as pairs $s_{y,\gamma}$ and $s^\dagger_{y+\gamma,-\gamma}$ on each side of the link, allows for the pairing of an annihilator a with an s on each site, thus cancelling out the Z outside the sites:

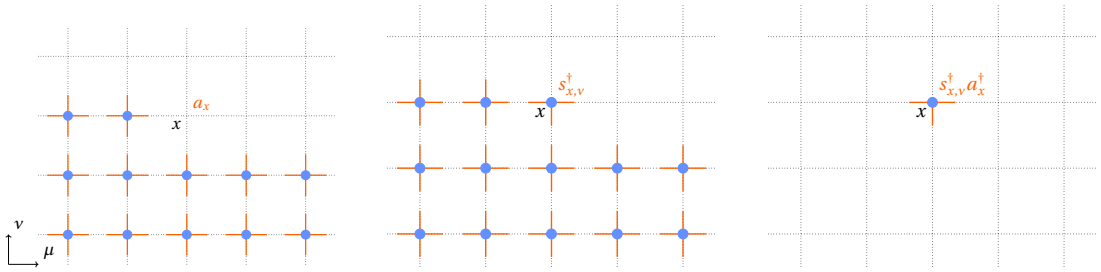
$$a^\dagger_{x+\eta,j} V^\dagger_{x,\eta} a_{x,k} = a^\dagger_{x+\eta,j} (s_{x+\eta,-\eta} s^\dagger_{x,\eta}) a_{x,k} \tag{2.22}$$

$$= (a^\dagger_{x+\eta,j} s_{x+\eta,-\eta})(s^\dagger_{x,\eta} a_{x,k}) \tag{2.23}$$

$$= |1\rangle^{x+\eta,j} \langle 0| \left(\prod_{y \in \left[(x+\eta,j),x+\eta:-\eta\right[} Z_y \right) r_{x+\eta,-\eta} r^\dagger_{x,\eta} \left(\prod_{y \in \left[(x,k),x:\eta\right[} Z_y \right) |0\rangle^{x,k} \langle 1| \tag{2.24}$$

$$= |1\rangle^{x+\eta,j} \langle 0| \left(\prod_{y \in \left[(x+\eta,j),x+\eta:-\eta\right[} Z_y \right) U^\dagger_{x,\eta} \left(\prod_{y \in \left[(x,k),x:\eta\right[} Z_y \right) |0\rangle^{x,k} \langle 1|. \tag{2.25}$$

The remaining Z operator are on sites x and $x+\eta$. The qubit-locality of the pair $s^\dagger_{x,\eta} a_{x,\eta}$, which is the local brick from which the hopping term is built, is illustrated in figure 2.1.



(a) $a_{x+\nu}$ (b) $s^\dagger_{x,\nu}$ (c) $s^\dagger_{x,\nu} a_x$

Figure 2.1.: Visualization of locality for $s^\dagger_{x,\nu} a_x$. The colored dots and lines corresponds to Z operators acting on fermions and gauge fields respectively. Each operator Z_y is applied exactly twice which cancels them out except on site x. Here, only one fermionic mode per site is represented, for clarity.

For the plaquette term—i.e. Eq. (2.21)—notice that it forms a small loop of four gauge field links. Developing each gauge operator $V_{y,\gamma}$ as a pair $s_{y,\gamma}$ and $s^\dagger_{y+\gamma,-\gamma}$, and reordering the resulting product of s, one gets two anti-commuting operators per site.

Hence, the string of Z cancels out outside the site they act on:

$$P_{x,\eta,\zeta} = V_{x,\eta} V_{x+\eta,\zeta} V^\dagger_{x+\zeta,\eta} V^\dagger_{x,\zeta} \tag{2.26}$$
$$= \left(s_{x,\eta} s^\dagger_{x+\eta,-\eta}\right)\left(s_{x+\eta,\zeta} s^\dagger_{x+\eta+\zeta,-\zeta}\right)\left(s_{x+\eta+\zeta,-\eta} s^\dagger_{x+\zeta,\eta}\right)\left(s_{x+\zeta,-\zeta} s^\dagger_{x,\zeta}\right) \tag{2.27}$$
$$= -s^\dagger_{x+\eta,-\eta}\left(s_{x+\eta,\zeta} s^\dagger_{x+\eta+\zeta,-\zeta}\right)\left(s_{x+\eta+\zeta,-\eta} s^\dagger_{x+\zeta,\eta}\right)\left(s_{x+\zeta,-\zeta} s^\dagger_{x,\zeta}\right) s_{x,\eta} \tag{2.28}$$
$$= -\left(s^\dagger_{x+\eta,-\eta} s_{x+\eta,\zeta}\right)\left(s^\dagger_{x+\eta+\zeta,-\zeta} s_{x+\eta+\zeta,-\eta}\right)\left(s^\dagger_{x+\zeta,\eta} s_{x+\zeta,-\zeta}\right)\left(s^\dagger_{x,\zeta} s_{x,\eta}\right) \tag{2.29}$$

where the minus sign that appears between the second and third line comes from the anti-commutation of $s_{x,\eta}$ with the other 7 operators. In order to better understand the structure of the local, minus signs in this term, it is helpful to break down the plaquette term into constituent, smaller qubit-local operators. Indeed, let us define the corner operators $c_{x,\eta,\zeta}$ as

$$c_{x,\eta,\zeta} = s^\dagger_{x,\zeta} s_{x,\eta} \tag{2.30}$$
$$= r^\dagger_{x,\zeta}\left(\prod_{y\in\left[x:\eta,x:\zeta\right[} Z_y\right) r_{x,\eta}. \tag{2.31}$$

These are local to x since the Z are on site x. A corner operator would be the result of a fermion having come from direction η, passed through site x, and left in the direction ζ. The plaquette operator can then be redefined as:

$$P_{x,\eta,\zeta} = -c_{x+\eta,\zeta,-\eta}\; c_{x+\eta+\zeta,-\eta,-\zeta}\; c_{x+\zeta,-\zeta,\eta}\; c_{x,\eta,\zeta}. \tag{2.32}$$

Thus, equations (2.25) and (2.32) allow the fermionic and bosonic dynamics terms (left-hand-side of the equations) to be expressed into simpler qubit-local dynamics (right-hand-side).

Notice that the only dependency of these local evolution operators w.r.t the JW order, is per-site, and could be made independent from one site to the other.

2.1.4. Gauge invariance

Gauge invariance was introduced in section 2.1.1 to motivate the need for a gauge field. It remains to be checked that above-defined local evolution operators are gauge invariant.

2.1.4.1. Gauge invariant operators

Gauge invariance is the commutation with gauge transformations, i.e. with space-dependent phases proportional to the occupation number. Because the annihilation and lowering operators act on the occupation number, they individually are not gauge invariant. However, the local evolution operators combine multiple annihilation and

lowering operators so that the total occupation number of a site is unchanged (only the distribution inside the site is modified)—e.g. a fermion leaving site x will reduce the number of fermions by one, but increase one of the gauge fields at x by one.

In order to formally show this, let us first write the commutation relations for the individual annihilation operators $a_{x,j}$

$$a_{x,j} g_\varphi = e^{i\varphi(x)} g_\varphi a_{x,j} \tag{2.33}$$
$$a^\dagger_{x,j} g_\varphi = e^{-i\varphi(x)} g_\varphi a^\dagger_{x,j}, \tag{2.34}$$

the gauge field operators on half-links $s_{x,\eta}$

$$s_{x,\eta} g_\varphi = e^{i\varphi(x)} g_\varphi s_{x,\eta} \tag{2.35}$$
$$s^\dagger_{x,\eta} g_\varphi = e^{-i\varphi(x)} g_\varphi s^\dagger_{x,\eta}, \tag{2.36}$$

and the gauge field operators $V_{x,\eta}$

$$V_{x,\eta} g_\varphi = e^{i(\varphi(x)-\varphi(x+\eta))} g_\varphi V_{x,\eta} \tag{2.37}$$
$$V^\dagger_{x,\eta} g_\varphi = e^{i(-\varphi(x)+\varphi(x+\eta))} g_\varphi V^\dagger_{x,\eta}. \tag{2.38}$$

Based on these commutation relations, we derive those of the local evolution operators. For the mass term:

$$\left(a^\dagger_{x,j} a_{x,k}\right) g_\varphi = a^\dagger_{x,j} \left(a_{x,k} g_\varphi\right) \tag{2.39}$$
$$= a^\dagger_{x,j} \left(e^{i\varphi(x)} g_\varphi a_{x,k}\right) \tag{2.40}$$
$$= e^{i\varphi(x)} \left(a^\dagger_{x,j} g_\varphi\right) a_{x,k} \tag{2.41}$$
$$= e^{i\varphi(x)} \left(e^{-i\varphi(x)} g_\varphi a^\dagger_{x,j}\right) a_{x,k} \tag{2.42}$$
$$= g_\varphi \left(a^\dagger_{x,j} a_{x,k}\right). \tag{2.43}$$

Hence, the mass term is gauge invariant.

For the hopping term:

$$\left(a^\dagger_{x+\eta,j} V^\dagger_{x,\eta} a_{x,j}\right) g_\varphi = a^\dagger_{x+\eta,j} V^\dagger_{x,\eta} \left(a_{x,j} g_\varphi\right) \tag{2.44}$$
$$= a^\dagger_{x+\eta,j} V^\dagger_{x,\eta} \left(e^{i\varphi(x)} g_\varphi a_{x,j}\right) \tag{2.45}$$
$$= a^\dagger_{x+\eta,j}\, e^{i\varphi(x)} \left(V^\dagger_{x,\eta} g_\varphi\right) a_{x,j} \tag{2.46}$$
$$= a^\dagger_{x+\eta,j}\, e^{i\varphi(x)} \left(e^{i(-\varphi(x)+\varphi(x+\eta))} g_\varphi V^\dagger_{x,\eta}\right) a_{x,j} \tag{2.47}$$
$$= e^{i\varphi(x+\eta)} \left(a^\dagger_{x+\eta,j} g_\varphi\right) V^\dagger_{x,\eta} a_{x,j} \tag{2.48}$$
$$= e^{i\varphi(x+\eta)} \left(e^{-i\varphi(x+\eta)} g_\varphi a^\dagger_{x+\eta,j}\right) V^\dagger_{x,\eta} a_{x,j} \tag{2.49}$$
$$= g_\varphi \left(a^\dagger_{x+\eta,j} V^\dagger_{x,\eta} a_{x,j}\right). \tag{2.50}$$

Hence, the hopping term is gauge invariant.

The electric term does not change the occupation number, hence it is directly gauge invariant:

$$E_{x,\eta} g_\varphi = g_\varphi E_{x,\eta}. \tag{2.51}$$

As for the plaquette term, we start by showing the gauge invariance of the corner operator:

$$c_{x,\eta,\zeta} g_\varphi = s^\dagger_{x,\zeta} s_{x,\eta} g_\varphi \tag{2.52}$$
$$= s^\dagger_{x,\zeta} \left(e^{i\varphi(x)} g_\varphi s_{x,\eta}\right) \tag{2.53}$$
$$= e^{i\varphi(x)} \left(s^\dagger_{x,\zeta} g_\varphi\right) s_{x,\eta} \tag{2.54}$$
$$= e^{i\varphi(x)} \left(e^{-i\varphi(x)} g_\varphi s^\dagger_{x,\zeta}\right) s_{x,\eta} \tag{2.55}$$
$$= g_\varphi \left(s^\dagger_{x,\zeta} s_{x,\eta}\right) \tag{2.56}$$
$$= g_\varphi c_{x,\eta,\zeta}. \tag{2.57}$$

Since the plaquette term is a product of four corner operators, its gauge invariance is ensured.

The QCA operators that will be defined in the next sections are linear combination or exponentials of the hopping, electric and magnetic terms. Therefore, their gauge invariance is ensured by the individual gauge invariance of those terms.

2.1.4.2. Gauge invariant states

In a gauge theory, gauge transformations should not be observable. Let $\mathcal{O}$ be an observable, ρ a density matrix representing a state and g_φ a gauge transformation. That gauge transformations should not be observable amounts to asking that $\mathrm{Tr}\left(\mathcal{O} g_\varphi \rho g^\dagger_\varphi\right) =$

$\mathrm{Tr}(\mathcal{O}\rho)$. There are two common ways to enforce this: namely to restrict the set of observables to the gauge invariant ones $[\mathcal{O}, g_\varphi] = 0$, so that $\mathrm{Tr}\left(\mathcal{O} g_\varphi \rho g_\varphi^\dagger\right) = \mathrm{Tr}\left(g_\varphi \mathcal{O} \rho g_\varphi^\dagger\right) = \mathrm{Tr}\left(g_\varphi^\dagger g_\varphi \mathcal{O} \rho\right) = \mathrm{Tr}(\mathcal{O}\rho)$ or to restrict the set of states to the gauge invariant ones, so that $\mathrm{Tr}\left(\mathcal{O} g_\varphi \rho g_\varphi^\dagger\right) = \mathrm{Tr}\left(\mathcal{O}\rho g_\varphi g_\varphi^\dagger\right) = \mathrm{Tr}(\mathcal{O}\rho)$. We opt for the second, demanding that for every gauge transformation,

$$g_\varphi \rho = \rho g_\varphi. \tag{2.58}$$

Let us draw the consequences of this demand that the states be gauge-invariant. Any density matrix ρ is a convex linear combination over pure states. In the case of a pure state $|\psi\rangle\langle\psi|$, this commutation relation amounts to forbidding superposition across any two eigenspaces of a gauge transformation, so that $g_\varphi |\psi\rangle\langle\psi| = e^{i\lambda} |\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| e^{i\lambda} = |\psi\rangle\langle\psi| g_\varphi$ with $e^{i\lambda}$ the eigenvalue of the eigenspace of g_φ to which $|\psi\rangle$ pertains. In other words, $|\psi\rangle = \sum_{c\in S} \alpha_c |c\rangle$ is a superposition of particular basis states $|c\rangle$, i.e. taken in some subset S such that for all φ there exists λ, such that for all $c \in S$, $g_\varphi |c\rangle = e^{i\lambda} |c\rangle$. Let $f(x)$ denote the sum of the occupation numbers, for both the fermions and the gauge fields, at each site x of c. Because the $\lambda = \sum_x \varphi(x) f(x)$ and $\varphi(x)$ is arbitrary, the gauge-invariance therefore imposes that $f(x)$ be the same for $c \in S$. Thus, gauge-invariance demands that there exists some fixed, classical occupation number function $f(x)$, and that pure states be considered physical if and only if, at each position x, the occupation number operator yields $f(x)$:

$$\left(\sum_{\eta\in\{\pm\mu,\pm\nu,\pm\rho\}} E_{x,\eta} + \sum_{j\in 0\ldots(d-1)} |1\rangle^{x,j}\langle 1| \right) |\psi_{\text{phys}}\rangle = f(x) |\psi_{\text{phys}}\rangle . \tag{2.59}$$

The physical pure states then form a subspace, call it the $f(x)$-subspace. The choice of a particular $f(x)$ can be interpreted physically as the choice of a classical fixed external charge. Counter-intuitively, the 'zero total charge' is usually not associated to the $f(x) = 0$ choice, but with the $f(x \text{ even}) = 0$ and $f(x \text{ odd}) = d$ convention, as we will soon discuss.

Having fixed $f(x)$ and thus S, one may wonder about the operators which allow us to prepare some basic state $c' \in S$ given initial basic state $c \in S$, e.g. by creating a fermion. As seen previously, the fermionic annihilators $a_{x,j}$ is not gauge invariant; it does not preserve occupation numbers and will take us out of S. Following ideas from [79], each fermion creation operator $a^\dagger_{x,j}$ could be turned into a gauge invariant state preparation by accompanying it with a gauge field lowering operator $V_{x,\eta}$, but this changes the occupation number at position $x+\eta$, which in turn has to be compensated by a $V_{x+\eta,\zeta}$, and so on until a boundary (possibly infinitely far) is reached. The following defined a gauge invariant state preparation:

$$\overline{a}^\dagger_{x,j,p} = a^\dagger_{x,j} \prod_{y:\eta\in p} V_{y,\eta} \tag{2.60}$$

where p is a gauge field path from position x to the space boundary (possibly infinite). If the lattice is finite, the last operator is understood to be a half-link transformation

s, instead of V, since there would be no end to the last link. (Notice that $a^\dagger_{x,j} s_{x,\eta}$ is also gauge invariant operator, but disallowed as it breaks the restriction that $E_{x,\eta} = -E_{x+\eta,-\eta}$, except at the boundary.)

The state preparation $\overline{a}^\dagger_{x,j,p}$ follows the prescribed anti-commutation relations. Indeed, recalling Eq. (2.7), we have that $a_{x,j}$ commutes with any $V_{y,\eta}$, hence $\overline{a}^\dagger_{x,j,p}$ also does. Moreover, within two operators $\overline{a}_{x,j,p}$ and $\overline{a}_{y,k,q}$, the fermionic parts $a_{x,j}$ and $a_{y,k}$ anti-commute, while every other pair of operators commutes, enforcing the fermionic anti-commutation relation (2.5).

Another gauge invariant state preparation is the creation of a gauge field loop, i.e. $\prod_{y:\eta\in p} V^\dagger_{y,\eta}$ where p is a cyclic gauge field path, or one that begins and ends at a boundary.

Pair creation. The state preparation $\overline{a}^\dagger_{x,j,p}$ can be understood as 'bringing a fermion from infinity' (or from the boundary) but it does not allow for the creation of an electron-positron pair in situ.

However, according to the Dirac sea convention, we may take as the zero total charge states those that lie in the $f(x)$-subspace where $f(x \text{ even}) = 0$ and $f(x \text{ odd}) = d$. Then, the canonical, Dirac sea vacuum is that where all gauge fields are set to zero, implying that even sites have no fermions and odd sites are full with fermions. For instance, in $1+1$, where $d = 2$ and representing only fermions for a minute, the state $\ldots|00\rangle^x|11\rangle^{x+\mu}\ldots$ is the Dirac sea vacuum for this $f(x)$-subspace.

Consider acting at an odd site with $a_{x+\eta,j}$, mapping $|1\rangle^{x+\eta,j}$ into $|0\rangle^{x+\eta,j}$. In order to remain in the $f(x)$-subspace, we must compensate this with some $V^\dagger_{x+\eta,\eta'}$, which changes the occupation number at $x+\eta+\eta'$ and so on along path p, generating field lines according to operator $\overline{a}_{x+\eta,j,p}$, i.e. the exact inverse of the earlier discussed creation of an electron $\overline{a}^\dagger_{x,j}$. It follows that this process can be interpreted as the creation of a positron. In other words a $|1\rangle^{x,j}$ at an even site, represents an electron, but a $|0\rangle^{x+\eta,j}$ at an odd site, represents a positron. And so $|1\rangle^{x+\eta,j}$ at an odd site, represents a positron-hole, i.e. the absence of a positron.

Finally, consider the hopping of a fermionic occupation number from an odd to an even site, mapping

$$|0\rangle^{x,i} \otimes |1\rangle^{x+\eta,j} \longmapsto |1\rangle^{x,i} \otimes |0\rangle^{x+\eta,j} \tag{2.61}$$

as implemented in a gauge-invariant and anti-commutation compliant manner by Eq. (2.25). This, therefore, must be interpreted as a positron-hole $|1\rangle^{x+\eta,j}$, moving to x even to create an electron $|1\rangle^{x+\eta,j}$ and leaving a positron $|0\rangle^{x+\eta,j}$ behind. This is an electron-positron pair creation. The reverse evolution is an electron-positron pair annihilation.

2.2. $2+1$ Quantum Cellular Automaton

Using the previously defined local, gauge invariant operators, it is possible to define a QCA that accounts for QED in $2+1$ dimensions. We proceed in three steps, following the same principles as that leading to the QED Lagrangian. First, a gauge invariant free dynamics for the fermions is defined through a generalization of a Dirac quantum walk (QW) to multiple walkers. Second, the electric contribution is defined as one of the simplest gauge invariant operator acting on the gauge field based on the electric operator. It is found to match the Trotterization of the electric part of the Kogut-Susskind Hamiltonian [37]. Third, the magnetic part is added as one the simplest gauge invariant operator acting on the gauge field with the lowering and raising operators. In fact, two constructions are provided for this magnetic term, both agreeing in the limit and matching a Trotterization of the magnetic Kogut-Susskind Hamiltonian.

Before delving into the Physics of the model, let us formally define quantum cellular automata.

2.2.1. Quantum cellular automata

The quantum configurations differ from classical configurations because they require a distinguished element of Σ to be called the *empty state* and such that only a finite number of cells are not empty.

Definition 14 (Finite unbounded configurations)**.** *Consider Σ the alphabet, with 0 a distinguished element of Σ, called the* empty *state. A* finite unbounded configuration *c over Σ is a function $c : \mathbb{Z}^d \longrightarrow \Sigma$, such that the set of the $(i_1,\dots,i_d) \in \mathbb{Z}^d$ for which $c_{i_1\dots i_d} \neq 0$, is finite. The set of all finite unbounded configurations will be denoted $\mathscr{C}_f$.*

The finite unbounded configurations are taken as basis to build the *Hilbert space of configurations* which allows for superposition of configurations.

Definition 15 (Hilbert space of configurations)**.** *The* Hilbert space of configurations *is that having orthonormal basis $\{|c\rangle\}_{c\in\mathscr{C}_f}$. It will be denoted $\mathscr{H}$.*

A QCA then acts on the Hilbert space of configuration with similar constraints as a classical CA, that is to say in a local, translation-invariant manner:

Definition 16 (QCA)**.** *A QCA is a linear operator over $\mathscr{H}$ which is translation-invariant, causal and unitary.*

Causality and translation-invariance in this context are formally defined in [12]. Locality is recovered from causality and unitarity as shown in [80].

In practice, to build a specific dynamics, a circuit version of QCA known as partitioned QCA is helpful. It works by partitioning the space into supercells on which a local unitary operator is applied. In one timestep, this may be done multiple times with different partitions and unitaries. There is no loss of generality since partitioned QCA are intrinsically universal [61].

In the following, everything is defined in the context of partitioned QCA.

2.2.2. Fermionic dynamics

Let us first recall the $2+1$ dynamics of the fermionic field, without any electromagnetic contribution, without any gauge field even, and restricting to the one particle sector. This is the well-known Dirac quantum walk (QW) [81, 82].

At each lattice site x lies a group of 2 qubits, each stating whether a fermion in mode $j \in 0\ldots1$ is present at the site (remember that in $2+1$ dimensions the Dirac Eq. is a PDE on a wave function having two complex amplitudes, corresponding to the two modes spin up and down). Again, this encoding captures the Pauli exclusion principle as there cannot be two fermions in the same mode at the same site. Moreover, as we focus on the one particle sector first, we temporarily look at the case where only one of the qubits can be in the state $|1\rangle$.

One time-step is divided in three sub steps: a vertical translation, a horizontal translation and a mass term. Moreover, each translation is decomposed into two swaps. Each of these terms thus acts on a pair of qubits: on a single site for the mass and the first swap (S), and across two neighboring sites for the second swaps (T). In the one particle sector, the possible input states are $|00\rangle$, $|01\rangle$ and $|10\rangle$. Number conservation forces $|00\rangle$ to be mapped to itself. Without loss of generality we can assume that this absence of particle triggers no phase. Hence, our two qubit operators of the Dirac QW are of the form $W = 1 \oplus M$ where 1 leaves $|00\rangle$ unchanged and M is the unitary acting on the subspace spanned by $|01\rangle$ and $|10\rangle$. The Dirac QW is given by:

$$\mathrm{QW} = \left[\bigotimes_x C_\epsilon\right]\left[\bigotimes_{(x,1),(x+\nu,0)} T_\nu \bigotimes_x S\right]\left[\left(\bigotimes_x H_\mu\right)\left(\bigotimes_{(x,1),(x+\mu,0)} T_\mu \bigotimes_x S\right)\left(\bigotimes_x H_\mu^\dagger\right)\right] \tag{2.62}$$

where $C_\epsilon = 1 \oplus e^{-im\epsilon Y}$ is the mass term, $H_\mu = 1 \oplus H$ with H the Hadamard operator (such that $HZH = X$), S swaps qubits $(x,0)$ and $(x,1)$, and T_η swaps qubits $(x,1)$ and $(x+\eta,0)$. It follows that $\bigotimes_{(x,1),(x+\eta,0)} T_\eta \bigotimes_x S = 1 \oplus e^{\epsilon Z \partial_\eta}$ is the displacement operators in the η direction by a factor ϵ, moving the first qubit in the positive direction and the second in the negative direction. The X, Y, Z are Pauli matrices and ∂_η the partial derivatives. Convergence towards the Dirac Eq. is rigorously proven in [81, 82].

With multiple walkers, the Dirac QW becomes the Dirac QCA. The dynamics needs to be extended to take into account the case where multiple qubits are in state $|1\rangle$. Since the QW gates act on at most two qubits, and due to number conservation, only the input state $|11\rangle$ requires our attention, and it can only be sent to itself, up to a phase. To find out exactly which phase has to be applied, let us move to the Heisenberg picture.

The Heisenberg picture is a choice of representation in which the evolution of a system is described in terms of evolving operators. Essentially, it tells about the future impact of our past actions. For instance, say that the overall evolution from time t to time $t+1$ is governed by a unitary operator $\mathbf{W}^\dagger$, e.g. mapping $|\psi\rangle$ to $|\psi'\rangle$. Then, the past action of creating a fermion at $(x,0)$ at time t, as implemented by $a^\dagger_{x,0}$, e.g. mapping $|\psi\rangle$ to $a^\dagger_{x,0}|\psi\rangle$, will have future impact $\mathbf{W}a^\dagger_{x,0}\mathbf{W}^\dagger$ at time $t+1$, i.e. $|\psi'\rangle$ to $\mathbf{W}a^\dagger_{x,0}\mathbf{W}^\dagger|\psi'\rangle$.

More specifically consider $\mathbf{S}$ the multi-particle sector extension of S which is such that $\mathbf{S}a^\dagger_{x,0}\mathbf{S}^\dagger = a^\dagger_{x,1}$ and $\mathbf{S}a^\dagger_{x,1}\mathbf{S}^\dagger = a^\dagger_{x,0}$, i.e. a 'fermionic swap'. Notice there exists $\mathbf{S}'$ which coincide with $\mathbf{S}$ and thus with S in the one-particle sector, but that do not obey these two equations. We discard them on the basis that $\mathbf{S}$ is the 'rightful non-interacting extension' of S, as the future impact of $a^\dagger_{x,0}$ is $a^\dagger_{x,1}$ regardless of there being other particles or not.

It follows that $\mathbf{S}a^\dagger_{x,0}a^\dagger_{x,1}\mathbf{S}^\dagger = \mathbf{S}a^\dagger_{x,0}\mathbf{S}^\dagger\mathbf{S}a^\dagger_{x,1}\mathbf{S}^\dagger = a^\dagger_{x,1}a^\dagger_{x,0} = -a^\dagger_{x,0}a^\dagger_{x,1}$. In particular, if we had $|\psi\rangle = |00\rangle$ at time t evolving into $|\psi'\rangle = \mathbf{S}|\psi\rangle = |00\rangle$ at time $t+1$, we realize that the past action of creating two fermions $a^\dagger_{x,0}a^\dagger_{x,1}$, e.g. mapping $|00\rangle$ to $|11\rangle$, will have future impact $-a^\dagger_{x,0}a^\dagger_{x,1}$, i.e. mapping $|00\rangle$ to $-|11\rangle$. Thus, $\mathbf{S}|11\rangle = -|11\rangle$ is the rightful qubit implementation of the fermionic swap, meeting the specifications imposed by the (anti-)commutation relations hypothesis. In order to build the Dirac QCA from the Dirac QW, we must proceed in the same manner for each term of the Dirac QW, as done in Appendix A.

We see that this phase got determined as a consequence of the (anti-)commutation relations hypothesis discussed in section 2.1, as well as the way we chose to implement the annihilation operators, under which Jordan-Wigner transform etc., as defined in that same section. This requires the presence of gauge field, which we had temporarily ignored for describing the Dirac QW, but we now restore for describing the Dirac QCA. We use bold fonts to denote the Dirac QCA counterparts of the Dirac QW operators.

When representing a QCA operator U acting on a 2-qubits state, the ordering is as follows:

$$\begin{matrix}|00\rangle\\|01\rangle\\|10\rangle\\|11\rangle\end{matrix} \tag{2.63}$$

The mass sub-step acts as C_ϵ on the states $|00\rangle$, $|01\rangle$ and $|10\rangle$. And the phase applied on state $|11\rangle$ is $c^2+s^2=1$ (using Appendix A). Therefore, the corresponding QCA unitary which we will denote $\mathbf{C}_\epsilon$ is:

$$\mathbf{C}_\epsilon = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & c & -s & 0\\ 0 & s & c & 0\\ 0 & 0 & 0 & 1\end{pmatrix} \begin{matrix}|00\rangle\\|01\rangle\\|10\rangle\\|11\rangle\end{matrix} \tag{2.64}$$

$$= C_\epsilon \oplus 1 \tag{2.65}$$

$$= \left(a_1 a_1^\dagger\right)\left(a_0 a_0^\dagger\right) + \left(a_1^\dagger a_1\right)\left(a_0^\dagger a_0\right) \tag{2.66}$$

$$+ c\left[\left(a_1 a_1^\dagger\right)\left(a_0^\dagger a_0\right) + \left(a_1^\dagger a_1\right)\left(a_0 a_0^\dagger\right)\right] + s(a_1^\dagger a_0 - a_0^\dagger a_1) \tag{2.67}$$

where $c=\cos(\epsilon m)$ and $s=\sin(\epsilon m)$, and the last line is $\mathbf{C}_\epsilon$ expressed in terms of the local evolution operator from Eq. (2.18). Note that this operator acts on-site, that is to say on the two qubits at the same position.

The transport sub-step takes a right-moving (resp. left-moving) qubit at position x (resp. $x+\epsilon$) and maps it to the right-moving (resp. left-moving) qubit at position $x+\epsilon$ (resp. x). It does so locally by first swapping the qubits on each site using the gate $\mathbf{S}$, then moving them through a gate $\mathbf{T}_\eta$ between neighboring sites while changing the gauge field accordingly:

$$\mathbf{S} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{2.68}$$

$$= \left(a_{x,1}a_{x,1}^\dagger\right)\left(a_{x,0}a_{x,0}^\dagger\right) - \left(a_{x,1}^\dagger a_{x,1}\right)\left(a_{x,0}^\dagger a_{x,0}\right) + a_{x,1}^\dagger a_{x,0} + a_{x,0}^\dagger a_{x,1} \tag{2.69}$$

$$\mathbf{T}_\eta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & K_\eta^\dagger & 0 \\ 0 & K_\eta & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{2.70}$$

$$= \left(a_{x,1}a_{x,1}^\dagger\right)\left(a_{x+\eta,0}a_{x+\eta,0}^\dagger\right) - \left(a_{x,1}^\dagger a_{x,1}\right)\left(a_{x+\eta,0}^\dagger a_{x+\eta,0}\right) \tag{2.71}$$

$$+ a_{x,1}^\dagger V_{x,\eta} a_{x+\eta,0} + a_{x+\eta,0}^\dagger V_{x,\eta}^\dagger a_{x,1} \tag{2.72}$$

where

$$K_{x,\eta} = \left(\prod_{y\in\left[x,x:\eta\right[} Z_y\right) U_{x,\eta} \left(\prod_{y\in\left[x+\eta,x+\eta:-\eta\right[} Z_y\right) \tag{2.73}$$

with U_η the gauge field lowering operator. The equations using fermionic annihilators and creators are based on the local evolution operators from equations (2.18) and (2.19). The product of Z_y comes from the hopping term defined in Eq. (2.25), with $x:\eta$ the link along which the swap takes place. The minus one, when the input is $|11\rangle$, is the exchange phase for crossing fermions. Again full justification is given in Appendix A.

The transport sub-step of the Dirac QCA is illustrated in figure 2.2.

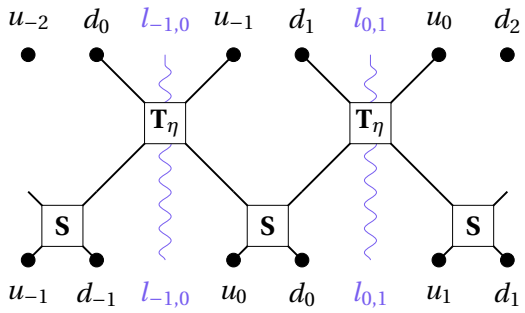


Figure 2.2.: Transport with d moving left (or down), u moving right (or up) and l the gauge field (given as a single field for conciseness).

The basis change $\mathbf{H}$ is similar to the mass term in that it acts only on a single site and can be written as a direct sum for the case with 0, 1 or 2 particles as follows:

$$\mathbf{H} = H_\mu \oplus -1 = 1 \oplus H \oplus -1 \tag{2.74}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{2.75}$$

$$= \left(a_1 a_1^\dagger\right)\left(a_0 a_0^\dagger\right) - \left(a_1^\dagger a_1\right)\left(a_0^\dagger a_0\right) \tag{2.76}$$

$$+ \frac{1}{\sqrt{2}}\left[\left(a_1 a_1^\dagger\right)\left(a_0^\dagger a_0\right) + \left(a_1^\dagger a_1\right)\left(a_0 a_0^\dagger\right) + (a_1^\dagger a_0 - a_0^\dagger a_1)\right]. \tag{2.77}$$

This last equation corresponds to the basis changed expressed using the local evolution operator (2.18);

The minus one is justified in Appendix A. Since $H^\dagger = H$, we have $\mathbf{H}^\dagger = \mathbf{H}$.

The complete Dirac QCA is:

$$\mathbf{D_F} = \mathbf{C}_\epsilon \mathbf{T}_\nu \mathbf{S} \mathbf{H} \mathbf{T}_\mu \mathbf{S} \mathbf{H}. \tag{2.78}$$

It is represented in figure 2.3.

Gauge invariance. Each of the operators constitutive of the Dirac QCA has been expressed as a linear combination of the local evolution operators given in subsection 2.1.3, which were proven to be gauge invariant in subsection 2.1.4. Therefore, the Dirac QCA is gauge invariant.

2.2.3. Electric contribution

Let us now define the electric contribution. To do so, we follow the same idea as in the Lagrangian formalism, which is to take some of the simplest gauge invariant

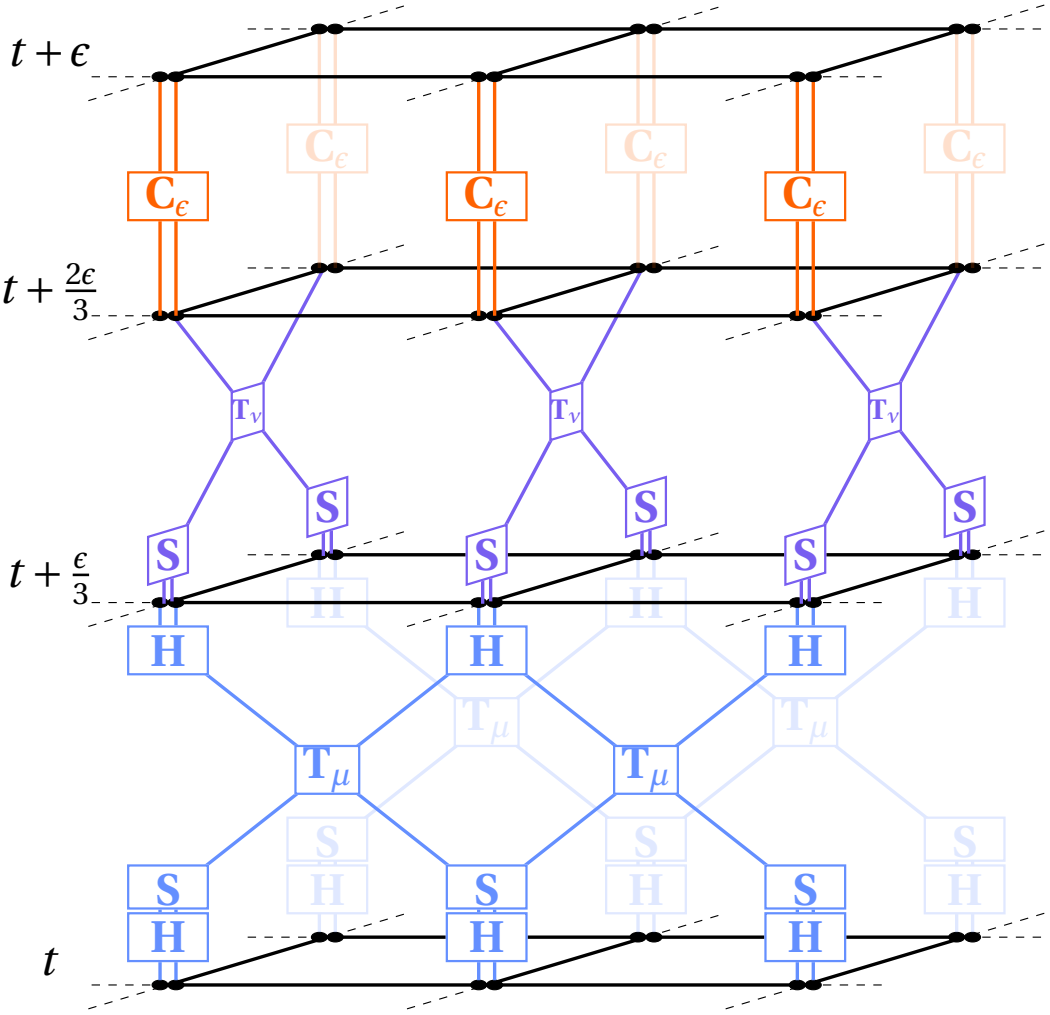


Figure 2.3.: The 3 steps of the free evolution in the multi-particle sector. The gauge field is omitted for clarity.

electric term. We then check that it matches the Trotterization of the Kogut-Susskind Hamiltonian. The construction proposed here is highly inspired by [53].

A simple electric contribution ought to act on the gauge field according to operator E. We could also demand that applying it on either side of a gauge field—i.e. (x,η) or $(x+\eta,-\eta)$ gives the same output. However, the electric operator itself does not match this requirement because $E_{x,\eta} = -E_{x+\eta,-\eta}$. The squared electric term E^2, does. The squared electric term itself is not unitary, but its exponential e^{iE^2}, is.

Notice also that the spacetime discretization should impact the amplitude of the phase: when any of the space or the time discretization parameter goes to zero, the exponential should tend towards the identity. Taking these considerations into account, one obtains:

$$\mathbf{D_E} = e^{\frac{i}{2}\epsilon^2 g_E^2 E^2} \tag{2.79}$$

where the ϵ^2 comes from the simultaneous discretization in space and time with

$\Delta_x = \Delta_t = \epsilon$, and g_E is the coupling constant as determined experimentally.

Without the electric contribution, the gauge field just keeps track of fermions passing by, but has no influence upon them. With the electric contribution, the gauge-field dependent phase, mediates the interaction.

Let us compare the electric contribution with the electric part of the Kogut-Susskind Hamiltonian [37] for QED:

$$H_E = \frac{g_E^2}{2}\Delta_x \sum_x (E_{x,\mu}^2 + E_{x,\nu}^2). \tag{2.80}$$

Integration over a Δ_t period of time—i.e. computing $e^{i\Delta_t H_E}$—and Trotterizing to separate the spatial sum into a product of exponentials, yield $\mathbf{D_E}$.

Remark 3 (Truncation of the electric field)**.** *If $\frac{1}{2}\epsilon^2 g_E^2 = \frac{2\pi}{k}$ exactly, with k an integer, then the phase of the electric contribution will wrap up around 2π as soon as E^2 reaches k. This when $\epsilon = \sqrt{\frac{4\pi}{k g_E^2}}$. If we restrict ourselves to such values of ϵ, i.e. decreasing it by augmenting k, then, as far as the electric contribution is concerned, the gauge field can equally well be represented with a k-dimensional Hilbert space $\mathscr{H}_k$. Indeed, when E outputs $k+l$, its square gives $k^2+2kl+l^2$, and the phase $\frac{1}{2}\epsilon^2 g_E^2 E^2$ simplifies into $\frac{1}{2}\epsilon^2 g_E^2 l^2$ because $\epsilon^2 g_E^2 k(k+2l)/2$ is proportional to 2π. Notice that this k still goes to infinity when taking ϵ to zero, augmenting proportionally to $1/\epsilon^2$. This idea of restricting the gauge field to finite-dimensions labelling roots of unity was suggested in [53]. Truncations in lattice gauge theory simulations were evaluated in [83].*

Gauge invariance. The electric contribution is gauge invariant as an exponential of a gauge invariant operator.

2.2.4. Magnetic contribution

In order to define the magnetic contribution, we follow the same path as for the electric contribution, that is to say define some of the simplest the gauge field-only term that is local, unitary and gauge invariant.

Formulation of the magnetic contribution. The word magnetic refers to the fact that it acts on the gauge field in a way dual to that of the electric operator—i.e. through lowering or raising the gauge field.

As discussed in section 2.1 operators that are defined solely using the lowering and raising operators need to form a loop (spatially) in order to both local and ensure gauge invariance. Indeed, raising the gauge field at one end of a link, implies lowering it at the other, hence imposing that the magnetic contribution be a loop; the smallest loop is realized by the plaquette local evolution operator $P_{x,\eta,\zeta}$ of Eq. (2.32).

Since the loop is oriented, one may wish to symmetrize. This is done through a sum $P_{x,\eta,\zeta} + P_{x,\eta,\zeta}^\dagger$, but this breaks unitarity. Just like for the electric field, unitarity is

restored through exponentiation, and the space and time discretization parameters need be used in the exponential to ensure that it goes to the identity when these go to zero. Taking these considerations into account, one obtains:

$$\mathbf{D_M} = e^{\frac{i}{2}\epsilon^2 g_M^2 (P_{x,\mu,\nu} + P_{x,\mu,\nu}^\dagger)} \tag{2.81}$$

with $\epsilon = \Delta_t = \Delta_x$ and $g_M^2/2$ a constant. Taking the limit of $\mathbf{D_M}$ when ϵ goes to zero yields:

$$\mathbf{D_M} = Id + i\epsilon^2 \frac{g_M^2}{2} \left(P_{x,\mu,\nu} + P_{x,\mu,\nu}^\dagger \right) + O\left(\epsilon^4\right). \tag{2.82}$$

Let us compare the obtained magnetic contribution with magnetic part of the Kogut-Susskind Hamiltonian:

$$H_M = \frac{g_M^2}{2} \Delta_x \sum_x (P_{x,\mu,\nu} + P_{x,\mu,\nu}^\dagger) \tag{2.83}$$

where $g_M = \frac{1}{\Delta_x g_E}$. Integrating this Hamiltonian over a Δ_t period of time—i.e. computing $e^{i\Delta_t H_M}$—and Trotterizing to separate the spatial sum leads to the same local operator $\mathbf{D_M}$.

Two formulations in terms of gates. In order to define $\mathbf{D_M}$ in terms of quantum gates, one needs to explicitly compute or closely approximate the exponential. We provide two constructions in order to do so. The first construction is to diagonalize the plaquette term so that taking its exponential simply amounts to exponentiating the eigenvalues, that is to say, we go from an electric basis to a magnetic one [84]. The quantum Fourier transform is used in the diagonalization. The second construction consist in a more subtle approach were the term $P + P^\dagger$ is written as the sum of two terms $\widetilde{P}$ and $\widetilde{Q}$ whose exponentials are simple to compute. This second construction yields a gate formalism reminiscent to that of a QW.

Ordering the operators. Two neighboring plaquette local evolution operators $P_{x,\mu,\nu}$ and $P_{x+\mu,\mu,\nu}$ both act on the two gauge fields of the link $(x+\mu,\mu)$. Therefore, the order of the operations could have been relevant. However, the plaquette local evolution operators actually commute. If one insists on not acting simultaneously with two different operators on a same system, then any arbitrary ordering can be chosen, such as applying the plaquette local evolution operators at even positions first, and then at odd positions.

Redefining the states. Before diving into the two constructions, let us introduce a new way of representing the gauge field affected by a loop of lowering operators, using U and not V:

$$U_{x,\mu} U_{x+\mu,\nu} U_{x+\nu,\mu}^\dagger U_{x,\nu}^\dagger. \tag{2.84}$$

Forgetting to denote the second gauge field of each link, which is just the opposite of the first, the loop applies the following transformation to the four links

$$|-a-n,-b-n,c+n,n\rangle \longrightarrow |-a-(n+1),-b-(n+1),c+(n+1),(n+1)\rangle\,. \tag{2.85}$$

This transformation can be seen as a shift where n is mapped to $n+1$. We introduce 'plaquette-like' states:

$$|\underline{abcn}\rangle = U^a U^b U^{\dagger c}\,|-n,-n,n,n\rangle\,. \tag{2.86}$$

We have:

$$U_{x,\mu}U_{x+\mu,\nu}U^\dagger_{x+\nu,\mu}U^\dagger_{x,\nu}\,|\underline{abcn}\rangle = |\underline{abc,n+1}\rangle \tag{2.87}$$

for a,b,c and n integers.

The plaquette local evolution operator of (2.12) and (2.21), is built using the previous loop of U combined with Z operators. These Z operators only add a plus or minus sign to the state $|\underline{abcn}\rangle$. However, depending on the Jordan-Wigner order, this sign may be influenced by the other gauge fields and qubits present at the four sites where the plaquette term is applied. In order to take this into account, we extend the plaquette-like state so as to add a qudit $|o\rangle$, such that $|\underline{abcno}\rangle$ entirely describes the four sites affected by the plaquette. We can then let $\varphi_{abcno}\in\{0,1\}$ be such

$$P\,|\underline{abcno}\rangle = (-1)^{\varphi_{abcno}}\,|\underline{abc,n+1,o}\rangle\,. \tag{2.88}$$

Starting from state $|\underline{abc,0,o}\rangle$, one reaches state $|\underline{abc,n,o}\rangle$ by applying the plaquette operator n times. We can then let $\psi_{abcno}\in\{0,1\}$ be such

$$(-1)^{\psi_{abcno}}\,|\underline{abcno}\rangle = P^n\,|\underline{abc,0,o}\rangle\,. \tag{2.89}$$

The ψ_{abcno} can be given in explicitly in terms of φ_{abcno}, so that $\psi_{abcno}+\varphi_{abcno} = \psi_{abc,n+1,o}$:

$$\psi_{abcno} = \begin{cases} \sum_{0\le k<n}\varphi_{abcko} & \text{when } n>0 \\ \sum_{n\le k<0}\varphi_{abcko} & \text{when } n<0 \end{cases} \tag{2.90}$$

This leads to the definition of 'plaquette states'

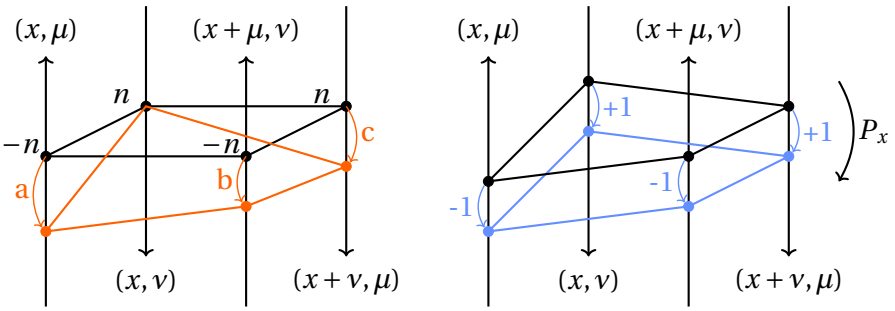
$$|\widetilde{abcno}\rangle = (-1)^{\psi_{abcno}}\,|\underline{abcno}\rangle \tag{2.91}$$

which verify the same relation as that of Eq. (2.87), with V operators instead of U:

$$P\,|\widetilde{abcno}\rangle = |\widetilde{abc,n+1,o}\rangle\,. \tag{2.92}$$

Again, these plaquette states help understand the plaquette local evolution operator as a shift, which will be useful for both decompositions of the magnetic contribution in terms of quantum gates.

The state and plaquette operator are illustrated in figure 2.4.



(a) Plaquette state $|\widetilde{abcn}\rangle$ (b) Plaquette operator

Figure 2.4.: Plaquette states and operator represented in the subspace $\mathbb{Z}^4$ containing four gauge field values.

Gauge field truncation. If truncating the gauge field to $\mathscr{H}_k$, one needs $|\widetilde{abc,k,o}\rangle = |\widetilde{abc,0,o}\rangle$ so that any sign discrepancy in Eq. (2.92) is avoided. This paragraph is just to overcome this technicality. In terms of phase the condition is that $\psi_{abcko} = \psi_{abc0o} = 0$, i.e. that $\psi_{abcko} = \sum_{0\leq n<k}\varphi_{abcno}$ be even. Each term φ_{abcno} is actually a sum $\varphi_{abcn} + \varphi_o$, where φ_{abcn} depends on the four links under transformation, whereas φ_o depends on the other gauge fields and qubits at the four sites, which are not modified by the plaquette operator. Both of these depend on the JW order chosen. Since φ_o is constant when acting only using the plaquette term, for an even k its contribution to the sum $\sum_{0\leq n<k}\varphi_o$ is even. Additionally, for any n, we have that $\varphi_{abc,n} = \varphi_{abc,n+2}$ as all the parities are equal. As a consequence $\varphi_{abc,n} + \varphi_{abc,n+1} + \varphi_{abc,n+2} + \varphi_{abc,n+3}$ is even. It follows that for k a multiple of 4, the sum $\sum_{0\leq n<k}\varphi_{abcn}$ is even. Hence, for $k = 4q$, with q an integer, the truncation is valid.

Relying on a specific JW order actually allows for any even k. Indeed, we can enforce that φ_{abcn} always be equal to 0: this is the case when $(x:-\eta)$ and $x:\eta$ are both inferior (or both superior) to $(x:-\zeta)$ and $(x:\zeta)$ for η and ζ two distinct directions. In this case, the four corner operators that form a plaquette defined in Eq. (2.30) will induce a phase $(-1)^{\varphi_{abcn}}$ through the following Z operators (disregarding the part which contributes to φ_o):

$$Z_{x:\eta}Z_{x+\eta:-\eta}Z_{x+\eta+\zeta:-\eta}Z_{x+\zeta:\eta}. \tag{2.93}$$

Notice that each link appear twice, hence they do not induce any phase, i.e. we have that $P|\widetilde{abcno}\rangle = (-1)^{\varphi_o}|\widetilde{abc,n+1,o}\rangle$. Thus, the truncation is well-defined for k even for that specific JW orders.

2.2.4.1. Quantum circuit implementation through diagonalization

The first construction moves from the electric to the magnetic basis [84]. In other words, it works by computing the eigenvectors and eigenvalues of the plaquette operator, so that taking the exponential of the operator simply amounts to exponentiating the eigenvalues.

A single plaquette local evolution can be seen as a shift operator upon plaquette

states as illustrated figure 2.4b. That shift amounts to a phase in the Fourier basis, therefore the Fourier transform diagonalizes the plaquette. To define this Fourier transform, the state space of the gauge field needs be truncated to $\mathbb{Z}_k$, for instance according to Remark 3, and in accordance with the restriction of subsection (2.2.4). Then the eigenvectors of a plaquette local evolution are

$$|abcp\rangle_\square = \frac{1}{\sqrt{k}} \sum_{n=0}^{k-1} e^{2\pi i n p/k} |\widetilde{abc, n}\rangle \tag{2.94}$$

for a, b, c and p integers in $0, ..., k-1$. These are the Fourier transform of the $|\widetilde{abc, n}\rangle$ states, that can be obtained through a quantum Fourier transform whose circuit representation is well-known. The corresponding eigenvalues are

$$\lambda_p = e^{2\pi i p/k}. \tag{2.95}$$

The eigenvectors of the hermitian conjugate of the plaquette operator are the same but with eigenvalues λ_{-p}. For the sum of the plaquette and its hermitian conjugate, the eigenvalues are:

$$e^{2\pi i p/k} + e^{-2\pi i p/k} = 2\cos\big(2\pi p/k\big). \tag{2.96}$$

Having found an eigenbasis of the plaquette term, it is now easy to exponentiate it. Doing so one gets the eigenvalue equation:

$$\exp\left(i\epsilon^2 \frac{g_M^2}{2}(P + P^\dagger)\right) |abcp\rangle_\square = \exp\left(i\epsilon^2 g_M^2 \cos\big(2\pi p/k\big)\right) |abcp\rangle_\square. \tag{2.97}$$

This defines a diagonal operator Diag that contains the eigenvalues

$$\exp\big(i\epsilon^2 g_M^2 \cos\big(2\pi p/k\big)\big). \tag{2.98}$$

The magnetic evolution for the QCA can thus be written as:

$$\mathbf{D}_\mathbf{M}^{(\mathbf{0})} = U_{\mathrm{QFT}}^\dagger \,\mathrm{Diag}\, U_{\mathrm{QFT}} \tag{2.99}$$

where U_{QFT} is the quantum Fourier transform. Hence, Eq. (2.99) thus defines a circuit of quantum gates for the magnetic term. In this construction, no approximation has been done, hence the limit is exactly the one given in Eq. (2.82).

2.2.4.2. Quantum walk-like circuit implementation

The second construction uses a reformulation of the plaquette operators to make it look like a quantum walk. Here we sometime abuse notations and write $|\widetilde{abcn}\rangle$ or even just $|\tilde{n}\rangle$ to talk about a state $|\widetilde{abcno}\rangle$. Indeed, the plaquette term can be divided into two operators, one which acts as $|\widetilde{2n}\rangle\langle\widetilde{2n+1}| + |\widetilde{2n+1}\rangle\langle\widetilde{2n}|$ and the other as $|\widetilde{2n+1}\rangle\langle\widetilde{2n+2}| + |\widetilde{2n+2}\rangle\langle\widetilde{2n+1}|$—i.e. the two operators act as shifted swaps between

pairs of sites. Let $\widetilde{P}$ and $\widetilde{Q}$ denote those operators:

$$\widetilde{P} = \sum_{abc\in\mathbb{Z}^3} \sum_{n\in 2\mathbb{Z}} \left|\widetilde{abc,n+1}\right\rangle\left\langle\widetilde{abc,n}\right| + \left|\widetilde{abc,n}\right\rangle\left\langle\widetilde{abc,n+1}\right| \tag{2.100}$$

$$\widetilde{Q} = \sum_{abc\in\mathbb{Z}^3} \sum_{n\in 2\mathbb{Z}+1} \left|\widetilde{abc,n+1}\right\rangle\left\langle\widetilde{abc,n}\right| + \left|\widetilde{abc,n}\right\rangle\left\langle\widetilde{abc,n+1}\right|. \tag{2.101}$$

We have that

$$\widetilde{P} + \widetilde{Q} = P + P^\dagger. \tag{2.102}$$

$\widetilde{P}$ and $\widetilde{Q}$ are hermitian, unitary and their eigenvectors are

$$|+_n\rangle = \frac{1}{\sqrt{2}}(|\widetilde{n}\rangle + |\widetilde{n+1}\rangle) \tag{2.103}$$

$$|-_n\rangle = \frac{1}{\sqrt{2}}(|\widetilde{n}\rangle - |\widetilde{n+1}\rangle) \tag{2.104}$$

with n even for $\widetilde{P}$ and odd for $\widetilde{Q}$. The corresponding eigenvalues are plus and minus one.

Now taking the exponential $\mathbf{D}_{\widetilde{\mathbf{P}}}$ of $\widetilde{P}$, we have, with n even:

$$\exp\left(i\epsilon^2\frac{g_M^2}{\sqrt{2}}\widetilde{P}\right)|+_n\rangle = \exp\left(i\epsilon^2\frac{g_M^2}{\sqrt{2}}\right)|+_n\rangle \tag{2.105}$$

$$\exp\left(i\epsilon^2\frac{g_M^2}{\sqrt{2}}\widetilde{P}\right)|-_n\rangle = \exp\left(-i\epsilon^2\frac{g_M^2}{\sqrt{2}}\right)|-_n\rangle \tag{2.106}$$

$$\mathbf{D}_{\widetilde{\mathbf{P}}}|\widetilde{n}\rangle = \exp\left(i\epsilon^2\frac{g_M^2}{2}\widetilde{P}\right)|\widetilde{n}\rangle \tag{2.107}$$

$$= \frac{1}{\sqrt{2}}\left(\exp\left(i\epsilon^2\frac{g_M^2}{2}\right)|+_n\rangle + \exp\left(-i\epsilon^2\frac{g_M^2}{2}\right)|-_n\rangle\right) \tag{2.108}$$

$$= \cos\left(\epsilon^2\frac{g_M^2}{2}\right)|\widetilde{n}\rangle + i\sin\left(\epsilon^2\frac{g_M^2}{2}\right)|\widetilde{n+1}\rangle \tag{2.109}$$

$$\mathbf{D}_{\widetilde{\mathbf{P}}}|\widetilde{n+1}\rangle = i\sin\left(\epsilon^2\frac{g_M^2}{2}\right)|\widetilde{n}\rangle + \cos\left(\epsilon^2\frac{g_M^2}{2}\right)|\widetilde{n+1}\rangle. \tag{2.110}$$

These equations are identical for $\mathbf{D}_{\widetilde{\mathbf{Q}}}$ when taking n odd.

This is reminiscent of a one dimensional quantum walk with coin

$$\begin{pmatrix}\cos(\theta) & i\sin(\theta)\\ i\sin(\theta) & \cos(\theta)\end{pmatrix}. \tag{2.111}$$

Such QW is homogeneous in the 'tilde' basis, but at first glance, it seems inhomoge-

neous in the canonical basis because of the operator

$$\left|\widetilde{abc,n+1},o\right\rangle\!\left\langle\widetilde{abc,n,o}\right| = (-1)^{\varphi_{abcno}}\left|\underline{abc,n+1,o}\right\rangle\!\left\langle\underline{abc,n,o}\right| \tag{2.112}$$

which induces a phase φ_{abcno}, dependent upon n, in the canonical basis. However, as explained in subsection 2.2.4, this phase can be made independent of n through a specific choice of JW order, recovering a homogeneous QW even in the canonical basis.

Using $\mathbf{D}_{\widetilde{\mathbf{P}}}$ and $\mathbf{D}_{\widetilde{\mathbf{Q}}}$, a way to implement the plaquette term is to apply those successively in one time step:

$$\mathbf{D}_{\mathbf{M}}^{(\mathbf{1})}\left|\widetilde{n}\right\rangle = \mathbf{D}_{\widetilde{\mathbf{Q}}}\mathbf{D}_{\widetilde{\mathbf{P}}}\left|\widetilde{n}\right\rangle. \tag{2.113}$$

Taking the limit when ϵ goes to zero after applying both the exponential of $\widetilde{P}$ and $\widetilde{Q}$ to $|\widetilde{n}\rangle$ (where n is even) gives:

$$\begin{aligned}\mathbf{D}_{\mathbf{M}}^{(\mathbf{1})}\left|\widetilde{n}\right\rangle &= \mathbf{D}_{\widetilde{\mathbf{Q}}}\mathbf{D}_{\widetilde{\mathbf{P}}}\left|\widetilde{n}\right\rangle && (2.114)\\ &= \mathbf{D}_{\widetilde{\mathbf{Q}}}\left(\left|\widetilde{n}\right\rangle + i\epsilon^2\frac{g_M^2}{2}\left|\widetilde{n+1}\right\rangle + O\left(\epsilon^4\right)\right) && (2.115)\\ &= \left|\widetilde{n}\right\rangle + i\epsilon^2\frac{g_M^2}{2}\left(\left|\widetilde{n-1}\right\rangle + \left|\widetilde{n+1}\right\rangle\right) + O\left(\epsilon^4\right). && (2.116)\end{aligned}$$

For n odd, $\mathbf{D}_{\widetilde{\mathbf{P}}}$ would yield the state $|\widetilde{n-1}\rangle$ instead of $|\widetilde{n+1}\rangle$ (in the second line of the equation) and $\mathbf{D}_{\widetilde{\mathbf{Q}}}$ the state $|\widetilde{n+1}\rangle$ instead of $|\widetilde{n-1}\rangle$ (in the third line). Therefore, the same limit would be reached.

This limit matches the one obtained in Eq. (2.82). Thus, both quantum gate implementations agree in the limit as $\mathbf{D}_{\mathbf{M}}^{(\mathbf{0})} = \mathbf{D}_{\mathbf{M}}^{(\mathbf{1})} + O(\epsilon^4)$.

Gauge invariance. Gauge invariance of the plaquette term has been verified in section 2.1.4.1. Its exponentiation is a linear combination of them, thus still gauge invariant.

2.2.5. Complete dynamics

Combining the fermionic dynamics, the electric and magnetic contribution, one obtains the following complete dynamics for the 2 + 1 QED QCA:

$$\mathbf{QCA} = \mathbf{D}_{\mathbf{M}}\mathbf{D}_{\mathbf{E}}\mathbf{D}_{\mathbf{F}} \tag{2.117}$$

where $\mathbf{D}_{\mathbf{F}}$ (fermionic term) refers to Eq. (2.78), $\mathbf{D}_{\mathbf{E}}$ (electric term) refers to Eq. (2.79) and $\mathbf{D}_{\mathbf{M}}$ (magnetic term) refers to Eq. (2.81) or (2.113) depending on the quantum gate implementation chosen.

2.3. 3+1 Quantum Cellular Automaton

This section extends the previous $2+1$ QED QCA construction, to reach a $3+1$ QED QCA. In $3+1$ dimensions, the Dirac Eq. is a PDE on a wave function having four complex amplitudes, i.e. there are four fermionic modes instead of two. As for the gauge field, no additional degree of freedom is required, but the third dimension needs to be taken into account when considering the electronic and plaquette terms.

In the following, to avoid mixing notations, every operator referring to the $3+1$ case will be overlined, e.g. the mass term of the $3+1$ Dirac QW is $\overline{C}_\epsilon$. Again those of the multi-particle sector QCA are in bold, e.g. $\overline{\mathbf{C}}_\epsilon$.

2.3.1. Fermionic dynamics

The procedure is the same here as in the $2+1$ case: (i) define the $3+1$ Dirac QW, (ii) extend each gate using the Heisenberg picture so that it acts on the full state space and not just in the one-particle sector—cf. Appendix A.

Let γ_j be the following generalized Pauli matrix:

$$\gamma_0 = Y \otimes I \tag{2.118}$$
$$\gamma_1 = Z \otimes X \tag{2.119}$$
$$\gamma_2 = Z \otimes Y \tag{2.120}$$
$$\gamma_3 = Z \otimes Z. \tag{2.121}$$

They respect the anti-commutation relation

$$\{\gamma_j, \gamma_k\} = 2\delta_{j,k} I_4 \tag{2.122}$$

with $\delta_{j,k}$ the Kronecker delta.

The state space for the Dirac QW is that of 4 qubits restricted to the one-particle sector, i.e. there are 5 possible states: $|0000\rangle$, $|0001\rangle$, $|0010\rangle$, $|0100\rangle$ and $|1000\rangle$. As in the $2+1$ case, state $|0000\rangle$ is mapped to itself because of number conservation. Hence, every operator is of the form $1 \oplus U$ where U acts on the remaining four dimensional subspaces. The Dirac QW has the same structure: a mass term follows transport operations in each direction, each of these transports being surrounded by a basis

change [81, 82, 85]:

$$\overline{\mathrm{QW}} = \left(\bigotimes_x \overline{C}_\epsilon\right) \tag{2.123}$$

$$\left(\bigotimes_x \overline{H}_\mu\right)\left(\bigotimes_{(x,1),(x+\mu,0)} \overline{T}_\mu \bigotimes_x \overline{S}\right)\left(\bigotimes_x \overline{H}_\mu^\dagger\right) \tag{2.124}$$

$$\left(\bigotimes_x \overline{H}_\nu\right)\left(\bigotimes_{(x,1),(x+\nu,0)} \overline{T}_\nu \bigotimes_x \overline{S}\right)\left(\bigotimes_x \overline{H}_\nu^\dagger\right) \tag{2.125}$$

$$\left(\bigotimes_x \overline{H}_\rho\right)\left(\bigotimes_{(x,1),(x+\rho,0)} \overline{T}_\rho \bigotimes_x \overline{S}\right)\left(\bigotimes_x \overline{H}_\rho^\dagger\right) \tag{2.126}$$

where $\overline{S}$ swaps qubits $(x,0)$ and $(x,1)$ with $(x,2)$ and $(x,3)$, and $\overline{T}_\eta$ swaps qubits $(x,2)$ and $(x,3)$ with $(x+\eta,0)$ and $(x+\eta,1)$ so that $\bigotimes_x \overline{T}_\eta \bigotimes_x \overline{S} = 1 \oplus e^{\epsilon(Z\otimes I)\partial_\eta}$, transporting the first two qubits in the positive direction and the last two in the opposite one.

The operators $\overline{H}_\eta$ are defined so that:

$$\overline{H}_\eta(1 \oplus (Z \otimes I))\overline{H}_\eta^\dagger = 1 \oplus \gamma_\eta. \tag{2.127}$$

One possible choice for them is as follows:

$$\overline{H}_\rho = 1 \oplus \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{2.128}$$

$$\overline{H}_\mu = \overline{H}_\rho(1 \oplus H \oplus H) \tag{2.129}$$

$$\overline{H}_\nu = \overline{H}_\rho(1 \oplus F \oplus F) \tag{2.130}$$

where H is the Hadamard matrix such that $HZH = X$ and

$$F = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix} \tag{2.131}$$

is a matrix such that $FYF = Z$. These last equality can be checked easily when noticing that $F = \frac{Y+Z}{\sqrt{2}}$. Then

$$FYF = \frac{1}{2}(Y+Z)Y(Y+Z) \tag{2.132}$$

$$= \frac{1}{2}(YYY + YYZ + ZYY + ZYZ) \tag{2.133}$$

$$= \frac{1}{2}(Y + Z + Z + iZX) \tag{2.134}$$

$$= Z. \tag{2.135}$$

The same line of reasoning applies to $H = \frac{X+Z}{\sqrt{2}}$. Note that all three $\overline{H}_\eta$ are Hermitian.

The derivation of the operators making up the $3+1$ QED QCA requires to consider any configuration for the 4 qubits, hence possibly more than two fermions crossing.

Fortunately, all of these 4-qubit operator can be reexpressed as products of 2-qubit gates, with the 2 qubits being adjacent in the JW order. Thanks to this, the $2+1$ methodology and results readily apply, see Appendix A.

The mass term is almost the same as for the $2+1$ case. In the $3+1$ Dirac QW it has the form

$$\begin{aligned}
\overline{C}_\epsilon &= 1 \oplus e^{-im\epsilon\gamma_0} && (2.136)\\
&= 1 \oplus (cI_4 - is\gamma_0) && (2.137)\\
&= 1 \oplus \begin{pmatrix} c & 0 & -s & 0 \\ 0 & c & 0 & -s \\ s & 0 & c & 0 \\ 0 & s & 0 & c \end{pmatrix} && (2.138)\\
&= 1 \oplus (1 \oplus X \oplus 1)(C_\epsilon \oplus C_\epsilon)(1 \oplus X \oplus 1) && (2.139)
\end{aligned}$$

with $c = \cos(m\epsilon)$ and $s = \sin(m\epsilon)$.

The mass term of the $3+1$ Dirac QCA is reached by seeking to represent the above as a circuit of 2-qubit gates. The same sequence of gates as in the QW, although expended to the multi-particle sector, is applied to the QCA. That is because the QCA should act as the QW in the one-particle sector.v We thus need to swap the second and third qubits, then apply the $2+1$ mass term $\mathbf{C}_\epsilon$ separately on the first and last two qubits, and then swap again the second and third qubits.

This is represented in figure 2.5 and the corresponding operator $\overline{\mathbf{C}}_\epsilon$ is:

$$\overline{\mathbf{C}}_\epsilon = (I \otimes \mathbf{S} \otimes I)(\mathbf{C}_\epsilon \otimes \mathbf{C}_\epsilon)(I \otimes \mathbf{S} \otimes I) \tag{2.140}$$

where $\mathbf{S}$ is the swap defined in Eq. (2.68) and $\mathbf{C}_\epsilon$ is the 2+1D mass term defined in Eq. (2.64).

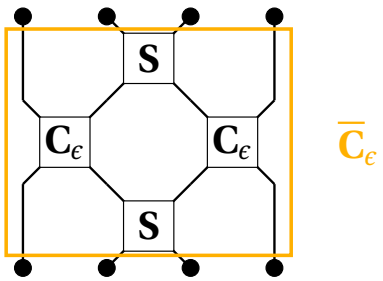


Figure 2.5.: Representation of the mass term of $3+1$ QED QCA. u, u' are moving right (or up) while d and d' are moving left (or down).

The transport term of the 3+1 Dirac QCA needs a similar change as the mass term. It will move the first two qubits in the η direction while moving the last two in the direction $-\eta$. This is done by first swapping the first two qubits with the last two using a gate $\overline{\mathbf{S}}$, then applying a transport operator which will swap these pairs of qubits with neighboring ones in the η direction using a gate $\overline{\mathbf{T}}_\eta$. This is illustrated in figure 2.6 and corresponds to the operators:

$$\overline{\mathbf{S}} = (I \otimes \mathbf{S} \otimes I)(\mathbf{S} \otimes \mathbf{S})(I \otimes \mathbf{S} \otimes I) \tag{2.141}$$

$$\overline{\mathbf{T}}_\eta = (I \otimes \mathbf{T}_\eta \otimes I)(\mathbf{S} \otimes \mathbf{S})(I \otimes \mathbf{T}_\eta \otimes I) \tag{2.142}$$

where $\mathbf{S}$ and $\mathbf{T}_\eta$ are defined through equations (2.68) and (2.70) respectively

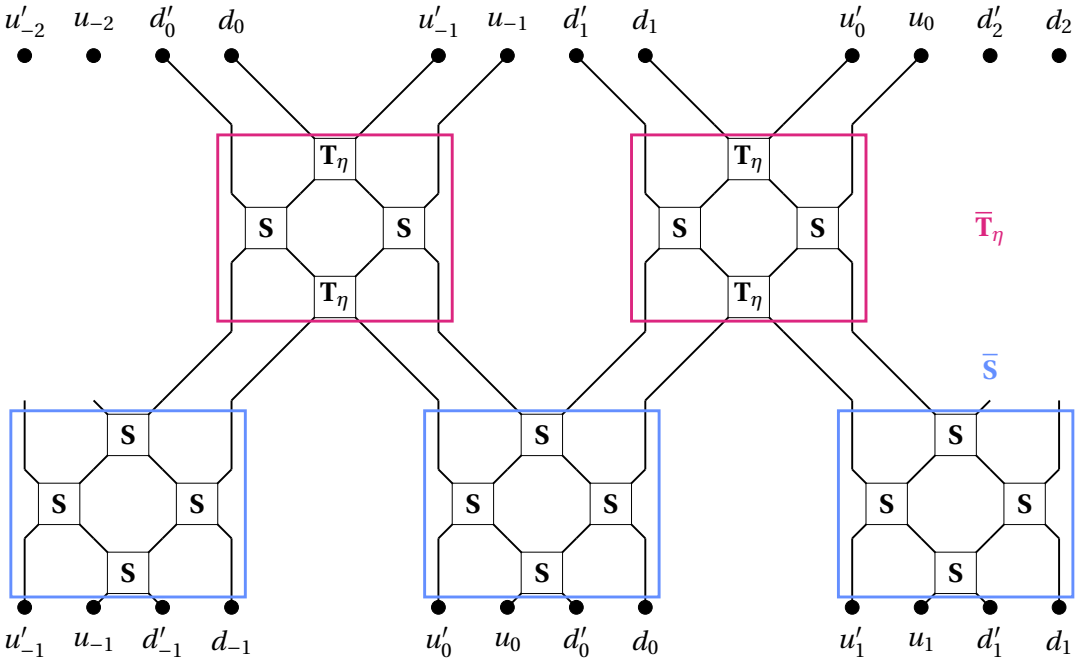


Figure 2.6.: Circuit for the transport term

The basis changes are of two kinds in the 3+1 dimensional case. The first kind is that of H_ρ from (2.128) which exchanges the second and last qubits of the QW. This can be realized through the operator $\overline{\mathbf{H}}_\rho$ represented as a circuit in figure 2.7 and defined as:

$$\overline{\mathbf{H}}_\rho = (I \otimes \mathbf{S} \otimes I)(I_2 \otimes \mathbf{S})(I \otimes \mathbf{S} \otimes I)). \tag{2.143}$$

The other two basis change—$\overline{\mathbf{H}}_\mu$ and $\overline{\mathbf{H}}_\nu$—share a common formalism, the QW counterpart $\overline{H_\rho}(1 \oplus H \oplus H)$ (resp. $\overline{H_\rho}(1 \oplus F \oplus F)$) is simply the operator H (resp. F) applied independently to the first and last two qubits, followed by the $\overline{H}_\rho$ operator.

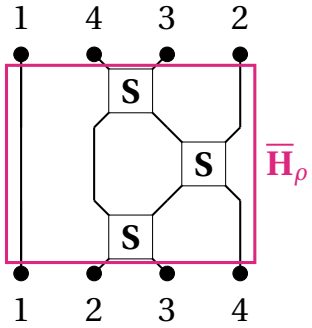


Figure 2.7.: Representation of the basis change $\overline{\mathbf{H}}_z$

This can be immediately translated into QCA operators:

$$\overline{\mathbf{H}}_\mu = \overline{\mathbf{H}}_\rho(\mathbf{H}\otimes\mathbf{H}) \tag{2.144}$$

$$\overline{\mathbf{H}}_\nu = \overline{\mathbf{H}}_\rho(\mathbf{F}\otimes\mathbf{F}) \tag{2.145}$$

$$\tag{2.146}$$

where $\mathbf{H}$ is defined in Eq. (2.74) and $\mathbf{F}$ is the generalization of F using the procedure in appendix A:

$$\mathbf{F} = 1\oplus F\oplus -1 \tag{2.147}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & \frac{i}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{2.148}$$

The full fermionic dynamics is therefore:

$$\overline{\mathbf{D}}_\mathbf{F} = \overline{\mathbf{C}}_\epsilon\left(\overline{\mathbf{H}}_\mu\overline{\mathbf{T}}_\mu\overline{\mathbf{S}}\overline{\mathbf{H}}_\mu^\dagger\right)\left(\overline{\mathbf{H}}_\nu\overline{\mathbf{T}}_\nu\overline{\mathbf{S}}\overline{\mathbf{H}}_\nu^\dagger\right)\left(\overline{\mathbf{H}}_\rho\overline{\mathbf{T}}_\rho\overline{\mathbf{S}}\overline{\mathbf{H}}_\rho^\dagger\right). \tag{2.149}$$

2.3.2. Electric and magnetic contributions

The electric contribution is exactly the same as in the 2+1D case, i.e. the exponentiated squared electric operator is applied at every link:

$$\overline{\mathbf{D}}_\mathbf{E} = e^{\frac{i}{2}g_E^2E^2}. \tag{2.150}$$

The magnetic contribution needs to be generalized to take into account the three dimensions, and thus the three possible directions for the plaquettes. Therefore, the magnetic contribution of the $3+1$ QED QCA is the same as in the $2+1$ case, but it is applied three times: one for each pair of directions. Let $\mathbf{D}_{\mathbf{M},\eta,\zeta}$ from Eq. (2.81) or (2.113) (depending on the formulation one chooses) denote the magnetic contribution

along the two spatial dimension η and ζ. We now have:

$$\overline{\mathbf{D}}_{\mathbf{M}} = \mathbf{D}_{\mathbf{M},\mu,\nu}\mathbf{D}_{\mathbf{M},\mu,\rho}\mathbf{D}_{\mathbf{M},\nu,\rho}. \tag{2.151}$$

Again this evolution coincides, in the limit, with the magnetic part of the Kogut-Susskind Hamiltonian:

$$H_M = \frac{g_M^2}{2} \sum_{\substack{x \\ \eta,\zeta\in\{\mu,\nu,\rho\} \\ \eta\neq\zeta}} P_{x,\eta,\zeta} \tag{2.152}$$

$$= \frac{g_M^2}{2}\sum_x \left(P_{x,\mu,\nu} + P^\dagger_{x,\mu,\nu}\right) + \quad \frac{g_M^2}{2}\sum_x \left(P_{x,\mu,\rho} + P^\dagger_{x,\mu,\rho}\right) + \frac{g_M^2}{2}\sum_x \left(P_{x,\nu,\rho} + P^\dagger_{x,\nu,\rho}\right). \tag{2.153}$$

2.3.3. Complete dynamics

Combining the $3+1$ Dirac QCA of (2.149) with the electric (2.150) and magnetic (2.151) contributions, one obtains the $3+1$ QED QCA:

$$\overline{\mathbf{QCA}} = \overline{\mathbf{D}}_{\mathbf{M}}\overline{\mathbf{D}}_{\mathbf{E}}\overline{\mathbf{D}}_{\mathbf{F}}. \tag{2.154}$$

Its gauge invariance is ensured by the same arguments as in the $2+1$ case.

3. Conclusion

Summary of achievements

Classical setting. In this thesis we formally defined gauge invariance in the context of cellular automata as a commutation relation between the evolution and a group of local transformations in equation (1.11). In order to obtain gauge invariance, the extension of cellular automata was introduced with a distinction between an absolute extension (definition 10), where the gauge field is added at each position, and a relative extension (definition 11), where the gauge field is added on the links between the positions.

In Physics one usually motivates the demand for a certain gauge symmetry from an already existing global symmetry. Mathematically, the gauge field introduced to ensure gauge invariance is often seen as a connection between gauge choices at neighboring points. However, there is no immediate reason for gauge invariance to arise from an already existing global invariance, nor is there an immediate reason for the gauge field to be interpretable as a connection. A relation between these two folklore perspectives was given through theorem 1 where globally invariant (or G–blind) cellular automata were then shown to be exactly those relatively extensible into gauge invariant ones.

Since globally invariant cellular automata are universal, this provides a first way to show the universality of gauge invariant cellular automata. The intrinsic universality was then proven a second time (in theorem 2), through the explicit construction of an absolute gauge extension. The intrinsic universality of the model is a strong result since it allows the implementation of the symmetry starting with any given dynamics.

A last contribution in the classical setting, was the formalization and preliminary study of the degree of freedom induced by the symmetry. Since two cellular automata can have the same dynamics up to the symmetry, a notion of equivalence was given in definition 12. This related to the well-known concept of gauge fixing in Physics, which is the choice of a dynamics among the equivalent ones.

3+1 quantum electrodynamics as a quantum cellular automaton. In the second chapter of this thesis we constructed a quantum cellular automata (QCA) accounting for QED in $2+1$ and $3+1$ dimensions. The construction follows the same principles used to build the Lagrangian formulation of QED—i.e. free anti-commuting fermions, gauge invariant, simplest electric and magnetic term. But here spacetime is discrete, and space and time are treated on equal footing. The evolution is described in terms of local quantum gates, whose wiring coincide exactly with the speed of light of the QED. To reach our goal, we needed three contributions.

The first contribution was the formulation of gauge invariant qubit-local evolution operators—equations (2.25) and (2.32)—that meet the specifications imposed by the (anti-)commutation relations (2.5), (2.6) and (2.7) of the fermionic and bosonic annihilators/lowering operators they are made of. It was, to us, a surprise that this could be achieved since it is in apparent contradiction with the no-go result of [70]. But, following ideas of [74, 86] the gauge field came to the rescue. This was used to obtain a $2+1$ Dirac QCA, i.e. a generalization of the $2+1$ Dirac QW to multiple walkers, recovering the free fermionic dynamics $\mathbf{D_F}$ (2.78) which is represented in figure 2.3.

The second contribution was to derive the electric $\mathbf{D_E}$ (2.79) and magnetic $\mathbf{D_M}$ (2.81) contributions, leading to the $2+1$ QED QCA in Eq. (2.117). The magnetic contributions was the most challenging, but in the end two possible quantum circuit representations were found. The first uses a diagonalization, through a Fourier transform, in order to exponentiate the plaquette terms (2.99), albeit up to truncation. The second approach formulates the magnetic contribution in terms of a quantum walk over the gauge field Hilbert space $\mathscr{H}_{\mathbb{Z}}$ (2.113) without the need for a truncation. Both approaches lead to the same continuum limit (2.82) and were checked to correspond to the integration of the magnetic part of the Kogut-Susskind Hamiltonian.

The third contribution was the extension of the QCA to a $3+1$ QED QCA (2.154) which required, in our model, raising the state space from 2 to 4 qubits per sites to represent fermions. On paper, this meant working out the consequences of the anti-commutation relations for fermions, under sophisticated changes of basis. Fortunately, these 4-qubit gates were decomposable as 2-qubit gates which we knew how to handle. The electric and magnetic contribution were straightforwardly extended from the $2+1$ case. Altogether, the $3+1$ QED QCA provides a first, *relativistic* discrete spacetime formulation of a quantum field theory.

Discussion

Notice that the distinction between fermions and interacting hardcore-bosons [87, 88] is wearing thin with this qubit-local model, and yet seems to persist as embodied by the Z terms of equations (2.25) and (2.30). Moreover, there is nothing fundamental in the arbitrary choice of local Jordan-Wigner order that remains, any order is essentially as good as another. Could the same dynamics be defined without such an order? This is intriguing, and one truly wonders whether the distinction between fermion and hardcore-bosons is physically observable or can be proven otherwise [73].

In chapter 2, we focused on the dynamics of the fermions and gauge field, without specifically studying the photonic dynamics. For instance, the quantum circuit does not inform us on the way the gauge field allow for photonic transport, or what the effective speed of light would be. A theory of light in the settings of QCA has already been defined in [89], it would be interesting to look for a connection between this theory and the excitations of the gauge field in our model.

In the introduction of chapter 2, the advantage of a *relativistic* quantum simulation was stipulated. In theory, the circuit simulation of QED presented here could allow

for a more efficient simulation of QED than Hamiltonian discretization, because of a hypothesized quadratic gain in the number of gates for the same time-lapse. For the same decoherence of the simulation device, such gain is significative in the number of time steps that could be simulated. However, all of this is still at the level of ideas and intuitions and would benefit from being backed by better theoretical and experimental arguments.

Looking back at our work in the classical setting, the example of dynamics for the gauge field were mostly trivial. The gauge field was introduced to ensure gauge invariance but not used to derive new dynamics. In the quantum version, such dynamics is in fact the mediator for interaction. In the examples given throughout chapter 1, the gauge field influences the matter field but not the other way around. Hence, defining a two-way interaction between gauge and matter field at the classical level, may hold interesting prospects.

Perspectives

Short-term and midterm research prospects An immediate continuation of this work would be to further parametrize the QED QCA, making it 'plastic' enough so that we may be able to take a discrete space continuous time limit of the model. This was first done for QW [54, 55], and used to prove that a 1+1 QED QCA recovers the Kogut-Susskind Hamiltonian in [56]. Going beyond QED and obtaining a QCA that implements quantum chromodynamics (QCD) would require non-Abelian gauge invariance. Gauge invariance was defined in cellular automata for any group of gauge transformation, be it Abelian or not. Hence, another continuation of this work is to extend the model to encompass QCD.

In the definition of the extension of a cellular automaton, there is no preferred direction of space, i.e. the edges are not oriented, and the local evolution rule is symmetric in all space directions. Such properties hint that relative gauge invariance could be defined on cellular automata that live on graphs [57], for example on triangular and tetrahedral spatial discretization of space, as was done for quantum walks [90].

An extension to graphs holds a particular interest for a fundamentally discrete, relativistic version of QED, defined on a curved space. Going further, it would also allow for a (quantum) graph dynamics—i.e. a (quantum) dynamics over the structure of the graph itself [91]—to be coupled with the matter dynamics. In the one particle sector, an example of this was built, where the space triangulation is dynamically induced by the quantum walk [6]. Such a coupling between matter and geometry, where the field (matter and gauge) distribution evolves according to QED, is reminiscent of general relativity and is thus an interesting perspective which does not seem out of reach.

Back to the classical setting, gauge invariance introduces some degrees of freedom, both on the choice of the evolution and on the choice of a specific configuration to describe a physical state. In Physics a canonical way to remove or constrain such degrees of freedom is gauge fixing—e.g. temporal/Weyl gauge. Gauge fixing was introduced in this manuscript, but there is no canonical way of doing so. Hence,

defining a canonical gauge fixing procedure offers a perspective of research. Moreover, an elegant derivation of Gauss' law (conservation law) can arise from constraining these degrees of freedom [92, 86]. Can Gauss' law find a formulation in terms of classical CA and be derived through a constraint of the degrees of freedom offered by gauge invariance?

Long-term applications These two and three-dimensional QED QCA are quantum circuits. $\mathbf{D_F}$, $\mathbf{D_E}$ and $\mathbf{D_M}$ can be expressed in terms of standard universal gates such as CNOT, PHASE, HADAMARD. Thus, the QCA is directly interpretable as a digital quantum simulation algorithm, to be run on a Quantum Computer. A perspective is thus the implementation of this QCA on quantum computers. This simulation scheme is efficient, in that it requires $O(s^d/\Delta_x^d\ t/\Delta_t)$ gates in order to simulate a chunk of space of size s, over t time steps with Δ_x the space resolution, Δ_t the time resolution, and d the space dimension. The output of this is a quantum state and the simulation may need to be run multiple times in order to obtain meaningful statistics. However, classically just the state space itself is an $O(e^{s^d/\Delta_x^d})$ as it grows exponentially with the number of quantum systems to be simulated. The classical time complexity is thus $O(e^{s^d/\Delta_x^d} t/\Delta_t)$. The exponential gain here clearly comes from the fact that the scheme simulates a multi-particle systems, just like in Hamiltonian-based multi-particle quantum simulation schemes. Quantum walk-based simulation schemes on the other hand, are by definition in the one-particle sector, and thus can only yield polynomial gains.

Gauge invariance is a symmetry. As such it introduces the ideas of equivalence and degrees of freedom. What if this degree of freedom is used to add redundancy to the system in a way that it can detect, and potentially correct errors? This idea has already been studied in the quantum setting [93, 94, 95] where gauge invariance amounts to invariance under certain local errors. It echoes the question of noise resistance in cellular automata [96, 97]. Consider that the gauge transformations are defined as noise which interfere with the evolution of the cellular automata. Gauge extending the cellular automata would provide a construction for noise resistance.

Gauge symmetry has been studied for almost a century, leading to some of the most established and successful models in Physics. During the same time period, cellular automata have also been the subject of countless research projects, leading to theoretical results as well as numerous applications. It is undoubtedly clear that both fields still have much to offer each on their own. I hope this work convinced you that they also have much to offer together.

Bibliography

[1] Pablo Arrighi, Giuseppe Di Molfetta, and Nathanaël Eon. "A gauge invariant reversible cellular automaton". In: *International Workshop on Cellular Automata and Discrete Complex Systems*. Springer. 2018, pp. 1–12 (cit. on p. 3).

[2] Pablo Arrighi, Giuseppe Di Molfetta, and Nathanaël Eon. "Non-abelian gauge-invariant cellular automata". In: *International Conference on Theory and Practice of Natural Computing*. Springer. 2019, pp. 211–221 (cit. on p. 3).

[3] Pablo Arrighi, Marin Costes, and Nathanaël Eon. "Universal gauge-invariant cellular automata". In: *MFCS*. Vol. 202. 2021, 9:1–9:14 (cit. on p. 3).

[4] Pablo Arrighi, Giuseppe Di Molfetta, and Nathanael Eon. "Gauge invariance in cellular automata". In: *Natural Computing* (2022), pp. 1–13 (cit. on p. 3).

[5] Nathanaël Eon, Giuseppe Di Molfetta, Giuseppe Magnifico, et al. *A relativistic discrete spacetime formulation of 3+1 QED*. 2022 (cit. on p. 3).

[6] Quentin Aristote, Nathanael Eon, and Giuseppe Di Molfetta. "Dynamical triangulation induced by quantum walk". In: *Symmetry* 12 (2020), p. 128 (cit. on pp. 3, 18, 78).

[7] Chris Quigg. *Gauge theories of the strong, weak, and electromagnetic interactions*. Princeton University Press, 2013 (cit. on p. 11).

[8] Mari Carmen Banuls, Rainer Blatt, Jacopo Catani, et al. "Simulating lattice gauge theories within quantum technologies". In: *The European physical journal D* 74.8 (2020), pp. 1–42 (cit. on pp. 11, 14, 47).

[9] K. Culik, L. P. Hurd, and S. Yu. "Computation theoretic aspects of cellular automata". In: *Physica D* 45 (1990), pp. 357–378 (cit. on p. 12).

[10] M. Delorme. "An Introduction to Cellular Automata, Cellular Automata: a Parallel Model". In: *Mathematics and Its Applications*. Kluwer, 1999 (cit. on p. 12).

[11] K. Kari. "Theory of cellular automata: A survey". In: *Theor. Comp. Sc.* 334 (2005), p. 2005 (cit. on p. 12).

[12] Pablo Arrighi. "An overview of quantum cellular automata". In: *Natural Computing* 18.4 (2019), pp. 885–899 (cit. on pp. 12, 57).

[13] Terry Farrelly. "A review of Quantum Cellular Automata". In: *Quantum* 4 (2020), p. 368 (cit. on p. 12).

[14] J. von Neumann. *Theory of Self-Reproducing Automata*. Champaign, IL, USA: University of Illinois Press, 1966 (cit. on p. 13).

[15] K. Nagel and M. Schreckenberg. "A cellular automaton model for freeway traffic". In: *J. Phys. I France* 2 (1992), pp. 2221–2229 (cit. on p. 13).

[16] Maria Vittoria Avolio, Alessia Errera, Valeria Lupiano, et al. "Development and Calibration of a Preliminary Cellular Automata Model for Snow Avalanches". In: *ACRI*. 2010 (cit. on p. 13).

[17] D.H. Rothman and S. Zaleski. *Lattice-gas cellular automata: simple models of complex hydrodynamics*. Cambridge University Press, 1997 (cit. on p. 13).

[18] Patrick C. Fischer. "Generation of Primes by a One-Dimensional Real-Time Iterative Array". In: *J. ACM* 12 (1965), pp. 388–394 (cit. on p. 13).

[19] E. F. Moore. "The firing squad synchronization problem". In: *Sequential Machines, Selected Papers*. Addison-Wesley, 1964, pp. 213–214 (cit. on p. 13).

[20] Marcus Pivato. "Conservation laws in cellular automata". In: *Nonlinearity* 15.6 (2002), p. 1781 (cit. on p. 13).

[21] Siamak Taati. "Conservation Laws in Cellular Automata". In: *Handbook of Natural Computing*. 2012 (cit. on p. 13).

[22] J. Kari. "Reversibility and surjectivity problems of cellular automata". In: *J. Comput. Syst. Sci.* 48.1 (1994), pp. 149–182. ISSN: 0022-0000. DOI: 10.1016/S0022-0000(05)80025-X (cit. on p. 13).

[23] J. Kari. "On the circuit depth of structurally reversible cellular automata". In: *Fundamenta Informaticae* 38.1-2 (1999), pp. 93–107 (cit. on p. 13).

[24] Anahí Gajardo, Jarkko Kari, and Andrés Moreira. "On time-symmetry in cellular automata". In: *J. Comput. Syst. Sci.* 78 (2012), pp. 1115–1126 (cit. on p. 13).

[25] Ville Salo and Ilkka Törmä. "Color Blind Cellular Automata". In: *Lecture Notes in Computer Science* (2013), pp. 139–154. ISSN: 1611-3349 (cit. on pp. 13, 24, 38, 39).

[26] N. Ollinger. "Universalities in cellular automata a (short) survey." In: *First Symposium on Cellular Automata "Journées Automates Cellulaires" (JAC 2008), Uzès, France, April 21-25, 2008. Proceedings*. Ed. by B. Durand. MCCME Publishing House, Moscow, 2008, pp. 102–118 (cit. on p. 13).

[27] Jean-Charles Delvenne, Petr Kurka, and Vincent D. Blondel. "Decidability and Universality in Symbolic Dynamical Systems". In: *Fundam. Informaticae* 74 (2006), pp. 463–490 (cit. on p. 13).

[28] IM Georgescu, Sahel Ashhab, and Franco Nori. "Quantum simulation". In: *Reviews of Modern Physics* 86.1 (2014), p. 153 (cit. on p. 14).

[29] Seth Lloyd. "Universal quantum simulators". In: *Science* 273.5278 (1996), pp. 1073–1078 (cit. on p. 14).

[30] Stephen P Jordan, Keith SM Lee, and John Preskill. "Quantum algorithms for quantum field theories". In: *Science* 336.6085 (2012), pp. 1130–1133 (cit. on p. 14).

[31] John Preskill. "Simulating quantum field theory with a quantum computer". In: *Proceedings of The 36th Annual International Symposium on Lattice Field Theory - PoS(LATTICE2018)* (2019) (cit. on p. 14).

[32] Alexei Y. Kitaev. "Fault tolerant quantum computation by anyons". In: *Annals of Physics* 303 (2003), pp. 2–30 (cit. on p. 14).

[33] Lucile Savary and Leon Balents. "Quantum spin liquids: a review." In: *Reports on progress in physics. Physical Society* 80 1 (2017), p. 016502 (cit. on p. 14).

[34] Anthony Ciavarella, Natalie Klco, and Martin J Savage. "Some Conceptual Aspects of Operator Design for Quantum Simulations of Non-Abelian Lattice Gauge Theories". In: *arXiv preprint arXiv:2203.11988* (2022) (cit. on p. 14).

[35] Daniel González-Cuadra, Torsten V Zache, Jose Carrasco, et al. "Hardware efficient quantum simulation of non-abelian gauge theories with qudits on Rydberg platforms". In: *arXiv preprint arXiv:2203.15541* (2022) (cit. on p. 14).

[36] Francesco Knechtli, Michael Günther, and Michael Peardon. *Lattice quantum chromodynamics: practical essentials*. Springer, 2017 (cit. on p. 14).

[37] J. B. Kogut and Leonard Susskind. "Hamiltonian Formulation of Wilson's Lattice Gauge Theories". In: *Physical Review D* 11 (1975), pp. 395–408 (cit. on pp. 14, 57, 63).

[38] Thomas Banks, Leonard Susskind, and J. B. Kogut. "Strong Coupling Calculations of Lattice Gauge Theories: (1+1)-Dimensional Exercises". In: *Physical Review D* 13 (1976), pp. 1043–1053 (cit. on p. 14).

[39] Esteban A. Martinez, Christine A. Muschik, Philipp Schindler, et al. "Real-time dynamics of lattice gauge theories with a few-qubit quantum computer". In: *Nature* 534 (2016), pp. 516–519 (cit. on p. 15).

[40] Federica M Surace, Paolo P Mazza, Giuliano Giudici, et al. "Lattice gauge theories and string dynamics in Rydberg atom quantum simulators". In: *Physical Review X* 10.2 (2020), p. 021041 (cit. on p. 15).

[41] E Rico, T Pichler, M Dalmonte, et al. "Tensor networks for lattice gauge theories and atomic quantum simulation". In: *Physical Review Letters* 112.20 (2014), p. 201601 (cit. on p. 15).

[42] Marcello Dalmonte and Simone Montangero. "Lattice gauge theory simulations in the quantum information era". In: *Contemporary Physics* 57.3 (2016), pp. 388–412 (cit. on p. 15).

[43] Mari Carmen Banuls and Krzysztof Cichy. "Review on novel methods for lattice gauge theories". In: *Reports on Progress in Physics* 83.2 (2020), p. 024401 (cit. on p. 15).

[44] Román Orús. "A Practical Introduction to Tensor Networks: Matrix Product States and Projected Entangled Pair States". In: *Annals of Physics* 349 (2013), pp. 117–158 (cit. on p. 15).

[45] Guifre Vidal. "Entanglement renormalization". In: *Physical review letters* 99.22 (2007), p. 220405 (cit. on p. 15).

[46] Matteo Rizzi, Simone Montangero, and Guifre Vidal. "Simulation of time evolution with multiscale entanglement renormalization ansatz". In: *Physical Review A* 77.5 (2008), p. 052328 (cit. on p. 15).

[47] Tobias J Osborne. "Continuum limits of quantum lattice systems". In: *arXiv preprint arXiv:1901.06124* (2019) (cit. on p. 15).

[48] Jens Eisert and David Gross. "Supersonic quantum communication". In: *Physical review letters* 102.24 (2009), p. 240501 (cit. on p. 15).

[49] Marc Cheneau and Laurent Sanchez-Palencia. "A Speed Test for Ripples in a Quantum System". In: *Physics* 13 (2020), p. 109 (cit. on p. 15).

[50] C Huerta Alderete, Shivani Singh, Nhung H Nguyen, et al. "Quantum walks and Dirac cellular automata on a programmable trapped-ion quantum computer". In: *Nature communications* 11.1 (2020), pp. 1–7 (cit. on p. 15).

[51] Tobias M. Wintermantel, Yao Wang, Graham Lochead, et al. "Unitary and Nonunitary Quantum Cellular Automata with Rydberg Arrays." In: *Physical review letters* 124 (2020) (cit. on p. 15).

[52] Julian Seymour Schwinger. "Gauge Invariance and Mass". In: *Physical Review* 125 (1962), pp. 2425–2429 (cit. on p. 16).

[53] Pablo Arrighi, Cédric Bény, and Terry Farrelly. "A quantum cellular automaton for one-dimensional QED". In: *Quantum Information Processing* 19 (2020), pp. 1–28 (cit. on pp. 16, 45–47, 62, 63).

[54] Giuseppe Di Molfetta and Pablo Arrighi. "A quantum walk with both a continuous-time limit and a continuous-spacetime limit". In: *Quantum Information Processing* 19.2 (2020), pp. 1–16 (cit. on pp. 16, 78).

[55] Michael Manighalam and Giuseppe Di Molfetta. "Continuous time limit of the DTQW in 2D+ 1 and plasticity". In: *Quantum Information Processing* 20.2 (2021), pp. 1–24 (cit. on pp. 16, 78).

[56] Kevissen Sellapillay, Pablo Arrighi, and Giuseppe Di Molfetta. "A discrete relativistic spacetime formalism for 1 + 1-QED with continuum limits". In: *Scientific Reports* 12 (2022) (cit. on pp. 16, 45, 78).

[57] Pablo Arrighi, Simon Martiel, and Vincent Nesme. "Cellular automata over generalized Cayley graphs". In: *Mathematical Structures in Computer Science* 28 (2017), pp. 340–383 (cit. on pp. 20, 78).

[58] Tommaso Toffoli and Norman Margolus. "Cellular automata machines - a new environment for modeling". In: *MIT Press series in scientific computation*. 1987 (cit. on p. 22).

[59] Kenichi Morita and Masateru Harao. "Computation universality of one-dimensional reversible (injective) cellular automata". In: *IEICE Transactions on Fundamentals of Electronics, Communications and Computer Sciences* 72 (1989), pp. 758–762 (cit. on p. 22).

[60] Kenichi Morita and Katsunobu Imai. "Logical Universality and Self-Reproduction in Reversible Cellular Automata". In: *ICES*. 1996 (cit. on p. 22).

[61] Pablo Arrighi and Jonathan Grattage. "Partitioned quantum cellular automata are intrinsically universal". In: *Natural Computing* 11 (2011), pp. 13–22 (cit. on pp. 22, 57).

[62] Pierre Guillon, Pierre-Etienne Meunier, and Guillaume Theyssier. "Clandestine Simulations in Cellular Automata". In: *JAC*. 2010 (cit. on p. 23).

[63] Guillaume Theyssier. "Automates cellulaires : un modèle de complexités". In: 2005 (cit. on p. 38).

[64] Nicolas Ollinger. "Intrinsically Universal Cellular Automata". In: *CSP*. 2008 (cit. on p. 38).

[65] Giuseppe Di Molfetta, M Brachet, and Fabrice Debbasch. "Quantum walks as massless Dirac fermions in curved space-time". In: *Physical Review A* 88.4 (2013), p. 042301 (cit. on p. 45).

[66] Giuseppe Di Molfetta and Armando Pérez. "Quantum walks as simulators of neutrino oscillations in a vacuum and matter". In: *New Journal of Physics* 18.10 (2016), p. 103038 (cit. on p. 45).

[67] Mohamed Hatifi, Giuseppe Di Molfetta, Fabrice Debbasch, et al. "Quantum walk hydrodynamics". In: *Scientific reports* 9.1 (2019), pp. 1–7 (cit. on p. 45).

[68] Andre Ahlbrecht, Andrea Alberti, Dieter Meschede, et al. "Molecular binding in interacting quantum walks". In: *New Journal of Physics* 14.7 (2012), p. 073050 (cit. on p. 45).

[69] Alessandro Bisio, Giacomo Mauro D'Ariano, Paolo Perinotti, et al. "Thirring quantum cellular automaton". In: *Physical Review A* 97.3 (2018), p. 032132 (cit. on p. 45).

[70] Leonard D. Mlodinow and Todd A. Brun. "Quantum field theory from a quantum cellular automaton in one spatial dimension and a no-go theorem in higher dimensions". In: *Physical Review A* (2020) (cit. on pp. 45, 49, 77).

[71] Todd A Brun and Leonard Mlodinow. "Quantum cellular automata and quantum field theory in two spatial dimensions". In: *Physical Review A* 102.6 (2020), p. 062222 (cit. on p. 45).

[72] Leonard Mlodinow and Todd A Brun. "Fermionic and bosonic quantum field theories from quantum cellular automata in three spatial dimensions". In: *Physical Review A* 103.5 (2021), p. 052203 (cit. on p. 45).

[73] Erez Zohar and Juan Ignacio Cirac. "Eliminating fermionic matter fields in lattice gauge theories". In: *Physical Review B* (2018) (cit. on pp. 45, 77).

[74] Terry Farrelly. "Insights from quantum information into fundamental physics". In: *arXiv preprint arXiv:1708.08897* (2017) (cit. on pp. 45, 49, 77).

[75] Giuseppe Di Molfetta, Marc Brachet, and Fabrice Debbasch. "Quantum walks in artificial electric and gravitational fields". In: *Physica A: Statistical Mechanics and its Applications* 397 (2014), pp. 157–168 (cit. on p. 47).

[76] Pablo Arnault, Giuseppe Di Molfetta, Marc Brachet, et al. "Quantum walks and non-Abelian discrete gauge theory". In: *Physical Review A* 94.1 (2016), p. 012335 (cit. on p. 47).

[77] Iván Márquez-Martín, Pablo Arnault, Giuseppe Di Molfetta, et al. "Electromagnetic lattice gauge invariance in two-dimensional discrete-time quantum walks". In: *Physical Review A* 98.3 (2018), p. 032333 (cit. on p. 47).

[78] C Cedzich, T Geib, AH Werner, et al. "Quantum walks in external gauge fields". In: *Journal of Mathematical Physics* 60.1 (2019), p. 012107 (cit. on p. 47).

[79] Kirill Melnikov and Marvin Weinstein. "Lattice Schwinger model: Confinement, anomalies, chiral fermions, and all that". In: *Physical Review D* 62 (2000), p. 094504 (cit. on p. 55).

[80] P. Arrighi, V. Nesme, and R. Werner. "Unitarity plus causality implies localizability (full version)". In: *Journal of Computer and System Sciences* 77.2 (2011), pp. 372–378 (cit. on p. 57).

[81] Giuseppe Di Molfetta and Fabrice Debbasch. "Discrete-time quantum walks: Continuous limit and symmetries". In: *Journal of Mathematical Physics* 53.12 (2012), p. 123302 (cit. on pp. 58, 71).

[82] Pablo Arrighi, Vincent Nesme, and Marcelo Forets. "The Dirac equation as a quantum walk: higher dimensions, observational convergence". In: *Journal of Physics A: Mathematical and Theoretical* 47.46 (2014), p. 465302 (cit. on pp. 58, 71).

[83] Elisa Ercolessi, Paolo Facchi, Giuseppe Magnifico, et al. "Phase transitions in Z n gauge models: towards quantum simulations of the schwinger-weyl qed". In: *Physical Review D* 98.7 (2018), p. 074503 (cit. on p. 63).

[84] Jan F. Haase, Luca Dellantonio, Alessio Celi, et al. "A resource efficient approach for quantum and classical simulations of gauge theories in particle physics". In: *Quantum* 5 (2021), p. 393 (cit. on pp. 64, 66).

[85] Ivan Márquez-Martín, Giuseppe Di Molfetta, and Armando Pérez. "Fermion confinement via quantum walks in (2+ 1)-dimensional and (3+ 1)-dimensional space-time". In: *Physical Review A* 95.4 (2017), p. 042112 (cit. on p. 71).

[86] Giuseppe Magnifico, Timo Felser, Pietro Silvi, et al. "Lattice quantum electrodynamics in (3+1)-dimensions at finite density with tensor networks". In: *Nature Communications* 12 (2021) (cit. on pp. 77, 79).

[87] Matteo Lugli, Paolo Perinotti, and Alessandro Tosini. "Fermionic state discrimination by local operations and classical communication". In: *Physical Review Letters* 125.11 (2020), p. 110403 (cit. on p. 77).

[88] Chiara Marletto and Vlatko Vedral. "Spin, Statistics, Spacetime and Quantum Gravity". In: *arXiv preprint arXiv:2112.03392* (2021) (cit. on p. 77).

[89] Alessandro Bisio, Giacomo Mauro D'Ariano, and Paolo Perinotti. "Quantum Cellular Automaton Theory of Light". In: *Annals of Physics* 368 (2014), pp. 177–190 (cit. on p. 77).

[90] Pablo Arrighi, Giuseppe Di Molfetta, Iván Márquez, et al. "Dirac equation as a quantum walk over the honeycomb and triangular lattices". In: *Physical Review A* 97.6 (2018), p. 062111 (cit. on p. 78).

[91] Pablo Arrighi, Marios Christodoulou, and Amélia Durbec. "On quantum superpositions of graphs, no-signalling and covariance". In: *arXiv preprint arXiv:2010.13579* (2020) (cit. on p. 78).

[92] Timo Felser, Pietro Silvi, Mario Collura, et al. "Two-Dimensional Quantum-Link Lattice Quantum Electrodynamics at Finite Density". In: *arXiv: Quantum Physics* (2019) (cit. on p. 79).

[93] A Yu Kitaev. "Fault-tolerant quantum computation by anyons". In: *Annals of Physics* 303.1 (2003), pp. 2–30 (cit. on p. 79).

[94] Chetan Nayak, Steven H Simon, Ady Stern, et al. "Non-Abelian anyons and topological quantum computation". In: *Reviews of Modern Physics* 80.3 (2008), p. 1083 (cit. on p. 79).

[95] Abhishek Rajput, Alessandro Roggero, and Nathan Wiebe. "Quantum Error Correction with Gauge Symmetries". In: *arXiv preprint arXiv:2112.05186* (2021) (cit. on p. 79).

[96] Masateru Harao and Shoichi Noguchi. "Fault tolerant cellular automata". In: *Journal of computer and system sciences* 11.2 (1975), pp. 171–185 (cit. on p. 79).

[97] A. Toom. "Cellular automata with errors: Problems for students of probability". In: *Topics in Contemporary Probability and Its Applications* (1995), pp. 117–157 (cit. on p. 79).

A. From quantum walk to quantum cellular automata operators

We explain the process to go from a quantum walk to quantum cellular automata operators, starting in the $2+1$ case.

The QCA gates act on 2 qubits and are number conserving, which constrains them. Indeed, the evolution for the input $|00\rangle$ will always be the identity without loss of generality, and the evolution for the input $|11\rangle$ is only a phase since it is the only state with occupation number equal to 2. Therefore, any QCA gate $\mathbf{W}^\dagger$ can be written as a direct sum $\mathbf{W}^\dagger = W^\dagger \oplus e^{i\varphi}$ with $W^\dagger = 1 \oplus M$ the quantum walk gate for one particle and φ a phase to be determined. To find out this phase exactly, we use the Heisenberg picture.

Let $\mathbf{W}^\dagger = 1 \oplus M \oplus e^{i\varphi}$ be a QCA gate over two qubits $(x,0)$ and $(x,1)$ with:

$$M = \begin{pmatrix} M_{00} & M_{01} \\ M_{10} & M_{11} \end{pmatrix} = \begin{pmatrix} M_{00} & -e^{i\theta} M_{10}^* \\ M_{10} & e^{i\theta} M_{00}^* \end{pmatrix} \text{ without loss of generality.} \tag{A.1}$$

The Heisenberg picture describes the future impact of our past actions. Consider the past action $a_{x,1}^\dagger$ at t:

$$a_{x,1}^\dagger = |1\rangle^{x,1} \langle 0| \otimes Z_{x,0} \bigotimes_{y \prec (x,0)} Z_y \tag{A.2}$$

$$= (|10\rangle\langle 00| - |11\rangle\langle 01|) \bigotimes_{y \prec (x,0)} Z_y. \tag{A.3}$$

Its future impact at time $t+1$ is

$$\mathbf{W} a_{x,1}^\dagger \mathbf{W}^\dagger = \left[(M_{11}|10\rangle + M_{01}|01\rangle)\langle 00| - e^{i\varphi}|11\rangle \left(\langle 01| M_{00}^* + \langle 10| M_{10}^* \right) \right] \bigotimes_{y \prec (x,0)} Z_y \tag{A.4}$$

$$= \left[|1\rangle\langle 0| \otimes \begin{pmatrix} M_{11} & 0 \\ 0 & -e^{i\varphi} M_{00}^* \end{pmatrix} + \begin{pmatrix} M_{01} & 0 \\ 0 & -e^{i\varphi} M_{10}^* \end{pmatrix} \otimes |1\rangle\langle 0| \right] \bigotimes_{y \prec (x,0)} Z_y. \tag{A.5}$$

$$= \left[|1\rangle\langle 0| \otimes \begin{pmatrix} e^{i\theta} M_{00}^* & 0 \\ 0 & -e^{i\varphi} M_{00}^* \end{pmatrix} + \begin{pmatrix} -e^{i\theta} M_{10}^* & 0 \\ 0 & -e^{i\varphi} M_{10}^* \end{pmatrix} \otimes |1\rangle\langle 0| \right] \bigotimes_{y \prec (x,0)} Z_y. \tag{A.6}$$

Suppose that the φ we seek to determine, is equal to θ. With this supposition, the above simplifies and we have that the future impact of $a_{x,1}^\dagger$ is just $\mathbf{W} a_{x,1}^\dagger \mathbf{W}^\dagger = M_{11} a_1^\dagger + M_{01} a_{x,0}^\dagger$. A contrario, with any other choice of φ we would be constructing some $\mathbf{W}'$ which,

albeit coinciding with $\mathbf{W}$ and thus W in the one-particle sector, would for instance leave a phase between $a^\dagger_{x,1}a^\dagger_{x,0}a_{x,0}$ and $a^\dagger_{x,1}a_{x,0}a^\dagger_{x,0}$ in the future impact of $a^\dagger_{x,1}$. The future impact of $a^\dagger_{x,1}$ would again yield a superposition of a particle at $(x,0)$ or at $(x,1)$, but with a phase depending on another particle being there or not. Such a $\mathbf{W}'$ would not, therefore, be the 'rightful non-interacting extensions of W' to the multi-particle sector. Only $\mathbf{W}$ is. In other words, we were seeking to determine the φ of the last entry of $\mathbf{W}$; setting it to θ fixes it to its non-interactive value.

The same process can be applied to the evolution $a^\dagger_{x,0}$ leading to

$$\mathbf{W}a^\dagger_{x,0}\mathbf{W}^\dagger = M_{00}a^\dagger_{x,0} + M_{10}a^\dagger_{x,1} \tag{A.7}$$
$$\mathbf{W}a^\dagger_{1}\mathbf{W}^\dagger = M_{01}a^\dagger_{x,0} + M_{11}a^\dagger_{x,1}. \tag{A.8}$$

Considering as past action the product of these two operators $a^\dagger_{x,0}a^\dagger_{x,1}$. Its future impact is

$$\mathbf{W}a^\dagger_{x,0}\mathbf{W}^\dagger\mathbf{W}a^\dagger_{x,1}\mathbf{W}^\dagger = (M_{00}a^\dagger_{x,0} + M_{10}a^\dagger_{x,1})(M_{01}a^\dagger_{x,0} + M_{11}a^\dagger_{x,1}) \tag{A.9}$$
$$= M_{00}M_{11}a^\dagger_{x,0}a^\dagger_{x,1} + M_{01}M_{10}a^\dagger_{x,1}a^\dagger_{x,0} \tag{A.10}$$
$$= (M_{00}M_{11} - M_{01}M_{10})a^\dagger_{x,0}a^\dagger_{x,1}. \tag{A.11}$$

Now, because state $|00\rangle$ evolves into $|00\rangle$, and because $|11\rangle = a^\dagger_{x,0}a^\dagger_{x,1}|00\rangle$, it must be that $|11\rangle$ evolves into $(M_{00}M_{11} - M_{01}M_{10})a^\dagger_{x,0}a^\dagger_{x,1}|00\rangle = (M_{00}M_{11} - M_{01}M_{10})|11\rangle$. Hence, the phase $e^{i\varphi} = e^{i\theta}$ applied to $|11\rangle$ can simply be written $M_{00}M_{11} - M_{01}M_{10}$.

In other words we have that for any QW gate $W = 1 \oplus M$ acting on qubits that follow each other in the JW order, the corresponding non-interactive multi-particle extension QCA gate is

$$\mathbf{W}^\dagger = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & M_{00} & M_{01} & 0 \\ 0 & M_{10} & M_{11} & 0 \\ 0 & 0 & 0 & M_{00}M_{11} - M_{01}M_{10} \end{pmatrix}. \tag{A.12}$$

Let us now use this to define the on-site and transport gates of the QCA.

A.1. On-site operators

First consider $\mathbf{S} = 1 \oplus X \oplus e^{i\varphi}$ with $S_{01} = X_{10} = 1$ and $X_{00} = X_{11} = 0$. We justified in subsection 2.2.2 that φ needs be π. With the above this readily follows from $X_{00}X_{11} - X_{01}X_{10} = -1$ Therefore $\mathbf{S}$ is:

$$\mathbf{S} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{A.13}$$

On-site QW gates that are mere permutations of qubits in the one-particle sector,

can be extended to the multi-particle sector directly by means as products of **S**, in the same way that any permutation can be obtained from local transpositions.

For the mass term and the basis changes, this is not the case, but Eq. (A.12) again readily applies. As an example, the mass term $C_\epsilon = 1 \oplus C$ has $C_{00}C_{11} - C_{01}C_{10} = c^2 + s^2 = 1$, which results in the following mass gate for the QCA:

$$\mathbf{C}_\epsilon = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & c & -s & 0 \\ 0 & s & c & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{A.14}$$

A.2. Transport operators

In this chapter the transport is implemented in two steps: first swap the qubits on-site so that the right-moving qubit is on the right-hand side of the site (**S**), then hop qubits across adjacent sites (**T**) whilst changing the gauge field accordingly.

The hopping term **T** is of the form:

$$a^\dagger_{x+\eta} V^\dagger_{x,\eta} a_x = |1\rangle^{x+\eta} \langle 0| \left(\prod_{y \in \left[x+\eta,(x+\eta,-\eta)\right[} Z_y \right) U^\dagger_{x,\eta} \left(\prod_{y \in \left[x,(x,\eta)\right[} Z_y \right) |0\rangle^x \langle 1|. \tag{A.15}$$

In the one particle sector, one gets the operator:

$$T_\eta = 1 \oplus T \text{ with } T = \begin{pmatrix} 0 & K^\dagger_\eta \\ K_\eta & 0 \end{pmatrix} \tag{A.16}$$

with

$$K_{x,\eta} = \left(\prod_{y \in \left[x,(x,\eta)\right[} Z_y \right) U_{x,\eta} \left(\prod_{y \in \left[x+\eta,(x+\eta,-\eta)\right[} Z_y \right). \tag{A.17}$$

I.e. T plays the same role as M in Eq. (A.12), up to operators updating the gauge field.

The same reasoning applies. Since

$$T_{00}T_{11} - T_{01}T_{10} = -K^\dagger_\eta K_\eta = -I \tag{A.18}$$

we have that

$$\mathbf{T}_\eta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & K^\dagger_\eta & 0 \\ 0 & K_\eta & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{A.19}$$

A.3. 3+1 dimensions

In $3+1$ dimensions, there are four qubits per site instead of two. A QW operators W that acted in the one particle sector $|0001\rangle, |0010\rangle, \ldots$, now needs to be extended to a QCA operator $\mathbf{W}$ that can handle the multi-particle sector $|0011\rangle, |1110\rangle, \ldots$, which seems to leave open many more possibilities than in the $2+1$ case. However, the $3+1$ QW operators we are dealing with easily be decomposed as circuits of 2-qubit gates, with the qubits following each other in the JW order. So, we extend these two qubit gates instead, through the same process as in $2+1$ dimensions, and then recombine them to form the extension of the $3+1$ QW operator.

The 2-qubit QW operators used will turn out to be same as those of the $2+1$ case, except for $1 \oplus F$ which was not defined previously. Its QCA version $\mathbf{F}$ is given through Eq. (A.12):

$$\mathbf{F} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 \\ 0 & \frac{i}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{A.20}$$

Let us first decompose the 4-qubit operators for the $3+1$ QW that was given in Eq. (2.126), as circuits of 2-qubit gates.

$$\overline{C}_\epsilon = 1 \oplus (1 \oplus X \oplus 1)(C_\epsilon \oplus C_\epsilon)(1 \oplus X \oplus 1) \tag{A.21}$$

$$\overline{S} = 1 \oplus (I \oplus X \oplus I)(X \oplus X)(I \oplus X \oplus I) \tag{A.22}$$

$$\overline{T}_{\eta,\epsilon} = 1 \oplus (I \oplus T_\eta \oplus I)(X \oplus X)(I \oplus T_\eta \oplus I) \tag{A.23}$$

$$\overline{H}_\rho = 1 \oplus (I \oplus X \oplus I)(I_2 \oplus X)(I \oplus X \oplus I) \tag{A.24}$$

$$\overline{H}_\mu = \overline{H}_\rho(1 \oplus (H \oplus H)) \tag{A.25}$$

$$\overline{H}_\nu = \overline{H}_\rho(1 \oplus (F \oplus F)). \tag{A.26}$$

These operators are written as a product of direct sums of gates, with the identity for the null state. The direct sum is used here instead of the tensor, because we are in the one-particle sector, i.e. besides $|0000\rangle$ which is acted upon trivially with the first 1, the basis states are $|0001\rangle, |0010\rangle, |0100\rangle, |1000\rangle$. Notice that each gate on the right-hand-side acts on neighboring qubits, e.g. a C_ϵ acts on $|0001\rangle, |0010\rangle$ etc. Indeed, whenever some 4 qubit operator an operator needed to act on non-adjacent qubits in the JW order, a prior reordering using X was introduced. For instance, the mass term

$$\overline{C}_\epsilon = 1 \oplus \begin{pmatrix} c & 0 & -s & 0 \\ 0 & c & 0 & -s \\ s & 0 & c & 0 \\ 0 & s & 0 & c \end{pmatrix} \tag{A.27}$$

acts on the first and third qubit on the one hand, and on the second and last qubit on

the other. In order to obtain a circuit of adjacent gates in the JW order, The second and third qubits are swapped, using the operation $1 \oplus X \oplus 1$, allowing for the application of the 2-qubit mass term on the first and last two qubits separately through $C_\epsilon \oplus C_\epsilon$. The swap is then reapplied such that the initial order is recovered. These swaps can be understood as crossing of wires in a circuit so that the 2-qubit gates have the correct input and output. Such swaps correspond, in the multi-particle sector, to the QCA operator $\mathbf{S}$. Hence, we can extend $1 \oplus X \oplus 1$ into $1 \otimes \mathbf{S} \otimes 1$, as this again swaps the two middle qubits while leaving the rest unchanged. Notice that the operator $\otimes$ is used instead of $\oplus$ since we are no longer in the one particle sector. Similarly, the second step of the circuit for the mass term is extended into $\mathbf{C}_\epsilon \otimes \mathbf{C}_\epsilon$. In the end, one obtains the following multi-particle sector, QCA operator for the mass term:

$$\overline{\mathbf{C}}_\epsilon = (1 \otimes \mathbf{S} \otimes 1)\,(\mathbf{C}_\epsilon \otimes \mathbf{C}_\epsilon)\,(1 \otimes \mathbf{S} \otimes 1)\,. \tag{A.28}$$

The same procedure readily yields the gates that compose the 3+1 QED QCA of section 2.3.1.