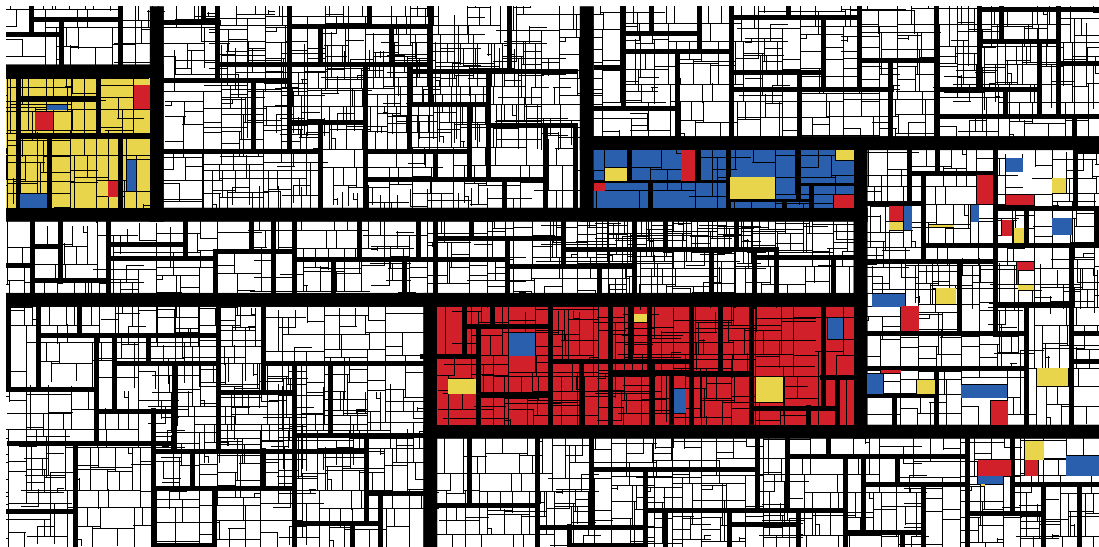




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QUANTUM WALKS ON CAYLEY GRAPHS:  
AN INFORMATION-THEORETICAL  
APPROACH TO QUANTUM FIELDS

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TABLE OF CONTENTS

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Table of contents	v
List of Figures	ix
Introduction, motivations and scopes	1
0.1 Emergence, operationalism and axiomatics in Physics . . . . .	1
0.2 The informational paradigm . . . . .	3
0.3 Quantum Cellular Automata and Quantum Walks . . . . .	5
0.4 The present thesis work . . . . .	6
List of contributions	11
<b>i QUANTUM WALKS ON CAYLEY GRAPHS</b>	<b>13</b>
<b>1 FUNDAMENTAL NOTIONS ON RANDOM WALKS</b>	<b>15</b>
1.1 Classical Random Walks . . . . .	16
1.1.1 Brownian motion . . . . .	17
1.1.2 Discrete-time classical rws on graphs . . . . .	19
1.2 Quantum Random Walks . . . . .	23
1.3 Discrete-time walks on the line . . . . .	28
1.3.1 The Simple Random Walk . . . . .	29
1.3.2 The Hadamard Walk . . . . .	29
1.3.3 The 1D Weyl Quantum Walk . . . . .	31
<b>2 GROUPS AND THEIR CAYLEY GRAPHS: SYMMETRIES AND GEOMETRIC PROPERTIES</b>	<b>33</b>
2.1 Fundamentals of Group Theory . . . . .	35
2.2 Cayley graphs and quasi-isometries . . . . .	42
2.3 Around quasi-isometric rigidity . . . . .	45

3	QUANTUM WALKS ON CAYLEY GRAPHS	47
3.1	Quantum walkers on groups . . . . .	48
3.2	Quantum Walks on free Abelian groups . . . . .	50
3.2.1	Representation in the Fourier space . . . . .	51
3.2.2	Differential equations and the continuum limit . . . . .	53
3.3	The 1D Dirac Quantum Walk . . . . .	55
4	DYNAMICS OF FREE QUANTUM FIELDS FROM PRINCIPLES OF INFORMATION PROCESSING	57
4.1	Free quantum fields as quantum walkers . . . . .	57
4.1.1	Principles of the theory . . . . .	58
4.1.2	Consequences of the principles . . . . .	61
4.2	The Weyl Quantum Walks . . . . .	64
4.3	The Dirac Quantum Walk . . . . .	66
ii	COARSE-GRAINING AND STRUCTURE RESULTS	69
5	COARSE-GRAINING OF QUANTUM WALKS ON CAYLEY GRAPHS	71
5.1	Tiling of qws on groups . . . . .	72
5.2	Fourier representation of virtually Abelian qws . . . . .	77
5.3	Example of a massless virtually Abelian qw . . . . .	79
6	ON THE SCALAR QUANTUM WALKS ON CAYLEY GRAPHS	83
6.1	The quadrangularity condition . . . . .	84
6.2	Classification of the Abelian scalar qws . . . . .	85
6.3	Scalar qws on the infinite dihedral group . . . . .	88
6.3.1	Derivation of the group and its Cayley graph . . . . .	89
6.3.2	Derivation of the scalar qws on $D_\infty$ . . . . .	93
6.3.3	Scalar qws on $D_\infty$ . . . . .	96
7	ISOTROPIC QUANTUM WALKS AND THE WEYL EQUATION	101
7.1	Generalities on isotropy for qws on Cayley graphs . . . . .	101
7.2	Unitarity conditions and isotropy . . . . .	105
7.3	The Euclidean isotropic qws with minimal complexity . . . . .	108
iii	EUCLIDEAN QUANTUM WALKS AND BEYOND	115
8	THE GROUP EXTENSION PROBLEM	117
8.1	Constructing extensions of groups . . . . .	117
8.2	Induced representations . . . . .	124

9	SCALAR EUCLIDEAN QUANTUM WALKS	127
9.1	$\mathbb{Z}^d$ -by-finite groups	128
9.1.1	One-dimensional case	129
9.2	2D and 3D cases with index 2	130
10	EUCLIDEAN QWS AND THE HYPERBOLIC CASE	137
10.1	Some scalar 2D Euclidean qws	137
10.2	Example of a massive virtually Abelian qw	141
10.3	qws on the Poincaré disk	144
Conclusions and outlooks		149
A	EXCLUSION OF CAYLEY GRAPHS OF $\mathbb{Z}^d$	155
A.1	Excluding $A_4$ - and $S_4$ -symmetric Cayley graphs	155
A.2	Exclusion of the truncated tetrahedron	165
A.3	Exclusion of $\mathbb{Z}_n, D_n, \mathbb{Z}_n \times \mathbb{Z}_2$ and $D_n \times \mathbb{Z}_2$ , with $n = 3, 4, 6$	168
A.4	Remaining presentations arising from $\mathbb{Z}_2, D_2$ and $D_2 \times \mathbb{Z}_2$	174
B	DERIVATION OF THE SCALAR QWS	177
B.1	Two space-dimensions	177
B.2	Three space-dimensions	178
C	DERIVATION OF THE SPINORIAL QWS	185
C.1	Derivation of the massive virtually Abelian qw	185
C.2	Derivation of the qw on the Poincaré disk	188
Bibliography		191
List of works		205
Acknowledgements		208





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LIST OF FIGURES

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Figure 1	The standard Cayley graph for the free group of rank 2 and a Cayley graph for $D_3$ . . . . .	43
Figure 2	Primitive cell of the body-centered cubic (BCC) lattice . . . . .	65
Figure 3	Planar Cayley graph for a massless qw . . . . .	80
Figure 4	Cayley graph of the infinite dihedral group admitting a scalar qw	92
Figure 5	Coarse-graining of the Cayley graph of the infinite dihedral group	93
Figure 6	Weyl-like dispersion relation of the qw on the infinite diheadral group . . . . .	99
Figure 7	Dirac-like dispersion relation of the qw on the infinite diheadral group . . . . .	99
Figure 8	Cayley graphs for $\mathbb{Z}^d$ , $d = 1, 2, 3$ , satisfying isotropy . . . . .	108
Figure 9	Planar Cayley graph for a qw with a massive dispersion relation	141
Figure 10	Example of Cayley graph quasi-isometric to the Poincaré disk .	145
Figure 11	Another example of Cayley graph quasi-isometric to the Poincaré disk . . . . .	147



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# INTRODUCTION, MOTIVATIONS AND SCOPES

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## 0.1 EMERGENCE, OPERATIONALISM AND AXIOMATICS IN PHYSICS

The idea—originally stemmed from natural philosophy and later borrowed by general sciences—that natural phenomena can be, if not *constituted*, at least properly *described* in terms of indivisible elementary chunks of matter, is called *atomism*. This belief is deeply related to the doctrine of *reductionism*, according to which, more in general, the understanding of (physical) reality can be divided into the comprehension of a number of elemental entities.

In Physics, a reductionist approach is as much an ambition as a simplification, and this is attested by the fact that in one of the very first and most important physical treatises, *Philosophiæ Naturalis Principia Mathematica* [1] by Sir Isaac Newton, the hypothesis of the existence of material points is straightforwardly assumed. This atomistic belief can be also tracked down in the discussion of the first known model of the kinetic theory of gases, which can be found in *Hydrodynamica* [2] by Daniel Bernoulli.

Thus, the idea produced one of the most fruitful and rich branch of Physics: Statistical Mechanics, initially developed by Ludwig Eduard Boltzmann [3]. The core assumption grounding Statistical Mechanics is still the existence of microscopic, fundamental bricks of matter which—mutually interacting or even solely composing according to a given law—give rise to macroscopic, *emergent* phenomena. The principle of *emergence* relies on properties or behaviours of a whole system which are not shared by its constituents, but arise when a change of scale is performed in the *description* of the system. One could then ask: which notions, in modern Physics, have to be considered as primitive and which ones are those emergent?

The advent of Quantum Mechanics (QM) and Special Relativity (SR) at the beginning of the XX century carried many questions and concerns from a conceptual point

of view, since both theories—contrarily to all the other ones formulated until then—immediately appeared to clash, if nothing else, with common sense and experience. On the one hand, many thinkers started to feel the urge of addressing the interpretative issues arisen; on the other hand, some were looking at least for primitive concepts which physical theories would hinge upon. As relevant examples, we can hereby mention two notable cases.

The problem of giving an operative interpretation to the elements of a physical theory was posed by the physicist Percy Williams Bridgman in *The logic of modern physics* [4] in 1927, where he postulates the principle according to “we mean by any concept nothing more than a set of operations; the concept is synonymous with the corresponding set of operations”. This principle is called *operationalism* and Bridgman, an experimental physicist, argued that the emphasis on an operational approach in Physics would have been of benefit for both phenomenological and theoretical advancements<sup>1</sup>.

In 1900 David Hilbert presented a celebrated list of unsolved problems in Mathematics [5]. Hilbert’s sixth problem is the *mathematical treatment of the axioms of physics*, remarkably suggested by “the investigations on the foundations of geometry”. In the first rank he includes the theories of probability and mechanics. In the 1930s, Andrey Nikolaevich Kolmogorov succeeded in giving to probability theory an axiomatic basis, also discussing the relation of the foundation of the theory to experimental data [6]. As far as classical mechanics concerns, Hilbert says that “Boltzmann’s work on the principles of mechanics suggests the problem of developing mathematically the limiting processes, there merely indicated, which lead from the atomistic view to the laws of motion of continua”.

Of course, the formulation of Quantum Mechanics (QM) posed far more severe problems, from both an interpretative and an axiomatic point of view. Hilbert worked on the mathematical axiomatics of QM, and in 1930 Paul Adrien Maurice Dirac unified [7] into the Hilbert-space framework the two different formulations available at the time: Erwin Schrödinger’s wave mechanics and Werner Karl Heisenberg’s matrix mechanics. John von Neumann’s book on the mathematical foundations of QM [8] then gathered and popularised Dirac–von Neumann axioms. Von Neumann was the first, in a joint paper [9] with Garrett Birkhoff, who endeavoured to endow the mathematical structure of QM with a rigorous physical meaning in terms of logical statements: the authors

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<sup>1</sup> In this respect, Bridgman takes as an example the basic tenet of SR that time is not absolute (in opposition to Newtonian mechanics). He argues that not only SR stated that absolute time does not exist, but furthermore in an operational view it is just a meaningless notion.

developed a new kind of propositional calculus (different from classical logic), called Quantum Logic.

The birth of a relativistic theory of quantum fields, or Quantum Field Theory (QFT), even exacerbated all this set of problems, as is clear. While QFT represents an effort to provide a physical description for high energy phenomena at small scales, it still lacks a well-founded mathematical foundation and an operational interpretation. For a critical discussion of the open problems in this regard (divergencies, renormalization, localizability etc.), the reader can refer to Refs. [10–13]. The most important attempts to formulate a well-posed mathematical framework for QFT are the popular Wightman’s axioms [14] and Haag-Kastler’s axioms [15, 16]. More generally, Algebraic QFT intends to resort to the formalism of  $C^*$ -algebras to found QFT. The states of the systems are modelled as “operator valued distributions”. The crucial assumptions in this context are the covariance of the fields under the Poincaré group and the commutativity of the algebras of local observables on two space-like (causally disconnected) space-time regions. Thus, the framework particularly relies on the spacetime structure strongly reminiscent of SR and of Einstein’s causality (which, in the present context, will be referred to as *locality*). Among the most relevant result, we mention the formalisation of the free (noninteracting) theory of relativistic quantum fields and the rigorous derivation of the Spin-Statistics Theorem [14]. Yet, the formulation of a full theory of interacting quantum fields is still missing. In fact, for example Haag’s Theorem and related results state the nonexistence, in a unique Hilbert’s space, of the interacting picture, even in the absence of interactions [17, 18]. This no-go result suggests that there is still a long way ahead. Put in Teller’s words: “Everyone must agree that as a piece of mathematics Haag’s theorem is a valid result that at least appears to call into question the mathematical foundation of interacting quantum field theory, and agree that at the same time the theory has proved astonishingly successful in application to experimental results” [12].

## 0.2 THE INFORMATIONAL PARADIGM

Hilbert’s sixth problem yet remains unanswered. Not only the most successful physical theories at our disposal still need a solid and complete mathematical ground, but also their primitive elements are more and more deficient of a precise operational meaning.

Since the 2000s, a wide community started to struggle to endow QM with operational axioms [19–26]. The guiding spirit was the lesson taught by Quantum Information Theory (QIT), which had been developed in the previous two decades. QIT’s key notions are

the quantification of the information content of physical systems and a suitable description of how this is processed by physical transformations. The motto of an influential 2001 conference discussing the foundations of QM was “Quantum foundations in the light of QIT” [20]. In 2011 G. M. D’Ariano, P. Perinotti and G. Chiribella presented an operational axiomatization of Quantum Theory (QT)<sup>2</sup> based on information-theoretical principles [27]. The authors proved that QT is a special kind of operational probabilistic theory, being equivalent to the standard Dirac–von Neumann QM. QT is there derived from six general principles of information processing where, remarkably, *causality* and *conservation of information* play a notable role. For a close examination of the axioms and their implications, we refer the reader to Refs. [22, 23, 25, 28]<sup>3</sup>.

The D’Ariano–Perinotti–Chiribella axiomatization showed that QT is a theory of systems (pieces of informations) and events (transformations) dressed with probabilities. The theory gains then an operational ground and enjoys Probability Theory (which is an extension of Logic [30]) as an integral part, making at the same time use of classical logic. This achievement represents an enormous success, and also it allows us to consider QT retaining standard logic (a ground of the common sense) and to think about systems as Bayesian inference rules.

Within a retrospective glance, the route for axiomatization has always been unravelled under the guidance of basic and solid first principles, acquiring the important lesson which this method of inquiry imparts. To this extent, the informational paradigm seems to rely on good and fruitful principles. Remarkably, Richard Phillips Feynman concerned himself with the information content of the physical systems. He expressed his dissatisfaction with the hypothesis of the existence of the continuum<sup>4</sup> in physics: “There might be something wrong with the old concept of continuous functions. How could there possibly be an infinite amount of information in any finite volume?” [31]. After all, he has been one of the pioneers of modern QFT, which is still suffering from the problems due to the continuum. Sir Archibald Wheeler, Feynman’s mentor, was strongly committed to the idea that the “elementary quantum phenomenon” is the “potential building element for all that is” [32]. He epitomized this conviction—that every *it* (physical quantity) “derives its ultimate significance from bits, binary yes-or-

<sup>2</sup> QT is here opposed to QM insofar that the *theory* is actually formulated without reference to any particular *mechanical* system; rather, it is a broad physical grammar apt to construct particular models or even different theories.

<sup>3</sup> It is worth mentioning the axiomatization by Samson Abramsky and Bob Coecke, that resorts to category theory [29].

<sup>4</sup> In the operational scope, the continuum is an idealization, or approximation, rather than an hypothesis about the physical world.

no indications”—in the popular motto *it from bit* [33], conveniently rephrased as “it from qubit” [34]. This belief leans on the Deutsch–Church–Turing thesis [35, 36] as presented in Ref. [37]: “Every finite experimental protocol is perfectly simulated by a finite quantum algorithm”.

The idea that physical law are a quantum computation running between a discrete set of events [38] is very appealing from a theoretical viewpoint, since it may possibly allow to overcome the issues arising in QFT because of the continuum and to build a theory of quantum fields grounding on solely informational principles. Recently, the research program of providing an information-theoretical foundation to QFT has been undertaken by several authors [39–45]. The core idea is to consider a general algorithm defining the discrete-time evolution of a network of quantum systems in mutual interaction, under some general physical assumption. The mathematical description capturing the notion of such sort of quantum computation is that of Quantum Cellular Automaton (QCA)<sup>5</sup> [48–51]. QCAs model the evolution on a graph where a Hilbert space is associated to each graph node. Essential features of QCAs are the translation-invariance of the evolution on the graph and locality (each node is connected with a finite number of other nodes). However, in general, it is a hard problem to explicitly construct and analyse the dynamics of discrete interacting quantum fields via QCAs (as we mentioned, the interacting case encounters difficulties also in Algebraic QFT). The simplest example of QCA is the Quantum Walk (QW) model [52–58], where the evolution rule is linear. The latter represents the case of free dynamics (it is thus called the “one-particle sector” of the QCA).

### 0.3 QUANTUM CELLULAR AUTOMATA AND QUANTUM WALKS

Discrete versions of QFTs have been broadly investigated from both a computational and a theoretical point of view. On the one hand, lattice gauge theories [59] offer a solid tool to provide numerical evaluations of infinite-dimensional path integrals occurring in QFT, via a discretization of the underlying spacetime: this allows one to eventually recover the continuum limit. On the other hand, discrete formulations of QFT provide insights on feasible ways to overcome the mathematical issues which QFT is still coping with, possibly offering experimental tests to falsify discrete microscopic theories. In

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<sup>5</sup> The germ of the idea of recovering quantum fields as emergent from a (possibly classical) cellular automaton can be found in Ref. [46], while cellular automata were previously introduced in Theoretical Physics by Ref. [47].

this context, whatever the lattice model is, the elementary steps are hypothetically taken at the Planck scale.

Models addressing the problem of constructing a discretised version of gauge theories can be found e.g. in Refs. [60–64]. Also experimental simulations of gauge theories on a lattice have been devised, exploiting for instance the effective dynamics of ultracold atoms [65–69]. Other attempts aim to reconstruct the effect of an electric field on a charged particle in a lattice or Weyl and Dirac dynamics using quantum walks on graphs (see Refs. [70–72]). QWs have also been studied to formulate both Abelian and non-Abelian discrete gauge theories for Dirac fermions [42, 73]. Furthermore, QW models proved to be a useful toolbox to treat the problem of recovering Lorentz invariance in a discrete spacetime [40, 74–76]. Finally, QWs are a suitable arena to study phenomena in curved spacetimes [77–80] and also interacting scenarios [81–83].

A further generalization of the QW model has been given with the notion of QCA. The QCA model consists in a numerable set of mutually interacting quantum systems, where a finite-dimensional Hilbert space is associated to each site. The evolution, defined by the graph of interactions, is reversible and local. QCAs have been proposed as an underlying mechanism for quantum fields in the spirit of Feynman’s paradigm of describing Physics as information processing [48]. It has been shown that it is possible to simulate a scalar field with a quantum algorithm in a polynomial time [84, 85]. In Ref. [44] the authors give an example of a one-dimensional QCA without a particle interpretation, particularly focusing on applications to discrete QFTs. A classification of QCAs, along with their dynamics, is still an open problem.

#### 0.4 THE PRESENT THESIS WORK

The framework presented in this thesis work is an information-theoretical construction resorting to QWs. The final objective is a discrete reconstruction of QFT as emergent from a more fundamental theory, built up with pure interactions between identical quantum systems and without assuming a background spacetime nor SR. What we will assume instead are the following requirements for the interactions: 1) locality, 2) homogeneity, 3) isotropy, and 4) unitarity. The assumptions of locality and homogeneity importantly imply that the graph of interactions for the present model is in fact a Cayley graph, namely a graphic representation of a group. Assuming the above hypotheses, Weyl, Dirac, and Maxwell equations has been derived from principles of information processing [86–88] (for the relation between the Weyl and Dirac QWs and the Klein–Gordon equation, see Ref. [89]). The aim of the present work is to develop



mathematical methods and prove structure results regarding a free QCA field theory on Cayley graphs as a discrete approach to standard QFTs.

### *Part i—Quantum Walks on Cayley graphs*

In Chapter 1 we provide some fundamental notions on discrete-time random walks on graphs. After reviewing Einstein’s formalisation of the first example of random walk, i.e. the Brownian motion, we define classical discrete-time random walks on graph as time-homogeneous Markov chains. Then we introduce the notion of discrete-time qw, along with some comments on the constraints derived from unitarity of the evolution. We conclude with some relevant example of random walks. The material presented in this chapter can be found in Refs. [55, 90–93].

In Chapter 2 we revisit the basics of Group Theory, serving as introductory tool to the study of Cayley graphs. These objects are the ambient space of the qws studied in the present thesis. Cayley graphs are investigated by Geometric Group Theory, a branch of Mathematics developed in the last three decades to the purpose of investigating groups as geometric objects. We here provide some concepts and results to study Cayley graphs as metric objects and to connect them to continuous manifold. This analysis will allow us to conveniently represent and analyse qws on Cayley graphs.

In Chapter 3 the evolution of qws on Cayley graphs is defined and discussed. The focus is on qws on Cayley graphs of Abelian groups (Abelian qws). These walks, via a group-theoretical method, admit a Fourier representation to study them in the momentum space. This allows to define differential equations for the evolution and recover the continuum limit. This kinematic and dynamical properties of Abelian qws are studied mainly following the discussion of Ref. [86]. The interesting example of the 1D Dirac qw is presented and finally the non-Abelian case is briefly introduced.

Chapter 4 consists of part of the formalisation and results of Refs. [41, 86, ME94]. The principles for the present discrete free theory of quantum fields are exposed and discussed with a deep degree of detail. The Cayley graph structure is derived (in the broader context of QCAs) and the notion of isotropy is particularly characterized. We conclude discussing the examples of the 3D Weyl and Dirac qws.

*Part ii—Coarse-graining and structure results*

In Chapter 5 the results of Refs. [ME95, ME96] are overhauled and expanded. We present a rigorous coarse-graining technique for qws, based on the notion of tiling of a Cayley graph. The coarse-graining comes to aid in order to represent a vast class qws with enlarged coin systems but on smaller groups. In the case of Euclidean qws, coinciding with qws on Cayley graphs of virtually Abelian groups, the procedure is particularly significant and useful, since it allows to reduce any Euclidean qw to an Abelian one. The procedure constitutes a classification of qws on flat spaces. This leads to a characterization of virtually Abelian qws and to a method for solving their dynamics in the Fourier space, which was lacking throughout the literature. A massless example is presented.

In Chapter 6, Ref. [ME97] is reviewed. The Abelian qws with a one-dimensional coin system (or scalar) are thoroughly classified, finding that their dynamics is trivial. This results extends the no-go theorem of Ref. [98]. The proof of the classification [ME97] is here emended, making the main result completely general. In addition, a structure result for a relevant class of 1D qws is given. We derive a family of scalar qws on the infinite dihedral group and finally study their kinematics and dynamics are studied, recovering the 1D Dirac qw in a suitable limit.

In Chapter 7 the analysis of Ref. [ME94] is reviewed and expanded. After a general result on the isotropy assumption, a structure theorem for the isotropic qws on  $\mathbb{Z}^d$  with a two-dimensional coin system is proved up to dimension  $d = 3$ . The isotropic spinorial qws on  $\mathbb{Z}^d$  are closely related to the Dirac qw (for  $d = 1$ ) and to the Weyl qw (for  $d = 2$ ), while remarkably there exist two qws in  $d = 3$ , and these are with the 3D Weyl qws. This results represents a derivation of the Weyl equation from principles of information processing. As a corollary, the qws on the infinite dihedral groups derived in Chapter 6 are found to coincide with parity invariant qws on the line.

The results of this part are structure classifications for qws on flat emergent space-times. We first connect virtually Abelian groups to Euclidean qws; then we classify the simplest Abelian qws from the point of view of the coin system, finding that their dynamics is trivial; finally, we can treat the Abelian qws with spin  $\frac{1}{2}$ , proving that in three dimensions the isotropic evolution implies unique graph and dynamics, namely the Weyl one.

*Part iii—Euclidean Quantum Walks and beyond*

In Chapter 8 we set the problem of constructing groups satisfying properties suitable to the coarse-graining procedure established in Chapter 5. This mathematical problem is called group extension. We treat this in full generality, and then contextualize the coarse-graining method in the scope of the mathematical notion of induced representations. The material exposed here is unpublished.

In Chapter 9, also based on unpublished material, we focus on the extensions of Abelian groups, paying particular attention to  $\mathbb{Z}^d$ . We explicitly construct the simplest extensions of  $\mathbb{Z}^d$  up to  $d = 3$ , and construct the unique Cayley graphs admitting a scalar qw.

In Chapter 10 we finally derive some of the spinorial walks classified in Chapter 7 from the scalar qws on the extensions of  $\mathbb{Z}^d$  constructed in Chapter 9. Then we present the example of a virtually Abelian qw, and via the coarse-graining method we study its kinematic properties, finding a massive behaviour. In addition, we give a first example of qw on the Cayley graph of a group which is quasi-isometric to the Poincaré disk—having negative curvature—and make some final observations on its relevance.

In this final part we investigate how to keep a minimal coin dimension without finding, in a flat emergent spacetime, a resulting trivial dynamics. This can be done considering virtually Abelian groups, which can be constructed, along with their Cayley graph admitting scalar qws, via the group extension procedure exposed. Thus one is able to explore the consequences of an isotropic evolution in flat spaces relaxing Abelianity, but still keeping the minimality of the coin dimension. A spinorial walker can be then recovered via a coarse-graining of the qw. Finally, we approach a possible future scenario of curved emergent spacetime, finding that the complexity of the problem of studying qws in the case of negative curvature is not higher than in the flat case. This can be a good ground for future enquiries in spaces with nonzero curvature.

All of the Figures appearing throughout the present work, excepting Figs. 1(a) and 11, are taken from the Drafter's contributions and belong to their respective owners (see Refs. [ME94, ME96, ME97]). For the sake of convenience, the contents of Appendices A and C follows almost verbatim that of Appendices in, respectively, Refs. [ME94] and [ME96].

We eventually draw our conclusive considerations and outlooks for this thesis work.



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## LIST OF CONTRIBUTIONS

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1. [ME97] Giacomo Mauro D'Ariano, Marco Erba, Paolo Perinotti, and Alessandro Tosini "Quantum walks with a one-dimensional coin". In: *Physical Review A* 93 (6 2016), p. 062334. URL: <https://link.aps.org/doi/10.1103/PhysRevA.93.062334>.
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3. [ME94] Giacomo Mauro D'Ariano, Marco Erba, and Paolo Perinotti. "Isotropic quantum walks on lattices and the Weyl equation". In: *Physical Review A* 96 (6 2017), p. 062101. URL: <https://link.aps.org/doi/10.1103/PhysRevA.96.062101>.
4. \_\_\_\_\_ Giacomo Mauro D'Ariano, Marco Erba, and Paolo Perinotti. Unpublished work on group extensions and scalar qws to appear soon (2018).



Part I

QUANTUM WALKS ON CAYLEY GRAPHS





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## FUNDAMENTAL NOTIONS ON RANDOM WALKS

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In the present chapter we shall introduce the reader to the notion of Random Walk (RW), starting from its first appearance as a (classical) physical model and then presenting its quantum version, that is to say the Quantum Walk (QW). In particular, this thesis work will be focused on discrete-time QWs on graphs, developing a mathematical framework for QWs on Cayley graphs and discussing the relevance of the model for a discrete approach to free Quantum Field Theories (QFTs).

In his seminal 1905 paper [90] (one of the popular *Annus Mirabilis papers*), Albert Einstein introduced the notion of RW as a (classical) continuous-time diffusive phenomenon in Euclidean space. He performed a statistical analysis of the erratic random motion of a particle triggered by the collisions generated in a bath of molecules. Such a description of RWs gives rise to the well-known Fokker–Planck equation [99, 100], a general diffusion-equation playing a major role in the study of e.g. diffusive processes (in gases and liquids) and lasers [101]. Moreover, RWs have been broadly investigated in Probability Theory in the context of stochastic processes [102, 103]. In particular, RWs can be modelled as discrete-time processes where a stochastic variable  $X_n$  is associated to each time-step  $n$  and the evolution is suitably defined by the sequential extraction of values for the  $X_n$  over a state space  $M$ .

The quantum analogue of the classical RW has been introduced in Ref. [54] in 1993, followed by other works [55, 56, 58, 104, 105] aiming to define and formalize

the concept of discrete-time qw on graphs. The peculiar trait of qws is that a finite-dimensional Hilbert space is associated to each node of the graph, associating an intrinsic degree of freedom (*spin*) to the system. This leads to an intertwining among the space-evolution and the internal one. We shall here give a general definition of a discrete-time qw model, and provide two relevant one-dimensional examples. In particular, our focus on theoretical applications of the qw model to free QFTs shall lead the discussion to the simplest example of discrete quantum field dynamics—i.e. the 1D Weyl qw—describing the Weyl field equation in a discrete scenario.

### 1.1 CLASSICAL RANDOM WALKS

Classical rws are dynamical stochastic processes modelling the motion of a system when driven by some classical random behaviour. As already said, rws were first theorized back in 1905 by Albert Einstein in his popular paper [90], where a statistical model was developed to the purpose of accounting for the observations of the botanist Robert Brown [106]. The latter observed under a microscope the erratic motion of some pollen grains suspended in water. Initially, the motion was thought to be due to the grains themselves, and contributed to revive the long-standing debate about the atomistic hypothesis. This phenomenon was named *Brownian motion*, after his discoverer. Einstein devised a one-dimensional microscopic model where the motion of the particles is the result of random “kicks” experienced in the presence of water’s molecules. He assigned to the Brownian particles a time-dependent probability distribution  $P(x, t)$  of finding at least one of them at position  $x$  after a time  $t$ . By doing so, he derived a diffusion equation for this statistical evolution, linking the probability distribution of the stochastic displacements experienced by the particles to their probability distribution at arbitrary times.

Let  $P(\mathbf{x}, t)$  be the probability distribution associated to a system’s position  $\mathbf{x}$  in  $d$  space-dimensions at time  $t$ . In this context, the general equation governing the evolution of the distribution  $P$  for a diffusive system is the well-known *Fokker–Planck diffusion equation* (also known as *Kolmogorov forward equation*), which is given by

$$\partial_t P(\mathbf{x}, t) = -\nabla \cdot (\mathbf{v}(\mathbf{x}, t)P(\mathbf{x}, t)) + \nabla \nabla \cdot (\mathbf{D}(\mathbf{x}, t)P(\mathbf{x}, t)), \quad (1)$$

where  $\mathbf{v}(\mathbf{x}, t)$  and  $\mathbf{D}(\mathbf{x}, t)$  are respectively the drift vector and the diffusion tensor. In Chapter. 3 we will present a method to extract a partial differential equation à la

Fokker–Planck for the evolution of a quantum system governed by a quantum RW (which will be defined in the next section).

### 1.1.1 *Brownian motion*

Einstein investigates the random motion of  $n$  particles suspended in a fluid and undergoing a diffusion caused by the thermal molecular motion. He assumes that the motion of each particle is independent from that of all the others. In addition, he introduces a time interval  $\tau$  which shall be very small compared to the time of the observable random motion, but also large enough to allow to consider the motions performed by the particles at times separated by  $\tau$  as mutually independent events. This latter hypothesis is equivalent to consider the random evolution a Markov process [107], as will be discussed in the next subsection.

The model is one-dimensional: in a time interval  $\tau$ , each particle experience a displacement  $\lambda$  (which can be either positive or negative), where a certain probability distribution  $\phi(\lambda)$  is associated to the displacements. In addition to the normalization condition

$$\int_{-\infty}^{+\infty} d\lambda \phi(\lambda) = 1, \quad (2)$$

Einstein also assumes that the parity property

$$\phi(\lambda) = \phi(-\lambda) \quad (3)$$

holds for the distribution  $\phi$ . This symmetry property between positive and negative displacements amounts to the assumption that there is no drift current in the fluid: none of the directions of motion is preferential.

The number of particles experiencing a displacement lying between  $\lambda$  and  $\lambda + d\lambda$  is then given by

$$dn = n\phi(\lambda)d\lambda.$$

If  $f(x, t)$  denotes the number of particles at  $x$  at time  $t$ , then the number of particles lying at time  $t + \tau$  between  $x$  and  $x + dx$  reads

$$f(x, t + \tau)dx = \int_{-\infty}^{+\infty} d\lambda f(x + \lambda, t)\phi(\lambda)dx. \quad (4)$$

Expanding now  $f$  for small values of  $\tau$  and  $\lambda$ , one obtains respectively

$$\begin{aligned} f(x, t + \tau) &= f(x, t) + \tau \partial_t f(x, t) + \dots, \\ f(x + \lambda, t) &= f(x, t) + \lambda \partial_x f(x, t) + \frac{\lambda^2}{2} \partial_x^2 f(x, t) + \dots \end{aligned}$$

Substituting these expressions into Eq. (4) and recalling the normalization (2), the former equation becomes, up to the chosen truncation order,

$$\tau \partial_t f(x, t) = \partial_x f(x, t) \int_{-\infty}^{+\infty} d\lambda \lambda \phi(\lambda) + \partial_x^2 f(x, t) \int_{-\infty}^{+\infty} d\lambda \frac{\lambda^2}{2} \phi(\lambda). \quad (5)$$

Defining now

$$D := \frac{1}{\tau} \int_{-\infty}^{+\infty} d\lambda \frac{\lambda^2}{2} \phi(\lambda)$$

and using the parity property (3), one finally obtains

$$\partial_t f(x, t) = D \partial_x^2 f(x, t), \quad (6)$$

which is the 1D Fokker-Planck equation (1) with a vanishing drift coefficient and a constant diffusion coefficient  $D$ .

**Remark 1.1.** *If one takes into account a generic distribution  $\phi$ , namely a distribution  $\phi(\lambda, x, t)$  for which in general the parity symmetry (3) does not hold, then the above calculations may be performed expanding also  $\phi$  and thus attaining the general Fokker-Planck equation in one dimension. Substituting*

$$\phi(\lambda, x + \lambda, t) = \phi(\lambda, x, t) + \lambda \partial_x \phi(\lambda, x, t) + \frac{\lambda^2}{2} \partial_x^2 \phi(\lambda, x, t) + \dots$$

into Eq. (4), and neglecting the higher order terms, one gets

$$\begin{aligned} \partial_t f(x, t) &= \partial_x \left( \int_{-\infty}^{+\infty} d\lambda \frac{\lambda}{\tau} \phi(\lambda, x, t) f(x, t) \right) + \partial_x^2 \left( \int_{-\infty}^{+\infty} d\lambda \frac{\lambda^2}{2\tau} \phi(\lambda, x, t) f(x, t) \right) =: \\ &=: \partial_x (v(x, t) f(x, t)) + \partial_x^2 (D(x, t) f(x, t)), \end{aligned}$$

namely the 1D Fokker-Planck equation (1).

Posing now  $f(x, 0) = 0$  for  $x \neq 0$  and being

$$\int_{-\infty}^{+\infty} dx' f(x', 0) = n$$

by definition of  $f$ , the partial differential equation problem (6) is solved by the Gaussian function

$$f(x, t) = \frac{n}{\sqrt{\pi 4Dt}} \exp\left(-\frac{x^2}{4Dt}\right).$$

The Brownian particles have then the same distribution of random errors, as one could have expected. Remarkably, the standard deviation of the position of the particles at arbitrary time  $t$  is given by

$$\sigma(x, t) = \sqrt{\langle x^2 \rangle} = \int_{-\infty}^{+\infty} dx' x'^2 f(x', t) = \sqrt{2Dt}, \quad (7)$$

namely it is proportional to the square root of the time  $t$ . This property is peculiar of the random diffusive motion and is in contrast with the ballistic dispersion without collisions in classical mechanics, which is given by

$$\sigma(s, t) = vt, \quad (8)$$

where  $s$  is the position of the projectile and  $v$  its velocity.

### 1.1.2 Discrete-time classical rws on graphs

Since in the present work we study discrete-time random walks in discrete spaces, we now provide a first (classical) model of rws as sequences of stochastic extractions on a discrete state space at discrete time-steps. These are conveniently described as a random evolution on a graph: the definition of the latter is given below.

**Definition 1.1** (Directed graph). A directed graph or digraph is a ordered pair  $\Gamma = (V, E)$ , where  $V$  and  $E$  are set such that  $E$  collects arbitrary ordered pairs  $(x_1, x_2)$  of elements  $x_1, x_2 \in V$ . The elements in  $V$  are called the vertices and those in  $E$  the edges of the graph.

Throughout this work we will focus on directed graphs: accordingly, we will omit the mention *directed* for the sake of brevity. The vertices are graphically represented as dots and are also called *sites* or *nodes*. The set  $E$  of edges defines the connectivity

between the vertices of the graph: an edge  $(x_1, x_2)$  is graphically indicated by an arrow having direction from  $x_1$  to  $x_2$ . We can thus give the following useful definition.

**Definition 1.2** (First-neighbourhood of a site and its complement). *Let  $\Gamma = (V, E)$  be a graph. We define the first-neighbourhood of each site  $x \in V$  as the set*

$$N_x := \{y \in V \mid (x, y) \in E\},$$

*namely all the vertices connected to  $x$  by arrows having  $x$  as tail. The elements contained in  $N_x$  are called first-neighbours of  $x$ . The complement of the first-neighbourhood of each site  $x \in V$  is the set defined as*

$$N_x^{-1} := \{y \in V \mid (y, x) \in E\}.$$

Following Einstein's assumption of statistical independence of the random events in a diffusive process (see Subsection 1.1.1), in order to define a discrete-time rw on a graph we first need to introduce in the present context the interesting notion of *memoryless* process, as defined below.

**Definition 1.3** (Markov chain). *Let  $\mathbf{X} = \{X_n\}_{n \in \mathbb{N}}$  denote a sequence of stochastic variables  $X_n$ , each taking values on a discrete space  $M$ , called state space.  $\mathbf{X}$  is called a Markov chain if the probability measure satisfies the following Markov property on the conditional probabilities:*

$$P(X_{n+1} = j \mid X_0 = i_0, \dots, X_n = i_n) = P(X_{n+1} = j \mid X_n = i_n) \quad \forall n \in \mathbb{N}. \quad (9)$$

The Markov property (9) states that the probability of each transition depends only on the value extracted at the previous step, without conserving memory of the history of the preceding steps. Furthermore, a Markov chain is said to be *time-homogeneous* if the conditional probabilities are independent from the time-step:

$$P(X_{n+1} = j \mid X_n = i) = p_{ij} \quad \forall n \in \mathbb{N}.$$

The previous quantities are called *transition probabilities* and define a stochastic matrix  $T$  whose matrix elements are given by

$$T_{ij} = p_{ij} \quad (i, j) \in M \times M.$$

$T$  is called *transition matrix* of the time-homogeneous Markov chain on  $M$ .



**Theorem 1.1.** *Let  $\mathbf{X} = \{X_n\}_{n \in \mathbb{N}}$  be a Markov chain on a state space  $M$ . Then there exists a time-homogeneous Markov chain  $\mathbf{X}' = \{X'_n\}_{n \in \mathbb{N}}$  on the state space  $M \times \mathbb{N}$  such that  $X_n = \Pi(X'_n)$  for all  $n \in \mathbb{N}$ , where  $\Pi$  denotes the projection on the subspace  $M$ .*

*Proof.*  $\mathbf{X} = \{X_n\}_{n \in \mathbb{N}}$  is a Markov chain with transition probabilities

$$p_{ij,n} := P(X_{n+1} = j | X_n = i),$$

which are in general dependent on the time-step  $n$ . Let us define the random variables

$$X'_n := (X_n, n) \quad n \in \mathbb{N}$$

and construct the new Markov chain defined by  $\mathbf{X}' = \{X'_n\}_{n \in \mathbb{N}}$ . By definition, one has

$$X_n = \Pi(X'_n), \quad P'(X'_n = (i, k)) = \delta_{nk} P(X_n = i) \quad \forall i \in M$$

and the transition probabilities

$$P'(X'_{r+1} = (j, l) | X'_r = (i, r)) = \delta_{rk} \delta_{l, r+1} p_{ij,r} =: p'_{(i,r),(j,l)}$$

do not explicitly depend on the time-step. Accordingly,  $\mathbf{X}'$  is a time-homogeneous Markov chain. ■

We now give a characterization of the transition matrix of the time-homogeneous Markov chain.

**Theorem 1.2.** *Let  $\mathbf{X}$  be a homogeneous Markov chain on  $V$  with transition matrix  $T$ . Then the relation*

$$P(X_{n+m} = j | X_n = i) = (T^m)_{ij}, \quad T^0 := I_V \tag{10}$$

holds for every  $n, m \in \mathbb{N}$  and for every  $i, j \in V$ .

*Proof.* We prove the relation by induction on  $m$ . Eq. (10) holds for  $m = 1$  by definition. Let us now suppose that the relation holds for  $m > 1$ . Then for every  $n \in \mathbb{N}$  one has

$$P(X_{n+m+1} = j | X_n = i) = \frac{P(X_{n+m+1} = j, X_n = i)}{P(X_n = i)} =$$



$$\begin{aligned}
 &= \sum_{l \in V} \frac{P(X_{n+m+1} = j, X_{n+m} = l, X_n = i)}{P(X_{n+m} = l, X_n = i)} \\
 &\cdot \frac{P(X_{n+m} = l, X_n = i)}{P(X_n = i)} = \\
 &= \sum_{l \in V} P(X_{n+m+1} = j | X_{n+m} = l, X_n = i) \cdot (T^m)_{il} = \\
 &= \sum_{l \in V} \underbrace{P(X_{n+m+1} = j | X_{n+m} = l, X_n = i)}_{=P(X_{n+m+1}=j|X_{n+m}=l) \text{ (Markov property)}} \cdot (T^m)_{il} = \\
 &= \sum_{l \in V} p_{lj} (T^m)_{il} \equiv \sum_{l \in V} (T^m)_{il} (T)_{lj} = \\
 &= (T^{m+1})_{ij} \quad \forall (i, j) \in V \times V.
 \end{aligned}$$

Then relation (10) holds for every  $m \in \mathbb{N}$ . ■

With the aid of Theorem 1.2 we can now show that

$$\begin{aligned}
 P(X_{n+m} = j | X_0 = i) &= (T^{n+m})_{ij} = (T^n T^m)_{ij} \equiv \\
 &\equiv \sum_{l \in V} P(X_n = j | X_0 = l) P(X_m = l | X_0 = i). \tag{11}
 \end{aligned}$$

Relations (11) are called the *Chapman–Kolmogorov equations*. As pointed out in Ref. [108], the Chapman–Kolmogorov equations are a set of necessary but not sufficient conditions for a Markov process: there exist examples of non-Markov process with long-time memory where Eqs. (11) holds.

## 1.2 QUANTUM RANDOM WALKS

qws are a dynamical model which intuitively describes the coherent evolution of a quantum system over a graph. The model was first formalized in Ref. [54], where it is shown that, due to quantum interference, the average path length can be much larger than the maximum allowed path in the corresponding classical rw. In Ref. [55] the authors analyse the so-called Hadamard Walk, which represent the quantum analogue of the symmetric rw (see Section 1.3). These works pointed out the potential relevance of qws in branches as quantum optics and quantum computation, and indeed contributed to the flourishing of literature concerning the qw model. Applications of qws can be found in quantum information and computation, e.g. qws can also serve as a solid tool to formulate quantum search algorithm [57, 109–111].

Generally, qws are defined on directed graphs  $\Gamma = (V, E)$ . A finite-dimensional Hilbert space  $\mathcal{H}_x$  is associated to each lattice site  $x \in V$ , while the state of the evolving system is defined on the total Hilbert space

$$\mathcal{H}_{\text{tot}} := \bigoplus_{x \in V} \mathcal{H}_x.$$

Each  $\mathcal{H}_x$  represents the internal degree of freedom of the system at site  $x$ , the so-called *coin system*: this is said a *cell structure* for the qw. We are now ready to give the formal definition of qw.

**Definition 1.5** (Discrete-time Quantum Walk on a graph). *Let  $\Gamma = (V, E)$  be a graph and let  $N_x^{-1}$  denote the complement of the first-neighbours of each node  $x \in V$ , to which is associated a finite-dimensional Hilbert space  $\mathcal{H}_x$ . A qw on  $\Gamma$  is a unitary operator  $W$  providing a time-homogeneous evolution on states at arbitrary time  $t$  on  $\Gamma$  defined as*

$$\begin{aligned} W : \bigoplus_{y \in N_x^{-1}} \mathcal{H}_y &\longrightarrow \mathcal{H}_x \\ \bigoplus_{y \in N_x^{-1}} |\psi_y(t)\rangle &\longmapsto |\psi_x(t+1)\rangle. \end{aligned}$$

This defines a time-discrete evolution on a graph  $\Gamma$  according to its neighbourhood schemes. By linearity of the operator  $W$ , for a generic state  $|\psi(x, t)\rangle \in \bigoplus_{y \in N_x^{-1}} \mathcal{H}_y$  one can block-decompose the evolution as

$$|\psi_x(t+1)\rangle = W |\psi(x, t)\rangle = W \bigoplus_{y \in N_x^{-1}} |\psi_y(t)\rangle = \sum_{y \in N_x^{-1}} A_{yx} |\psi_y(t)\rangle, \quad (12)$$

where the  $A_{xy}$  are  $\dim \mathcal{H}_x \times \dim \mathcal{H}_y$  (complex) matrices, called the transition matrices of the qw.

This coincides with the first historical definition of *linear QCA* (see e.g. Ref. [98]). Throughout the literature, the usual choice is  $\mathcal{H}_x \cong \mathbb{C}^s \forall x \in V$ , where the integer  $s$  is called the dimension of the coin system of the walk. In addition, the graph  $\Gamma$  is taken

of constant degree  $k$ . In the following of this work, unless otherwise stated, we will assume this choice. Accordingly, the form of the walk operator is the following:

$$W = \begin{pmatrix} \ddots & & \ddots & & & & \\ & \ddots & & \ddots & & & \\ A_{x_{i-1-j}x_{i-1}} & \cdots & A_{x_{i-1}x_{i-1}} & \cdots & A_{y_{i-1+l}x_{i-1}} & & \\ & A_{x_{i-j}x_i} & \cdots & A_{x_i x_i} & \cdots & A_{x_{i+l}x_i} & \\ & & A_{x_{i+1-j}x_{i+1}} & \cdots & A_{x_{i+1}x_{i+1}} & \cdots & A_{x_{i+1+l}x_{i+1}} \\ & & & \ddots & & \ddots & \\ & & & & \ddots & & \ddots \end{pmatrix}$$

where  $k = j + l + 1$ . This is the analogue of a Markov chain.

The total Hilbert space of the qw then satisfies the unitary equivalence

$$\mathcal{H}_{\text{tot}} \cong \ell^2(V) \otimes \mathbb{C}^s,$$

where  $\ell^2(V)$  is the space of square-summable complex functions defined on the set of vertices of the graph  $\Gamma$ . Moreover, given the dual vector space  $\ell^2(V)^*$  of all the linear functionals on  $\ell^2(V)$  along with an isomorphism

$$\begin{aligned} \Phi: \ell^2(V) &\longrightarrow \ell^2(V)^* \\ |x\rangle &\longmapsto \Phi_x, \end{aligned}$$

we will use the notation  $\langle x | x' \rangle := \Phi_x(x')$  and  $\langle x | := |x\rangle^\dagger$ . In the contexts of physical relevance, one has  $|N_x| = k$  for every  $x \in V$ , but for now we relax this hypothesis, taking  $|N_x|$  just finite  $\forall x \in V$ . We now wish to find a representation on  $\ell^2(V) \otimes \mathbb{C}^s$  for the time evolution. Let  $\{|x\rangle\}_{x \in V}$  denote the canonical basis of  $\ell^2(V)$  and  $A$  a walk operator acting on  $\ell^2(V) \otimes \mathbb{C}^s$ . Then for any states

$$|y'\rangle \in \ell^2(V), \quad |\Psi(y', t)\rangle := \sum_{x' \in N_{y'}^{-1}} |x'\rangle |\psi_{x'}(t)\rangle \in \ell^2(V) \otimes \mathbb{C}^s,$$

using Eq. (12) one can represent the time evolution as

$$\begin{aligned}
\langle y' | A | \Psi(y', t) \rangle &= \langle y' | A \sum_{x' \in N_{y'}^{-1}} |x'\rangle | \psi_{x'}(t) \rangle = | \psi_{y'}(t+1) \rangle = \\
&= \sum_{x' \in N_{y'}^{-1}} A_{x'y'} | \psi_{x'}(t) \rangle = \langle y' | \sum_{x' \in N_{y'}^{-1}} \sum_{y \in N_{x'}} |y\rangle A_{x'y} | \psi_{x'}(t) \rangle = \\
&= \langle y' | \left( \sum_{x \in V} \sum_{y \in N_x} |y\rangle \langle x| \otimes A_{xy} \right) \sum_{x' \in N_{y'}^{-1}} |x'\rangle | \psi_{x'}(t) \rangle = \\
&= \langle y' | \left( \sum_{x \in V} \sum_{y \in N_x} |y\rangle \langle x| \otimes A_{xy} \right) | \Psi(y', t) \rangle.
\end{aligned}$$

Thus the walk operator can be finally written in terms of the neighbourhood schemes as

$$A = \sum_{x \in V} \sum_{y \in N_x} \Delta_{xy} \otimes A_{xy}, \quad (13)$$

where the  $\Delta_{xy}$  are the shift operators, translating  $x$  to  $y$ .

From the form (13) and imposing the unitarity conditions  $A^\dagger A = A A^\dagger = I \otimes I_s$ , one can easily find constraints on the transition matrices  $\{A_{xy}\}_{x \in V}^{y \in N_x}$  which are equivalent to the unitarity of  $A$ . One has, for  $x_1 \neq x_2$ ,

$$\begin{aligned}
0 &= \langle x_1 | A^\dagger A | x_2 \rangle = \langle x_1 | \sum_{x, x' \in V} \sum_{\substack{y \in N_x \\ y' \in N_{x'}}} \delta_{y, y'} |x\rangle \langle x'| \otimes A_{xy}^\dagger A_{x'y'} | x_2 \rangle = \\
&= \langle x_1 | \sum_{x, x' \in V} \sum_{y \in N_x \cap N_{x'}} |x\rangle \langle x'| \otimes A_{xy}^\dagger A_{x'y'} | x_2 \rangle = \sum_{y \in N_{x_1} \cap N_{x_2}} A_{x_1 y}^\dagger A_{x_2 y},
\end{aligned}$$

and for  $y_1 \neq y_2$

$$\begin{aligned}
0 &= \langle y_1 | A A^\dagger | y_2 \rangle = \langle y_1 | \sum_{x, x' \in V} \sum_{y, y' \in N_x} \delta_{x, x'} |y\rangle \langle y'| \otimes A_{xy} A_{x'y'}^\dagger | y_2 \rangle = \\
&= \langle y_1 | \sum_{x \in V} \sum_{y_1, y_2 \in N_x} |y\rangle \langle y'| \otimes A_{xy} A_{x'y'}^\dagger | y_2 \rangle = \sum_{x \in N_{y_1}^{-1} \cap N_{y_2}^{-1}} A_{x y_1} A_{x y_2}^\dagger.
\end{aligned}$$

Summarizing the previous calculations, we can finally write the unitarity constraints for the transition matrices in a compact form:

$$\sum_{y \in N_x \cap N_{x'}} A_{xy}^\dagger A_{x'y} = \delta_{x,x'} I_s, \quad (14)$$

$$\sum_{x \in N_y^{-1} \cap N_{y'}^{-1}} A_{xy} A_{x'y}^\dagger = \delta_{y,y'} I_s. \quad (15)$$

The set of conditions (14) and (15) are quadratic in the transition matrices and their solution constitutes generally a hard problem. Structure theorems for the form of the solutions are lacking even in the *scalar* case, namely when  $A_{xy} \in \mathbb{C} \forall x, y \in V$ . Clearly, the solutions will depend on the neighbours schemes of the graph and some general solutions can be found in the presence of particular symmetries: for example, this is the case of the standard graph for the free group [93]). In other cases, some particular solutions has been found (see e.g. Ref. [70, 112]). On some level, the constraints (14) and (15) are the counterpart for QWs of the Chapman–Kolmogorov equations (11) for Markov chains. On the other hand, we remark that the comparison is not perfectly fitting, since the transition matrices of a QW do not represent probabilities and do not even need to be positive operators.

The next definition is relevant to introduce a key feature for QWs: translation-invariance.

**Definition 1.6** (Graph automorphism). *Let  $\Gamma = (V, E)$  be a graph. A graph automorphism  $\lambda$  is a permutation of the elements of  $V$  preserving the set of edges  $E$ , namely such that for every  $v_1, v_2 \in V$*

$$(v_1, v_2) \in E \iff (\lambda(v_1), \lambda(v_2)) \in E.$$

Suppose now to have a graph  $\Gamma$  of degree  $k$ . Then each  $N_x$  can be identified with the same set  $N$ , with  $|N| = k$ . The graph is then homogeneous in the nodes and it is meaningful to define the notion of translation-invariance for a QW on  $\Gamma$ .

**Definition 1.7** (Translation-invariant QW). *Let*

$$A = \sum_{x \in V} \sum_{y \in N} \Delta_{xy} \otimes A_{xy}$$

be the evolution operator of a QW on a graph  $\Gamma = (V, E)$  of degree  $k$  and with neighbourhood scheme  $N$ . Define the operator

$$\Theta_v := \sum_{u \in V} \Delta_{uv} \otimes I_s$$

where the choice of the set  $\mathcal{T}_v := \{v_u \in V\}_{u \in V}$  is such that  $\Theta_v$  induces on  $\ell^2(V)$  an automorphism of the graph  $\Gamma$ . The  $\Theta_v$  represent the translations on the graphs, namely each  $\Theta_v$  shifts the node  $u$  into  $v_u$ . The QW is said translation-invariant if it satisfies the following condition:

$$[A, \Theta_v] = 0 \quad \forall \mathcal{T}_v.$$

We conclude this section outlining a general structure theorem, which has been proven in Ref. [113]. The result characterizes the unitary evolution operators on quantum labelled graphs—namely graphs where an arbitrary Hilbert space is associated to each node—which are also *causal*, that is to say that the first-neighbourhoods are of finite cardinality. We remark that these hypothesis are more general than the ones of the present QW model, including e.g. the QCA case. The theorem states that any unitary evolution operator  $U$  on a quantum labelled graph can be locally implemented: it can be namely decomposed into a finite number of operations on non-overlapping groups of sites. In particular, there exist  $|\phi\rangle$  and some isometric operators  $V_1, \dots, V_n$  such that for every state  $|\psi\rangle$  the following relation holds:

$$V_n \cdots V_1 |\psi\rangle = |\phi\rangle U |\psi\rangle.$$

As a relevant consequence, any  $U$  can be put into the form of a quantum circuit made up with more elementary operators.

### 1.3 DISCRETE-TIME WALKS ON THE LINE

We conclude the present chapter presenting some examples of both classical and quantum rws *on the line*: this is a widespread nomenclature to refer to rws on a graph having  $\mathbb{Z}$  as vertex set and being of degree 2. In the following, we shall simply indicate such a graph as *the integer lattice*.

### 1.3.1 The Simple Random Walk

Let  $\mathbf{Y} = \{Y_i\}_{i \in \mathbb{N}}$  be a sequence of statistically independent random variables with state space  $\{-1, +1\}$  and probability distribution  $\{p, 1 - p\}$ . The sequence  $\mathbf{X} = \{X_n\}_{n \in \mathbb{N}}$  where

$$X_n = \sum_{i=0}^{n-1} Y_i, \quad n \in \mathbb{N}$$

is called the *simple rw with parameter  $p$* . The walker performs a step to the right in the integer lattice with probability  $p$  and a step to the left with probability  $1 - p$ . The mean value of the position of the walker in the simple rw after  $n$  steps is given by

$$\langle X_n \rangle = \left\langle \sum_{i=0}^{n-1} Y_i \right\rangle = \sum_{i=0}^{n-1} \langle Y_i \rangle = \sum_{i=0}^{n-1} (+1 \cdot p - 1 \cdot (1 - p)) = n(2p - 1),$$

while the standard deviation, since the  $Y_i$  are identically distributed and statistically independent random variables, is given by

$$\begin{aligned} \sigma_{X_n} &= \sqrt{\sum_{i=0}^{n-1} \sigma_{Y_i}^2} = \sqrt{n (\langle Y_0^2 \rangle - \langle Y_0 \rangle^2)} = \\ &= \sqrt{n ((+1)^2 p + (-1)^2 (1 - p) - (2p - 1)^2)} = \sqrt{n 4p(1 - p)}. \end{aligned}$$

We notice that in this case for the standard deviation we recover the same diffusive behaviour of Eq. (7), namely  $\sigma_{X_n}$  scales as the square root of the time  $n$ .

The simple rw with parameter  $p = 1/2$  is called the *symmetric rw*. In this case there is no drift motion and the mean value is  $\langle X_n \rangle = 0$  for all  $n$ , as in the case of Brownian motion. Indeed, the 1D Brownian motion is the continuous-time analogue of the symmetric rw on the real line  $\mathbb{R}$ .

### 1.3.2 The Hadamard Walk

The Hadamard walk has been introduced in 2001 as the quantum counterpart of the symmetric rw [55]. A two-dimensional coin system represented by  $\mathbb{C}^2$  is associated

to each node of the integer lattice, and therefore the total Hilbert space is  $\mathcal{H}_{\text{tot}} \cong \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ . The neighbourhood scheme at each node is parametrized as

$$N_x = \{x - 1, x + 1\} \quad x \in \mathbb{Z}.$$

The walk operator consists of a transformation on the coin system sequentially composed to an operation on the whole space  $\mathcal{H}_{\text{tot}}$ . Denoting by  $\{|R\rangle, |L\rangle\}$  the computational basis for  $\mathbb{C}^2$ , the operation on the coin is the Hadamard gate  $H$ , acting as

$$\begin{aligned} H |R\rangle &= \frac{1}{\sqrt{2}} (|R\rangle + |L\rangle), \\ H |L\rangle &= \frac{1}{\sqrt{2}} (|R\rangle - |L\rangle). \end{aligned}$$

Let  $\{|x\rangle\}_{x \in \mathbb{Z}}$  denote the canonical basis for  $\ell^2(\mathbb{Z})$ : the operation  $T$  on the whole  $\mathcal{H}_{\text{tot}}$  is defined as

$$\begin{aligned} T |x\rangle |R\rangle &= |x + 1\rangle |R\rangle, \\ T |x\rangle |L\rangle &= |x - 1\rangle |L\rangle. \end{aligned}$$

The walk operator for the Hadamard qw is then defined as

$$W := T(I \otimes H),$$

which is clearly unitary. The Hadamard walk is an example of *linear* qw [114], namely the direction along which the node-components of a state are translated is controlled by the corresponding spin state.

The Fourier transform of the state  $\psi(x, t) := |x\rangle |u(t)\rangle$  at  $x$  reads

$$\tilde{\psi}(k, t) = \sum_{x \in \mathbb{Z}} e^{-ikx} \psi(x, t), \quad k \in [-\pi, +\pi].$$

The above defined states form a basis for  $\mathcal{H}_{\text{tot}}$ . Defining the two transition matrices

$$M_+ := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \quad M_- := \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ 1 & -1 \end{pmatrix},$$



one can thus represent the evolution in the Fourier domain as

$$\begin{aligned} W\tilde{\psi}(k, t+1) &= \sum_{x \in \mathbb{Z}} e^{-ikx} (M_+ \psi(x+1, t) + M_- \psi(x-1, t)) = \\ &= \left( e^{ik} M_+ \sum_{x \in \mathbb{Z}} e^{-k(x+1)} \psi(x+1, t) + e^{-ik} M_- \sum_{x \in \mathbb{Z}} e^{-k(x-1)} \psi(x-1, t) \right) = \\ &= \left( e^{ik} M_+ + e^{-ik} M_- \right) \tilde{\psi}(k, t) =: M_k \tilde{\psi}(k, t). \end{aligned}$$

Then the dynamics of the walk is suitably Fourier-represented by the finite-dimensional matrix

$$M_k = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{ik} & e^{ik} \\ e^{-ik} & -e^{-ik} \end{pmatrix}. \quad (16)$$

In Chapters 2 and 3 we shall set the above method in the scope of a group-theoretical analysis of qws, and we shall generalize it for a broad variety of lattices and dimensions. We will also show how one can extract information about the dynamics and the kinematics of the qw from a matrix such as (16). In Ref. [55] it is proved that the probability distribution is almost uniform on the interval  $(-t/\sqrt{2}, t/\sqrt{2})$  (where  $t$  denotes the time), namely the qw spreads in linear time, quadratically faster than a classical rw (see Subsection 1.1.1).

### 1.3.3 The 1D Weyl Quantum Walk

The one-dimensional Weyl qw was firstly presented in Ref. [86]. In the Fourier space, it exactly describes the one-dimensional Weyl equation in the momentum representation. The evolution operator is given by

$$A = T_+ \otimes A_+ + T_- \otimes A_-,$$

where the

$$T_{\pm} := \sum_{x \in \mathbb{Z}} |x \pm 1\rangle \langle x|$$

are the translations one the lattice and the transition matrices, in the computational basis  $\{|0\rangle, |1\rangle\}$  for  $\mathbb{C}^2$ , are given by

$$A_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad A_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (17)$$

It is straightforward to see that the 1D Weyl QW is translation-invariant. In addition, it is also linear according to the definition of Ref. [114].

In the Fourier domain, the walk is represented by the matrix

$$A_k = \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix} = \cos k I_2 + i \sin k \sigma_z = e^{ik\sigma_z}, \quad k \in [-\pi, +\pi].$$

The Hamiltonian defined as  $H(k) = -k\sigma_z$  generates the discrete-time evolution, obeying the partial differential equation

$$i\partial_t |\psi(k, t)\rangle = H(k) |\psi(k, t)\rangle = -k\sigma_z |\psi(k, t)\rangle,$$

which is the Weyl equation in the momentum representation.

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## GROUPS AND THEIR CAYLEY GRAPHS: SYMMETRIES AND GEOMETRIC PROPERTIES

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*Definite portions of a manifoldness, distinguished by a mark or by a boundary, are called Quanta. Their comparison with regard to quantity is accomplished in the case of discrete magnitudes by counting, in the case of continuous magnitudes by measuring. [...] The question of the validity of the hypotheses of geometry in the infinitely small is bound up with the question of the ground of the metric relations of space. In this last question, which we may still regard as belonging to the doctrine of space, is found the application of the remark made above; that in a discrete manifoldness, the ground of its metric relations is given in the notion of it, while in a continuous manifoldness, this ground must come from outside. Either therefore the reality which underlies space must form a discrete manifoldness, or we must seek the ground of its metric relations outside it, in binding forces which act upon it.*

---

BERNHARD RIEMANN, "ON THE HYPOTHESES WHICH  
LIE AT THE BASES OF GEOMETRY" [115]<sup>a</sup>

---

<sup>a</sup> For a discussion on the implications of Riemann's ideas for modern physics, most especially for Einstein's formulation of General Relativity, we can refer the reader to [116].

This thesis presents a formalism based on a group-theoretical study of qws. The ambient space of the qws under analysis are mathematical objects called *Cayley graphs*, which are graphical representations of groups. Cayley graphs turn out to be a handy and useful tool in the particular case of discrete groups. A group can be associated with several Cayley graphs, while each Cayley graph represents a unique group. A Cayley graph is conveniently and univocally defined by a *presentation*, which is a shorthand notation for discrete groups. A presentation consists of two sets: a generating set  $S_+$  for the group (an alphabet) and a set  $R$  of *relators*, namely words built up by composition of generators (and their inverses) which amounts to the identity element of the group. The aim of this work is to provide a mathematical framework for free discrete QFTs based on principles of quantum information processing. In Chapter 4 we will expose the physical principles assumed by our framework, leading us to consider the evolution of quantum systems on Cayley graphs of finitely generated groups, namely having  $|S_+| < \infty$ .

Interestingly, the investigation on classical rws on groups is a stand-alone research topic in discrete group theory [117–121]. More in general, the area of Mathematics devoted to the study of the geometric properties of finitely generated groups is rather young, dating back to the 1980s, and is called *Geometric Group Theory*. This discipline enriched the branch of Group Theory with the study of discrete groups as metric spaces and their treatment as geometric objects [122–126]. Geometric Group Theory is very fascinating and prosperous, and benefits from areas of Mathematics such as Riemannian geometry, low-dimensional topology, combinatorics, analysis, probability, logic, as well as from the traditional group theory.

Cayley graphs of finitely generated groups can be deeply connected to continuous manifolds via an equivalence relation called *quasi-isometry*. Considering Cayley graphs as discrete ambient spaces for the evolution of quantum fields allows one to recover a continuous space-time through equivalence classes of quasi-isometric manifolds. The aim of this chapter is to present to the reader the fundamental notions of Group Theory, along with useful results in Geometric Group Theory. Both disciplines shall be key to provide a convenient representation of the evolution of the quantum systems under consideration, to prove general results for qws on Cayley graphs and finally to devise novel qws.

## 2.1 FUNDAMENTALS OF GROUP THEORY

We shall give in the following some basic definitions and results of Group Theory. Let us start with the very definition of what a group is.

**Definition 2.1** (Group). *Let  $G$  be a set and  $\cdot$  a binary operation, called composition law, on  $G$ . The pair  $(G, \cdot)$  is a group if it satisfies the following group axioms:*

–  $G$  is closed under composition:

$$\begin{aligned} \cdot &: G \times G \longrightarrow G \\ (g_1, g_2) &\longmapsto g_1 \cdot g_2 \equiv g_1 g_2; \end{aligned}$$

– Composition is associative:  $\forall g_1, g_2, g_3 \in G, (g_1 g_2) g_3 = g_1 (g_2 g_3)$ ;

– Existence of the identity element:  $\exists e \in G$  such that  $\forall g \in G, eg = ge = g$ ;

– Existence of the inverse:  $\forall g \in G \exists g^{-1} \in G$  such that  $g^{-1}g = gg^{-1} = e$ .

As a consequence of the group axioms, it is straightforward to show that both the identity and the inverses are unique. A particular case of group is that of vector spaces  $V$ , which are groups having the sum as the composition law.

**Definition 2.2** (Element/group order). *Given a group  $G$ , the order of an element  $g \in G$  is defined as*

$$r_g := \min\{r \in \mathbb{N}_+ \mid g^r = e\}.$$

If  $r_g$  does not exist, the order of  $g$  is said to be infinite. The cardinality  $|G|$  is called the order of the group  $G$ .

Groups where the relation

$$g_1 g_2 = g_2 g_1 \quad \forall g_1, g_2 \in G$$

holds are called *Abelian* or *commutative* groups.

**Example 2.1** (Cyclic groups). *An important class of discrete Abelian groups is given by cyclic groups  $\mathbb{Z}_n$ , namely groups generated by composition of a single element  $c$ . For each  $\mathbb{Z}_n$  finite, there exists  $n \in \mathbb{N}$  such that  $c^n = e$ : the finite cyclic groups  $\mathbb{Z}_n$  have precisely order  $n$ . The group  $\mathbb{Z}_\infty \cong \mathbb{Z}$  is the only infinite cyclic group.*

We now introduce some notions apt to conveniently represent the structure groups mapping it into a vector space.

**Definition 2.3** (Group morphisms). *Let  $(G, \cdot)$  and  $(H, *)$  be two groups. A group homomorphism  $\varphi$  from  $G$  to  $H$  is a map preserving the group composition, namely such that*

$$\begin{aligned}\varphi : G &\longrightarrow H \\ g &\longmapsto \varphi(g),\end{aligned}$$

and  $\varphi(g_1 \cdot g_2) = \varphi(g_1) * \varphi(g_2) \ \forall g_1, g_2 \in G$ . When  $H = G$ , such a homomorphism is said an endomorphism. A bijective homomorphism is called an isomorphism, while a bijective endomorphism is called an automorphism. We denote that two groups  $G$  and  $H$  are isomorphic using the notation  $G \cong H$ .

As a consequence of this definition, a homomorphism  $\varphi$  from  $G$  to  $H$  maps the identity element  $e_G$  to  $e_H$  and then also

$$\varphi(g^{-1}) = \varphi(g)^{-1} \quad \forall g \in G.$$

Thus group homomorphisms preserve the group structure. In the following, we will drop the symbol for the group composition operation without loss of clarity. The collection of the automorphisms of a given group  $G$ , denoted by  $\text{Aut}(G)$ , forms itself a group. We are now ready to give the definition of the representation of a group.

**Definition 2.4** (Group representation). *Let  $G$  be a group,  $V$  a vector space over a field  $K$  and  $\text{GL}(V)$  the automorphism group of  $V$ . A representation of  $G$  on  $V$  is a group homomorphism  $\rho$  from  $G$  to  $\text{GL}(V)$ . A representation is called faithful if it is injective.*

For any space vector  $V$  over a field  $K$ ,  $\text{GL}(V)$  is called the *general linear group* of  $V$  and, if  $\dim V = n < \infty$ , it is isomorphic to the group of  $n \times n$  invertible matrices with entries from  $K$ , and is denoted by  $\text{GL}(n, K)$ . Besides, we denote by  $\text{O}(n, K)$  and  $\text{SO}(n, K)$  the subgroups of  $\text{GL}(n, K)$  whose elements are orthogonal and respectively with unit determinant.  $\text{U}(n)$  and  $\text{SU}(n)$  denote the matrix group of unitary matrices and respectively with unit determinant.

**Theorem 2.1.** *The group of automorphisms of  $\mathbb{Z}^d$  is isomorphic to  $\text{GL}(d, \mathbb{Z})$ . [126]*

We now wish to characterize the action of a group representation on the ground vector space. In the following chapters we will consider the right-regular representations

$T$  of groups  $G$  on  $\ell^2(G)$ , defined as follows. We will denote by  $\{|g\rangle\}_{g \in G}$  the canonical basis for  $\ell^2(G)$  and, consistently with the choice of right multiplication for  $G$ , we will define

$$T_{g'} |g\rangle = |gg'^{-1}\rangle \quad \forall g, g' \in G,$$

satisfying  $T_g T_{g'} = T_{gg'}$ . By construction, the right-regular representation is unitary, and indeed  $T_g^\dagger = T_{g^{-1}}$ . If  $G$  is a finite group, we will adopt the convention  $\ell^2(G) \equiv \mathbb{C}^{|G|}$  and the canonical basis will be denoted by  $\{|i\rangle\}_{i=0}^{|G|-1}$ .

**Definition 2.5** (Group action). *A left group action  $\mu$  of a group  $G$  on a set  $X$  is a map*

$$\begin{aligned} \mu : G \times X &\longrightarrow X \\ (g, x) &\longmapsto \mu(g, x) \equiv gx; \end{aligned}$$

*satisfying the group action axioms:*

- $g_1(g_2x) = (g_1g_2)x$  for all  $g_1, g_2 \in G$  and  $x \in X$ ;
- $ex = x$  for all  $x \in X$ .

*It is immediate to correspondingly define the right group action.*

**Definition 2.6** (Transitive action). *The action of a group  $G$  on a non-empty set  $X$  is called transitive if for every  $x, y \in X$  there exists a  $g \in G$  such that  $gx = y$ .*

**Definition 2.7** (Orbit). *Let  $G$  be a group admitting an action on a set  $X$ . The orbit of an element  $x \in X$  under  $G$  is defined as the set*

$$\mathcal{O}_G(x) := \{gx \in X \mid g \in G\}.$$

Clearly, if a group  $G$  admits a transitive action on a set  $X$ , then one has

$$\mathcal{O}_G(x) = X \quad \forall x \in X.$$

**Theorem 2.2** (Cayley's Theorem [127]). *Let  $G$  be a finite group. Then  $G$  is isomorphic to a subgroup of the group of all the permutations of  $|G|$  elements acting on  $G$ .*

**Definition 2.8** ( $G$ -module). *Let  $V$  a vector space,  $G$  a group and  $\mu$  a linear group action of  $G$  on  $V$ . The pair  $(V, \mu)$  is called  $G$ -module.*

For any representation  $\rho$  of a group  $G$  on  $V$ , one can construct the associated  $G$ -module  $(V, \mu)$  defining

$$\mu(g, \mathbf{v}) := \rho(g)\mathbf{v} \quad g \in G, \mathbf{v} \in V.$$

A  $G$ -module having no nontrivial submodules is called *irreducible*: the next definition introduces the analogous notion for a representation.

**Definition 2.9** (Irreducible representation). *An irreducible representation (shortly, irrep)  $\Pi$  of a group  $G$  over a vector space  $V$  is a group homomorphism from  $G$  to  $\mathbb{GL}(V)$  having no nontrivial invariant subspace.*

A  $G$ -module homomorphism is a map  $f : V \rightarrow W$  such that

$$f(\mu(g, \mathbf{v})) = \nu(g, f(\mathbf{v})).$$

The previous object is particularly useful to characterize the finite-dimensional irreps of Abelian groups, as we shall see in the following.

**Lemma 2.1** (Schur's Lemma). *Let  $G$  be a group,  $(V, \mu)$  and  $(W, \nu)$  irreducible  $G$ -modules and  $f$  a  $G$ -module homomorphism from  $V$  to  $W$ . Then  $f$  is either invertible or the null map.*

*Proof.*  $(\ker f, \mu)$  and  $(\text{Im} f, \nu)$  are submodules of  $(V, \mu)$  and  $(W, \nu)$ , respectively. Then, one has the following two cases: either i)  $(\ker f, \mu)$  is trivial and then  $\text{Im} f = W$ , implying  $f$  invertible, or ii)  $\ker f = V$  and then  $(\text{Im} f, \nu)$  is trivial, implying that  $f$  is the null map. ■

**Corollary 2.1.** *Let  $G$  be a group and  $(V, \mu)$  be a finite-dimensional and irreducible  $G$ -module taken over an algebraically closed field  $K$ . Then every  $G$ -module homomorphism  $f : V \rightarrow V$  is equal to a scalar multiplication.*

*Proof.*  $f$  has at least an eigenvalue  $\lambda$ . Since the transformation  $f - \lambda I_V$  is not invertible, by Theorem 2.1 it must be null, implying that  $\exists \lambda \in K : f = \lambda I_V$ . ■

**Proposition 2.1.** *Let  $G$  be an Abelian group. Then the finite-dimensional irreducible representations of  $G$  over an algebraically closed field  $K$  are one-dimensional.*

*Proof.* Let  $\Pi : G \rightarrow \mathbb{GL}(V)$  be a finite-dimensional irreducible representation of and Abelian group  $G$ . Then

$$\Pi(g_1)\Pi(g_2) = \Pi(g_1g_2) = \Pi(g_2g_1) = \Pi(g_2)\Pi(g_1) \quad \forall g_1, g_2 \in G. \quad (18)$$



Let us define the irreducible  $G$ -module  $(V, \mu)$  such that

$$\mu(g, \mathbf{v}) := \Pi(g)\mathbf{v} \quad \forall g \in G, \forall \mathbf{v} \in V.$$

Then, by equation (18) and for all  $g \in G$ , the map  $\Pi(g)$  is a  $G$ -module endomorphism. By Corollary 2.1 one has

$$\exists \lambda_g \in K : \Pi(g) = \lambda_g I_V, \quad \forall g \in G$$

and then, since  $\Pi$  is irreducible,  $\dim V = 1$ . ■

In the following chapters we will consider *completely reducible* unitary representations  $\rho$ , namely such that  $\rho(g)$  is a direct sum of irreps being unitary operators  $\forall g \in G$ .

If a subset  $H \subseteq G$  is itself a group under the group law of  $G$ , then  $H$  is called a *subgroup* of  $G$ , which we indicate by  $H \leq G$ . The existence of a subgroup induces partitions on the whole group.

**Definition 2.10** (Cosets of a subgroup). *Let  $G$  be a group and  $H$  a subgroup of  $G$ . The left cosets of  $H$  in  $G$  are the equivalence classes defined by the equivalence relation*

$$g_1 \sim g_2 \iff \exists h \in H : g_1 h = g_2 \quad g_1, g_2 \in G.$$

*It is immediate to correspondingly define the right cosets.*

It is a direct check to show that the previous relation is reflexive, symmetric and transitive. The set of the cosets of a subgroup  $H$  in  $G$  is denoted by  $G/H$ . The left cosets of  $H$  in  $G$  are of the form  $c_j H$  for some  $c_j \in G$  (called *coset representatives*). Furthermore, by definition, every element of  $G$  belongs to one and only one coset of  $H$ , and therefore the cosets are disjoint and induce a partition of  $G$ . Defining an alphabet  $J$  such that  $\bigcup_{j \in J} c_j H = G$ , the cardinality of  $J$  is called the *index* of  $H$  in  $G$ .

**Definition 2.11** (Normal subgroup). *A subgroup  $N$  of a group  $G$  is called a normal subgroup if*

$$g^{-1} n g \in N \quad \forall n \in N, \forall g \in G. \tag{19}$$

*We indicate this property by  $N \trianglelefteq G$ .*

**Proposition 2.2.** *Let  $\varphi : G \rightarrow H$  be a group homomorphism. Then  $\ker\varphi \trianglelefteq G$ .*

*Proof.* First we prove that  $\ker\varphi$  is a subgroup of  $G$ . By definition  $\varphi(e) = e$ , then  $e \in \ker\varphi$ . Moreover, for every  $g, g' \in \ker\varphi$  one has

$$\begin{aligned}\varphi(g)\varphi(g') &= e = \varphi(gg') \implies gg' \in \ker\varphi, \\ \varphi(g^{-1}) &= \varphi(g)^{-1} = e \implies g^{-1} \in \ker\varphi.\end{aligned}$$

Then  $\ker\varphi$  is a subgroup of  $G$ . Finally, since for every  $g \in G$  and  $n \in \ker\varphi$  one has that

$$\varphi(gng^{-1}) = \varphi(g)\varphi(n)\varphi(g^{-1}) = \varphi(g)\varphi(g^{-1}) = \varphi(gg^{-1}) = \varphi(e) = e,$$

consequently  $\ker\varphi$  is also normal in  $G$ . ■

A subgroup is normal if it is invariant under the operation defined in relation (19), which is called *conjugation* and defines an equivalence relation called the *conjugacy*. If one aggregates elements of a group belonging to the same cosets of a normal subgroup, this preserves the group composition and induces an additional group structure.

**Definition 2.12** (Quotient group). *Given a group  $G$  and a normal subgroup  $N$ , the quotient group  $G/N$  is the set of all the left cosets of  $N$  in  $G$  endowed with the composition rule  $(g_1N)(g_2N) = g_1g_2N$  for any  $g_1N, g_2N \in G/N$ .*

**Definition 2.13** (Projective representation). *Let  $G$  be a group and  $V$  a vector space over a field  $K$ . A projective representation of  $G$  on  $V$  is a group homomorphism  $\rho$  from  $G$  to  $\mathbb{PGL}(V)$ , where*

$$\mathbb{PGL}(V) := \mathbb{GL}(V)/\mathbb{Z}$$

and  $\mathbb{Z} \triangleleft \mathbb{GL}(V)$  is the subgroup of the transformations proportional to the identity.

**Definition 2.14** (Semidirect product). *Let  $G, H, N$  be groups such that  $N \trianglelefteq G$  and  $H \leq G$ . If*

$$\forall g \exists! n \in N \wedge \exists! h \in H : g = nh,$$

then  $G$  is called a semidirect product of  $N$  and  $H$ .

In Chapters 8 and 9 we shall address the problem of constructing a group  $G$  starting from the hypothesis that it contains a normal subgroup  $N$ : this is called the *extension problem*. In that context, semidirect products are also said *split extensions*. Given a

semidirect product  $G$  between  $N \trianglelefteq G$  and  $H$ , then for  $n_1, n_2 \in N$  and  $h_1, h_2 \in H$  one can set the convenient definition

$$n_1 h_1 n_2 h_2 = n_1 h_1 n_2 h_1^{-1} h_1 h_2 =: n_1 \varphi_{h_1}(n_2) h_1 h_2,$$

where

$$\begin{aligned} \varphi : H &\longrightarrow \text{Aut}(N) \\ h &\longmapsto \varphi_h \end{aligned} \tag{20}$$

is a group homomorphism. It is useful to denote a semidirect product explicitly referring to the homomorphism (20), and we will use the following notation:

$$G = N \rtimes_{\varphi} H.$$

A special case of a semidirect product is for  $\varphi = \text{id}$ : in this case

$$nh = hn \quad \forall n \in N, \forall h \in H$$

and the resulting group  $G = N \times H := N \rtimes_{\text{id}} H$  is called a *direct product*.

**Example 2.2** (Free Abelian groups). *The group*

$$G = \underbrace{\mathbb{Z} \times \dots \times \mathbb{Z}}_{d \text{ times}} \cong \mathbb{Z}^d$$

is called the free Abelian group of rank  $d$ . This terminology will become clearer in Section 2.2, where the definition of free group will be given in the context of group presentations. Being each isomorphic copy of  $\mathbb{Z}$  in  $G$  Abelian, the resulting group  $G$  is also Abelian.

**Remark 2.1.** Define  $\text{Inn}(G)$  as the subgroup of  $\text{Aut}(G)$  such that

$$\forall \phi_g \in \text{Inn}(G) \exists g \in G : \phi_g(g') = gg'g^{-1}, \quad g' \in G.$$

$\text{Inn}(G)$  is called the inner automorphism group and is normal in  $\text{Aut}(G)$ : indeed, for every  $g' \in G$ ,  $\phi_g \in \text{Inn}(G)$  and  $\alpha \in \text{Aut}(G)$ , one has

$$\alpha \circ \phi_g \circ \alpha^{-1}(g') = \alpha \left( g \alpha^{-1}(g') g^{-1} \right) = \alpha(g) g' \alpha(g^{-1}) = \alpha(g) g' \alpha(g)^{-1} \equiv$$

$$\equiv \phi_{\alpha(g)}(g').$$

The quotient  $\text{Out}(G) := \text{Aut}(G)/\text{Inn}(G)$  is called the outer automorphism group of  $G$ . The automorphisms which are not inner are called outer automorphisms. Notice that, in general,  $\text{Out}(G)$  is not a subgroup of  $\text{Aut}(G)$ , and then generally the outer automorphisms are not elements of  $\text{Out}(G)$ .

## 2.2 CAYLEY GRAPHS AND QUASI-ISOMETRIES

**Definition 2.15** (Generating set). Given a group  $G$ , a generating set  $S_+$  for the group is a subset of  $G$  such that any of its elements can be written as a word (i.e. a combination under the group law) of elements of  $S_+$  and their inverses. If  $S_-$  denotes the set collecting the inverses of the elements of  $S_+$ , then the set  $S := S_+ \cup S_-$  is called a set of generators for  $G$ . The cardinality of the smallest generating set for a group  $G$  is called the rank of  $G$ .

Uniqueness of the inverses implies that  $S^+$  and  $S^-$  are in one-to-one correspondence. The next definitions are introductory to a very powerful tool, the *presentation of a group*, which is connected to Cayley graphs and turns out to be very useful in order to characterize and visualize groups in a graphical fashion.

**Definition 2.16** (Free group). Given a set  $S_+$ , the free group  $F_{S_+}$  generated by  $S_+$  is the group whose elements are all the words that can be written using  $S = S_+ \cup S_-$  as an alphabet, considering two words different unless their equality follows from the group axioms.

Given an arbitrary group, the equality of two words on a generating set could follow from either the group axioms or by virtue of some other relations which characterize the group itself, such as  $c^m = e$  for some integer  $m$  (cyclic conditions) or  $g_1g_2 = g_2g_1$  (Abelianity). Free groups lack such relations and equalities between their elements follow solely from the group axioms.

**Definition 2.17** (Conjugate closure). Given a group  $G$  and a subset  $R$  of words on  $G$ , the conjugate closure  $N_R$  of  $R$  in  $G$  is the subgroup generated by the conjugates of  $R$ , namely by the elements of the set  $\{grg^{-1} \mid g \in G, r \in R\}$ .

Let us consider a generic element  $grg^{-1} \in N_R$ , for  $g \in G$  and  $r \in R$ . Then for every  $g' \in G$  one has

$$g' \left( grg^{-1} \right) g'^{-1} = (g'g) r (g'g)^{-1} \in N_R,$$

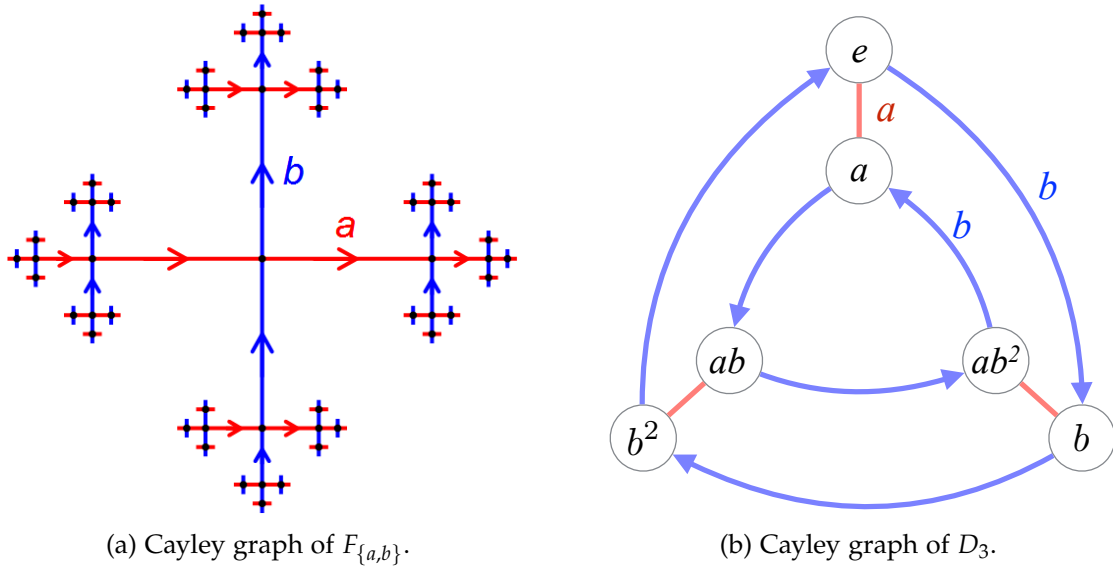


Figure 1: (Left) A possible Cayley graph for the free group of rank 2 (the simplest non-Abelian free group). (Right) A Cayley graph of the dihedral group  $D_3 = \langle a, b \mid a^2, b^3, aba^{-1}b \rangle$ .

namely the conjugate closure  $N_R$  is normal in  $G$ . Accordingly, we can give the following definition.

**Definition 2.18** (Presentation of a group). *Given a generating set  $S_+$  and a set  $R$  of words on  $S_+$ , let  $F_{S_+}$  be the free group on  $S_+$  and  $N_R$  the conjugate closure of  $R$  in  $F_{S_+}$ . Then  $\langle S_+ \mid R \rangle$  is called a presentation of the quotient group  $G = F_{S_+} / N_R$ .*

Presentations are in a bijective correspondence with Cayley graphs, defined in the following.

**Definition 2.19** (Cayley graph). *The Cayley graph  $\Gamma(G, S_+)$  of a group  $G$  with respect to the generating set  $S_+$  is the edge-coloured directed graph constructed as follows:*

1.  $G$  is the vertex set.
2. A coloured edge directed from  $g$  to  $gh$  is assigned to each  $h \in S$  and  $\forall g \in G$ .

One can see that different presentations of the same group corresponds to different Cayley graphs. For example,

$$\langle g_1, g_2 \mid g_1 g_2 g_1^{-1} g_2^{-1} \rangle$$

is a presentation for  $\mathbb{Z}^2$  whose corresponding Cayley graph is given by the simple square lattice, while

$$\langle g_1, g_2, g_3 \mid g_i g_j g_i^{-1} g_j^{-1}, g_2 (g_1 g_3)^{-1} \rangle \quad \forall i, j \in \{1, 2, 3\}$$

is the presentation for  $\mathbb{Z}$  associated with the hexagonal (honeycomb) lattice.

Groups (and consequently their Cayley graphs) equipped with a metric can be studied as metric spaces.

**Definition 2.20** (Word length and word metric). *Let  $G = \langle S \mid R \rangle$  be a finitely generated group. The word length  $l^w$  is the norm on  $G$  defined as*

$$l^w(g) := \min \left\{ n \in \mathbb{N} \mid g = h_{i_1} \cdots h_{i_n}, h_{i_j} \in S \right\}. \quad (21)$$

The norm  $l^w$  induces the word metric  $d_G$  on  $G$ , defined as

$$d_G(g, g') := l^w(g^{-1}g'). \quad (22)$$

The counting metric is not equivalent to the Euclidean metric due to the so-called Weyl tile argument [128]<sup>1</sup>. Take for example the simple hypercubic  $n$ -dimensional lattice  $\Lambda^n$  equipped with the counting metric and  $\mathbb{R}^n$  with the usual metric: intuitively, the two metrics are equivalent modulo a constant bound equal to  $\sqrt{n}$ . In fact, denoting with  $\mathcal{E}$  the natural map from  $\Lambda^n$  to  $\mathbb{R}^n$ , one has the following bounds:

$$\frac{1}{\sqrt{n}} d_{\Lambda^n}(g_1, g_2) \leq d_{\mathbb{R}^n}(\mathcal{E}(g_1), \mathcal{E}(g_2)) \leq \sqrt{n} d_{\Lambda^n}(g_1, g_2) \quad \forall g_1, g_2 \in \Lambda^n.$$

This suggests that the gap between the two metrics is quantitatively under control. In the present thesis we study qws on Cayley graphs which “reconstruct” Euclidean continuous spaces, and we shall make use of a convenient notion of embedding: the *quasi-isometry* [123].

---

<sup>1</sup> Actually, Weyl’s argument has not been formulated using the counting metric, but rather counting the tiles in between two lattice points. However, in the case of a square lattice the argument still works.

**Definition 2.21** (Quasi-isometry). *Let  $(G, d_G)$  and  $(M, d_M)$  two metric spaces. A quasi-isometry is a function  $\mathcal{E} : G \rightarrow M$  satisfying, for some fixed  $a \geq 1$  and  $b, c \geq 0$ , the two following conditions:*

$$\frac{1}{a}d_G(g, g') - b \leq d_M(\mathcal{E}(g), \mathcal{E}(g')) \leq ad_G(g, g') + b \quad \forall g, g' \in G; \quad (23)$$

$$\forall m \in M \exists g \in G : d_M(m, \mathcal{E}(g)) \leq c. \quad (24)$$

Two metric spaces  $G$  and  $M$  are called quasi-isometric if there exists a quasi-isometry from  $G$  to  $M$ .

**Lemma 2.2.** *Quasi-isometry induces an equivalence relation.*

*Proof.* The statement can be proved via a direct check of the properties of reflexivity, symmetry and transitivity for the relation “being quasi-isometric to”. ■

**Definition 2.22** (Virtually  $P$  group). *Let  $P$  be a group property. A group  $G$  is called virtually  $P$  if there exists a subgroup  $H \leq G$  satisfying  $P$  and such that the index  $|G/H|$  is finite.*

When we denote a property  $G$  with a group  $G$ , it will stand for “being isomorphic to  $G$ ”.

**Definition 2.23** ( $N$ -by- $Q$  group). *Let  $N$  and  $Q$  be two group properties. A group  $G$  is called  $N$ -by- $Q$  if there exists  $N \trianglelefteq G$  satisfying  $N$  and such that the quotient group  $G/N$  satisfies  $Q$ .*

### 2.3 AROUND QUASI-ISOMETRIC RIGIDITY

In this final section we focus on the quasi-isometric classes of Euclidean spaces.

**Theorem 2.3** (Fundamental theorem of finitely generated Abelian groups). *Every finitely generated Abelian group is isomorphic to a direct product of finitely many cyclic groups. [126]*

**Proposition 2.3** (Poincarè [129]). *Let  $G$  be a group containing a subgroup  $H$  of finite index  $l$ . Then the normal core of  $H$  in  $G$ , namely the set*

$$N_H := \bigcap_{g \in G} gHg^{-1},$$

*is a normal subgroup and of finite index  $l'$  in  $G$ , where  $l'$  is a multiple of  $l$  and a divisor of  $l!$ .*

**Corollary 2.2.** *Let  $G$  be a group and  $P$  a property inherited by subgroups of finite index. Then  $G$  is  $P$ -by-finite if and only if  $G$  is virtually  $P$ .*

**Proof.**

( $\Rightarrow$ ) It follows by definition.

( $\Leftarrow$ ) Let  $H$  be of finite index in  $G$  and satisfying  $P$ . It is easy to see that the normal core  $N_H$  is a subgroup of  $H$ , and since by Proposition 2.3 one has  $|G/N_H| < +\infty$ , also  $|H/N_H| < +\infty$  holds. By hypothesis  $N_H$  satisfies  $P$ , then the thesis follows.

■

**Corollary 2.3.** *A group is  $\mathbb{Z}^d$ -by-finite if and only if it is virtually  $\mathbb{Z}^d$ .*

**Proof.** The property of “being isomorphic to  $\mathbb{Z}^d$ ” is inherited by subgroup of finite index: by Theorem 2.3, any subgroup  $M$  of  $N \cong \mathbb{Z}^d$  must be isomorphic to  $\mathbb{Z}^{d'}$  with  $d' \leq d$ , thus  $|N/M| = +\infty$  unless  $d = d'$ . ■

It is easy to see that further properties  $P$  inherited by subgroups of finite index are: *cyclicity, Abelianity, and freeness.*

**Definition 2.24** (Virtually isomorphic groups). *Two groups  $G, G'$  are called virtually isomorphic if there exists a group  $Q$  such that both  $G$  and  $G'$  are virtually finite-by- $Q$ .*

**Lemma 2.3** (Milnor-Schwarz [130]). *Let  $G, G'$  two virtually isomorphic finitely generated groups. Then they are quasi-isometric.*

Let  $G$  be a virtually  $G'$  group, then both  $G$  and  $G'$  are virtually finite-by- $G'$ : in particular, they are virtually isomorphic. Then, for example, quasi-isometry are blind to finite group: every finite group is virtually trivial, and in particular quasi-isometric to a point.

**Definition 2.25** (Quasi-isometric rigidity). *A group  $G$  is said quasi-isometrically rigid if every group  $G'$  being quasi-isometric to  $G$  is also virtually isomorphic to  $G$ .*

**Theorem 2.4** (Quasi-isometric rigidity of  $\mathbb{Z}^d$  [131]). *If a finitely generated group  $G$  is quasi-isometric to  $\mathbb{Z}^d$ , then it has a finite index subgroup isomorphic to  $\mathbb{Z}^d$ .*



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## QUANTUM WALKS ON CAYLEY GRAPHS

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The evolution of systems on (generalized) Cayley graphs in the context of Cellular Automata has been extensively studied in Ref. [132]. A general survey on qws on Cayley graphs has been given in Ref. [93], while a particular focus on finite groups can be found in Refs. [112, 133].

In the present chapter we use the concepts presented in Chapters 1 and 2 to provide a mathematical framework for qws on Cayley graphs. First, we shall exploit the group-theoretical machinery to suitably represent the qws on Cayley graphs. Then we will provide a general analysis, justified by group-representation theory, of the Fourier representation of the Abelian qws—namely those qws on the Cayley graphs of Abelian groups. This will allow to study Abelian qws in the momentum space, diagonalizing the walk operator and defining differential equations for their time evolution. In this way one can extract kinematic and dynamical information from the evolution operator and also take the continuum limit. We will conclude presenting an application of these methods to the one-dimensional Dirac qw, a relevant example of discrete evolution on the line recovering the Dirac field equation in the continuum limit.

## 3.1 QUANTUM WALKERS ON GROUPS

Let  $\Gamma(G, S_+)$  be the Cayley graph of a group  $G$ . The discrete-time evolution of a qw on  $\Gamma$  with evolution operator  $A$  is expressed by

$$\psi_g(t+1) = \sum_{g' \in G} A_{gg'} \psi_{g'}(t), \quad (25)$$

where  $\psi(t) \in \mathbb{C}^s$  is the component on site  $g$  of the state of the system at time  $t$  and the  $A_{gg'} \in \mathbb{M}_s(\mathbb{C})$  are the transition matrices of the walk operator  $A$ . Denoting the total state of the system at time  $t$  as  $|\Psi(t)\rangle \in \ell^2(G) \otimes \mathbb{C}^s$  and defining  $A_h^g := A_{gg'}$  if  $h = g^{-1}g'$  for  $h \in S_+$ , equation (25) reads

$$\begin{aligned} \langle g | \Psi(t+1) \rangle &= \langle g | A | \Psi(t) \rangle = \sum_{g' \in G} A_{gg'} \langle g' | \Psi(t) \rangle = \\ &= \sum_{h \in S_+} A_h^g \langle gh | \Psi(t) \rangle = \langle g | \left( \sum_{g' \in G} \sum_{h \in S_+} |g'h^{-1}\rangle \langle g' | \otimes A_h^{g'} \right) | \Psi(t) \rangle =: \\ &=: \langle g | \left( \sum_{g' \in G} \sum_{h \in S_+} \Delta_h^{g'} \otimes A_h^{g'} \right) | \Psi(t) \rangle, \end{aligned}$$

resulting in the following final form for the evolution operator in terms of the generators contained in  $S_+$ :

$$A = \sum_{g \in G} \sum_{h \in S_+} \Delta_h^g \otimes A_h^g. \quad (26)$$

The latter is the general form for a qw on a group  $G$  with respect to a generating set  $S_+$ . Now suppose that the dimension of the coin systems is constant, say  $s$ . In Chapter 1 we defined (Definition 1.7) translation-invariance for qws on arbitrary graphs having constant degree (being homogeneous in the neighbours schemes). qws on groups are in this sense homogeneous by definition. In addition, they satisfies translation-invariance. This is because the translation operators along any  $g' \in G$  which induce an automorphism of the Cayley graphs are defined as

$$\Theta_{g'} := \sum_{g \in G} |g'g\rangle \langle g | \otimes I_s.$$

By direct computation, it is easy to check that the commutation

$$[A, \Theta_{g'}] = 0$$

holds for every  $g' \in G$ . In the case where also the evolution is homogeneous in the lattices sites, namely the transition matrices are  $A_h^g \equiv A_h \forall g \in G$ , then

$$A = \sum_{h \in S_+} \left( \sum_{g \in G} \Delta_h^g \right) \otimes A_h \equiv \sum_{h \in S_+} T_h \otimes A_h, \quad (27)$$

where  $T$  is the right-regular representation of  $G$  (see Chapter 2). Now, for a homogeneous evolution Eq. (25) reads

$$\psi_g(t+1) = \sum_{h \in S} A_h \psi_{g,gh}(t). \quad (28)$$

**Definition 3.1** (Quantum walk on a Cayley graph). *Let  $G$  be a finitely presented group. A qw on the Cayley graph  $\Gamma(G, S_+)$  with an  $s$ -dimensional coin system is the quadruple*

$$W = \{G, S_+, s, \{A_h\}_{h \in S}\}$$

such that

1.  $s \in \mathbb{N}$ ;
2. the transition matrices  $A_h \in \mathbb{M}_s(\mathbb{C})$  are non-vanishing  $\forall h \in S$ ;
3. the operator

$$A = \sum_{h \in S} T_h \otimes A_h \quad (29)$$

over  $\mathcal{H} := \ell^2(G) \otimes \mathbb{C}^s$  is unitary.

First, we showed that the evolution operator in Eq. (27) gives an equivalent representation to the time evolution defined in Eq. (28). A Cayley graph is a homogeneous space where the evolution is defined, and this fact is mirrored by the two definitions. This is a standard choice in the literature, and we refer the reader to Refs. [70, 86, 93, 112] for some examples. On the other hand, we notice that the evolution operator in

Eq. (26) is not homogeneous; yet can be, in general, acceptably called a qw on a Cayley graph.

**Remark 3.1.** *Sometimes authors studying qws on Cayley graphs are not in agreement with the definition: the summation in Eq. (27) is usually taken over a symmetric  $S_+$ , as in (29) (see Refs. [70, 86, 93]), but one can find also cases where this assumption is dropped [112]. This ambiguity may in part descend from the fact that, although in the mathematical literature there is general consensus on the definition of Cayley graphs via a symmetric generating set  $S$ , it is perfectly fine and lossless take non-symmetric generating sets  $S_+$ .*

Last remark motivates the following definition to the purpose of clearing out the nomenclature.

**Definition 3.2** (Monoidal qw on a Cayley graph). *A qw on a Cayley graph  $\Gamma(G, S_+)$  is called monoidal if its evolution operator has the form of (27), with  $S_+$  not necessarily symmetric.*

Specializing Eqs. (14) and (15) to the present case, the requirement of unitarity amounts to imposing the following set of conditions on the transition matrices:

$$\sum_{h \in S} A_h A_h^\dagger = \sum_{h \in S} A_h^\dagger A_h = I_s, \quad (30)$$

$$\sum_{hh'^{-1}=h''} A_h A_{h'}^\dagger = \sum_{h^{-1}h'=h''} A_h^\dagger A_{h'} = 0, \quad (31)$$

where  $h'' \in \{g \in G \mid g = hh'^{-1} \neq e : h, h' \in S\}$  (all the possible fixed paths of length two in the set of generators). The constraints in Eqs. (30) and (31) are a set of equations quadratic in the transition matrices  $\{A_h\}_{h \in S}$ . As pointed out in Chapter 1, in general there does not exist a closed-form solution, even in the case  $s = 1$ . On the contrary, in Chapters 9 and 10 we will give some example of cases where it is more convenient to convert the problem from a scalar one to a matricial one.

### 3.2 QUANTUM WALKS ON FREE ABELIAN GROUPS

In this section we will restrict to qws on Cayley graphs of free Abelian groups, generalizing in Chapter 6 the results here exposed to the case of arbitrary Abelian groups. We here follow the treatment of Ref. [ME94] for the general application of Fourier analysis to qws on Cayley graphs of free Abelian groups resorting to the methods presented in Chapter 2.

### 3.2.1 Representation in the Fourier space

Let  $G$  be a free Abelian group. By the classification of finitely generated Abelian groups (Theorem 2.3),  $G \cong \mathbb{Z}^d$  for some integer  $d \geq 1$ . Let then  $\Gamma(G, S_+)$  be an arbitrary Cayley graph of  $G$ . Throughout this section we will use Abelian notation, denoting the group composition law with the additive notation and the elements  $\mathbf{x} \in G$  as boldfaced  $d$ -dimensional real vectors. In particular, we will consider  $G$  as a space-vector.

The right-regular representation of each  $\mathbf{x} \in G$  is given by

$$T_{\mathbf{x}} = \sum_{\mathbf{y} \in G} |\mathbf{y} - \mathbf{x}\rangle \langle \mathbf{y}|.$$

Then, let the unitary operator

$$A = \sum_{\mathbf{h} \in S} T_{\mathbf{h}} \otimes A_{\mathbf{h}}$$

represent a qw on the Cayley graph  $\Gamma$ . By Proposition 2.1 the unitary irreps of  $G$  are one-dimensional. We now constructively show how to decompose the right-regular representation, which is unitary by definition, into the one-dimensional unitary irreps of  $G$ . The latter are classified by the joint eigenvectors given by the relation

$$T_{\mathbf{y}} |\mathbf{k}\rangle = e^{i\mathbf{k} \cdot \mathbf{y}} |\mathbf{k}\rangle \quad \mathbf{y} \in G, \quad (32)$$

where each  $k_y := \mathbf{k} \cdot \mathbf{y} \in [-\pi, +\pi]$  and  $\mathbf{k}$  is an element of  $G^*$ , the dual space of  $G$ . Taking the following expansion for the eigenvectors

$$|\mathbf{k}\rangle = \sum_{\mathbf{x} \in G} c(\mathbf{x}, \mathbf{k}) |\mathbf{x}\rangle,$$

and substituting it into Eq. (32), one obtains

$$T_{\mathbf{y}} |\mathbf{k}\rangle = \sum_{\mathbf{x} \in G} c(\mathbf{x}, \mathbf{k}) |\mathbf{x} - \mathbf{y}\rangle = \sum_{\mathbf{x} \in G} c(\mathbf{x} + \mathbf{y}, \mathbf{k}) |\mathbf{x}\rangle = \sum_{\mathbf{x} \in G} e^{i\mathbf{k} \cdot \mathbf{y}} c(\mathbf{x}, \mathbf{k}) |\mathbf{x}\rangle.$$

Therefore, the relation  $e^{-i\mathbf{k} \cdot \mathbf{y}} c(\mathbf{x} + \mathbf{y}, \mathbf{k}) = c(\mathbf{x}, \mathbf{k})$  leads to

$$e^{i\mathbf{k} \cdot \mathbf{x}} c(0, \mathbf{k}) = c(\mathbf{x}, \mathbf{k}).$$

Accordingly, substituting and imposing the normalization for the  $|\mathbf{k}\rangle$ , we obtain

$$|\mathbf{k}\rangle = \frac{1}{(2\pi)^{d/2}} \sum_{\mathbf{x} \in G} e^{i\mathbf{k}\cdot\mathbf{x}} |\mathbf{x}\rangle, \quad |\mathbf{x}\rangle = \frac{1}{(2\pi)^{d/2}} \int_B d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{x}} |\mathbf{k}\rangle, \quad (33)$$

where  $B$  is the *first Brillouin zone*, which we shall determine in the following.

In general, the generators in  $S_+$  are not linearly independent, then we define all the sets

$$D_n := \{\mathbf{h}_{n_1}, \dots, \mathbf{h}_{n_d}\} \subseteq S_+,$$

collecting linearly independent elements, where  $n$  labels the specific subset. For every  $n$ , we can then define the dual set

$$\tilde{D}_n := \{\tilde{\mathbf{h}}_{n_1}, \dots, \tilde{\mathbf{h}}_{n_d}\}, \quad \tilde{\mathbf{h}}_{n_l} \cdot \mathbf{h}_{n_m} = \delta_{lm}.$$

We now can expand each  $\mathbf{x} \in G$  and  $\mathbf{k} \in G^*$  as

$$\mathbf{x} = \sum_{j=1}^d x_j \mathbf{h}_{n_j}, \quad \mathbf{k} = \sum_{j=1}^d k_j \tilde{\mathbf{h}}_{n_j},$$

for some  $n$ , where  $x_j \in \mathbb{N}$  for every  $j$  and  $\mathbf{k} \in B$ . Two eigenstates  $|\mathbf{k}\rangle, |\mathbf{k}'\rangle$  are equal if there exists  $\theta \in [0, 2\pi]$  such that

$$|\mathbf{k}\rangle = e^{i\theta} |\mathbf{k}'\rangle.$$

Thus, from Eq. (33), one can derive

$$e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} = e^{i\theta} = e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}} \quad \forall \mathbf{x}, \mathbf{y} \in G,$$

which is equivalent to the condition

$$\exists \mathbf{l} \in \mathbb{N}^d : k_{n_j} - k'_{n_j} = 2\pi l_j \quad j = 1, \dots, d.$$

Since the choice of  $D_n, \tilde{D}_n$  is arbitrary, the Brillouin zone  $B \subseteq \mathbb{R}^d$  is the polytope defined by

$$B = \bigcap_{\tilde{\mathbf{h}} \in \tilde{D}} \{\mathbf{k} \in \mathbb{R}^d \mid -\pi|\tilde{\mathbf{h}}|^2 \leq \mathbf{k} \cdot \tilde{\mathbf{h}} \leq \pi|\tilde{\mathbf{h}}|^2\}, \quad \tilde{D} := \bigcup_n \tilde{D}_n.$$

The evolution operator  $A$  can be thus diagonalized as follows

$$A = \int_B d\mathbf{k} |\mathbf{k}\rangle \langle \mathbf{k}| \otimes A_{\mathbf{k}},$$

where the matrix

$$A_{\mathbf{k}} := \sum_{\mathbf{h} \in S} e^{i\mathbf{h} \cdot \mathbf{k}} A_{\mathbf{h}}$$

must be unitary for every  $\mathbf{k}$ . Being  $A_{\mathbf{k}}$  polynomial in  $e^{i\mathbf{h} \cdot \mathbf{k}}$ , imposing unitarity straightforwardly amounts to find the same general set of constraints of Eqs. (30) and (31).

Clearly, in general  $A_{\mathbf{k}} \in \mathbf{U}(s)$  and its eigenvalues will be of the form  $e^{i\omega_l(\mathbf{k})}$ , for some integer  $1 \leq l \leq s$ . The functions in the set

$$\{\omega_1(\mathbf{k}), \dots, \omega_s(\mathbf{k})\}, \quad \mathbf{k} \in B \tag{34}$$

are called the *dispersion relations* of the qw. We sometimes collectively refer to the set in Eq. (34) as the dispersion relation of the qw *tout court*. As one can see from the unitarity constraints in Eqs. (30) and (31), the operator  $A$  is defined up to a global phase factor, and then in particular one can always choose  $A_{\mathbf{k}} \in \mathbf{SU}(s)$  without loss of generality. This fact, in the case of interest of  $s = 2$  (see Chapter 4 and following), implies that the dispersion relation of a qw with a two-dimensional coin system is of the form  $\pm\omega(\mathbf{k})$ . In particular, this are interpretable as the particle and antiparticle branches of the dispersion relation.

### 3.2.2 Differential equations and the continuum limit

The study of Markov processes produced particularly interesting results in the investigation of quantum dynamical systems, for example leading to generalized Schrödinger equations in the form of Fokker–Planck (the reader may refer e.g. to Ref. [134]). Abelian-

ity in the context qws allows one to study the evolution of the eigenstates in the continuum limit and also define differential equations.

Let us introduce the interpolating effective Hamiltonian  $H_I(\mathbf{k})$  through the relation

$$\exp(-iH_I(\mathbf{k})) := A_{\mathbf{k}}.$$

$H_I(\mathbf{k})$  generates a discrete-time unitary evolution interpolating through a continuous time  $t$  as

$$\exp(-iH_I(\mathbf{k})t) |\psi(\mathbf{k}, 0)\rangle = |\psi(\mathbf{k}, t)\rangle.$$

Then we can write a Schrödinger-like differential equation

$$i\partial_t |\psi(\mathbf{k}, t)\rangle = H_I(\mathbf{k}) |\psi(\mathbf{k}, t)\rangle \quad (35)$$

and expand to the first order in  $\mathbf{k}$ , obtaining

$$i\partial_t |\psi(\mathbf{k}, t)\rangle = [H_I(\mathbf{0}) + \nabla_{\mathbf{k}'} H_I(\mathbf{k}')|_{\mathbf{k}'=\mathbf{0}} \cdot \mathbf{k} + O(|\mathbf{k}|^2)] |\psi(\mathbf{k}, t)\rangle. \quad (36)$$

Now, identifying  $\mathbf{k}$  with the momentum of the system, one can interpret Eq. (36) as a wave-equation in the wave-vector representation. Now, considering narrowband states  $|\psi(\mathbf{k}, t)\rangle$  with  $|\mathbf{k}| \ll 1$  has the meaning that small wave-vectors correspond to small momenta. Then, if one identifies the lattice step with an hypothetical Planck scale, taking the limit of small momenta is equivalent to the relativistic limit for the qw's evolution.

In the case  $s = 2$ , let  $|u(\mathbf{k})\rangle^\pm$  be the positive and negative frequency eigenstates of  $H_I(\mathbf{k})$ , namely such that

$$H_I(\mathbf{k}) |u(\mathbf{k})\rangle^\pm = \pm\omega(\mathbf{k}) |u(\mathbf{k})\rangle^\pm.$$

Then a so-called *(anti)particle state* is defined as

$$|\psi(t)\rangle^\pm = \int_B \frac{d\mathbf{k}}{(2\pi)^{d\mathcal{G}}} \mathcal{G}(\mathbf{k}, t) |\mathbf{k}\rangle \langle u(\mathbf{k})|.$$



Taking the normalized distribution  $g(\mathbf{k}, t)$  smoothly peaked around a given  $\mathbf{k}_0 \in B$ , the evolution given by Eq. (35) leads to a dispersive Schrödinger differential equation for the qw:

$$i\partial_t \tilde{g}(\mathbf{x}, t) = \pm \left[ \mathbf{v} \cdot \nabla + \frac{1}{2} \mathbf{D} \cdot \nabla \nabla \right] \tilde{g}(\mathbf{x}, t), \quad (37)$$

where  $\tilde{g}(\mathbf{x}, t)$  is the Fourier transform of  $e^{-i\mathbf{k}_0 \cdot \mathbf{x} + i\omega(\mathbf{k}_0)t} g(\mathbf{k}, t)$ . Eq. (37) is a Fokker-Planck equation, with drift vector and diffusion matrix given respectively by

$$\mathbf{v} = \nabla_{\mathbf{k}} \omega(\mathbf{k})|_{\mathbf{k}=\mathbf{k}_0}, \quad \mathbf{D} = \nabla_{\mathbf{k}} \nabla_{\mathbf{k}} \omega(\mathbf{k})|_{\mathbf{k}=\mathbf{k}_0}. \quad (38)$$

### 3.3 THE 1D DIRAC QUANTUM WALK

We give here an example of what we discussed in the Subsections 3.2.1 and 3.2.2, presenting the 1D Dirac qw [86, 135, 136]. The evolution operator is defined as

$$A = T_+ \otimes A_+ + T_- \otimes A_- + I \otimes A_e,$$

where

$$T_{\pm} := \sum_{x \in \mathbb{Z}} |x \pm 1\rangle \langle x|$$

are the shifts on the integer lattice and the transition matrices are represented, in the computational basis, as

$$A_+ = \begin{pmatrix} n & 0 \\ 0 & 0 \end{pmatrix}, \quad A_- = \begin{pmatrix} 0 & 0 \\ 0 & n \end{pmatrix},$$

$$A_e = \begin{pmatrix} 0 & im \\ im & 0 \end{pmatrix},$$

for real factors such that  $n^2 + m^2 = 1$ . We notice the presence of the identical transition  $T_e$ , associated with a massive dispersive behaviour around  $k = 0$ . In the Fourier representation, the one-dimensional Dirac qw acts on the coin system as:

$$A_k = \begin{pmatrix} ne^{ik} & im \\ im & ne^{-ik} \end{pmatrix} = n \cos k I_2 + i(n \sin k \sigma_z + m \sigma_x). \quad (39)$$

The spectrum (dispersion relation) of  $A_k$  is

$$\{+\arccos(n \cos k), -\arccos(n \cos k)\}, \quad k \in [-\pi, +\pi].$$

We notice that for small wave-vector  $k \approx 0$  and mass factor  $m \approx 0$ , the dispersion relation behaves as

$$\arccos(\sqrt{1-m^2} \cos k) \approx \sqrt{k^2 + m^2},$$

namely approximates the relativistic Dirac dispersion relation. Defining the interpolating Hamiltonian for (39), in the limit of small masses  $m \approx 0$  and wave-vectors Eq. (36) reads

$$i\partial_t |\psi(\mathbf{k}, t)\rangle = \left(i\sqrt{1-m^2}k\sigma_z + m\sigma_x\right) |\psi(\mathbf{k}, t)\rangle \approx (ik\sigma_z + m\sigma_x) |\psi(\mathbf{k}, t)\rangle,$$

which is the one-dimensional Dirac equation in the momentum representation.

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## DYNAMICS OF FREE QUANTUM FIELDS FROM PRINCIPLES OF INFORMATION PROCESSING

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The informational paradigm evokes the idea to reduce the elements of physical theories to information-theoretical concepts. In this regard, a “good” theory should hinge upon operational notions such as preparations of systems (control by an agent), transformations (events) and measurements (observations). This idea is very intriguing, and QT proved to be a general theory of systems suitable to describe a vast spectrum of other particular theories and models. Within this spirit, we present in this chapter some generally accepted physical principles, translating them into the framework of a network of quantum systems in mutual interaction. The aim of this construction is to provide a rigorous mathematical formalization for free discrete QFTs. The content of this Chapter is an original review and expansion of the framework presented in Refs. [41, ME94, 137].

### 4.1 FREE QUANTUM FIELDS AS QUANTUM WALKERS

The core of the present framework is a set denumerably many quantum system in mutual interaction, defining a network. The evolution of the systems can be seen algorithmically as a discrete-time information processing, transforming the total state defined on the network at discrete steps. The propagation of information is required to be local, namely the speed at which information is allowed to flow is bounded. The algorithm governing the evolution of the quantum network shall act homogeneously

on the system, namely the state of each node is transformed in the same way by the process. Also, the propagation of the information must be uniform: each system must interact in the same way with the systems it is connected to. Finally, the evolution is required to be unitary, as a crucial feature of (quantum) physical processes to conserve probability. The above discussed requirements are ubiquitously assumed for physical laws and in general in the study of physical models, and not only their assumption but also their consequences are very often tacitly accepted.

Such a quantum evolution is described by a QCA theory. In principle, the automaton can evolve fields of any statistics. If the automaton evolution is linear in the fields, then one is considering the so-called *one-particle sector* and the theory described is free (non-interacting). In this case, the QCA reduces to a qw. The evolution is then represented by a unitary operator acting on the Fock space of the system. In the following we expose in detail the principles of the model and their consequences for the mathematical framework.

#### 4.1.1 Principles of the theory

We proceed in a constructive way, building up the space associated to the free field and the operator governing the evolution. Let  $G$  be a denumerably infinite set, where to each  $g \in G$  is assigned a finite-dimensional Hilbert space  $\mathcal{H}_g \cong \mathbb{C}^{s_g}$  for  $s_g$  integer. Each site  $g$  is in mutual interaction with a set of neighbours, denoted by  $N_g$ . We denote the set of edges defining the connectivity of the network at site  $g$  as  $S_g$ , with  $h \in S_g$  if there exists  $g' \in N_g$  such that  $(g, g')$  is a directed edge of the network, namely  $g$  interacts with  $g'$ . If this is the case, we formally write  $g' = gh$ . A path  $\sigma$  on the network can be then written as a strings of letters

$$\sigma = gh_1 \cdots h_m \quad g \in G, h_1 \in S_g, \dots, h_m \in S_{gh_1 \cdots h_{m-1}},$$

where the alphabets are the set of edges defining the neighbourhood scheme at each step.

The state  $\psi_g$  of the system on the site  $g$  has the following formal structure as a column vector:

$$\psi_g = \begin{pmatrix} \psi_{g,1} \\ \psi_{g,2} \\ \vdots \\ \psi_{g,s_g} \end{pmatrix}.$$

In the linear sector, the one time-step of the discrete evolution of a state is given by

$$\psi_g(t+1) = \sum_{g' \in N_g} A_{gg'} \psi_{g'}(t), \quad (40)$$

where the transition matrices  $A_{gg'}$  are  $s_g \times s_{g'}$  matrices. In the following, we will state the principles assumed for the evolution of the state of this quantum network. We will describe the principles in full generality, each in a completely independent way from another, afterwards combining them to finally draw the implications.

**Reciprocity.** The evolution is symmetric for the sites, meaning that if site  $g$  interacts with sites  $g'$ , then also  $g'$  interacts with  $g$ . Mathematically speaking, one has

$$A_{gg'} \neq 0 \iff A_{g'g} \neq 0 \quad \forall g, g' \in G. \quad (41)$$

This implies that if  $g' \in N_g$  then also  $g \in N_{g'}$ . This also allows to formally pose

$$g' = gh \iff g = g'h^{-1} \quad \forall h \in S_g.$$

**Locality.** Assuming a local evolution means to bound the cardinality of each set of first-neighbours  $N_g$  to finite quantities, namely

$$|N_g| < \infty \quad \forall g \in G.$$

The state of the system on site  $g$  thus depends only on the state on a finite number of other sites and the information processing is locally well under control.

**Homogeneity.** A homogeneous evolution can be informally phrased as the universality of the physical law from the point of view of the network nodes: evolution must

not allow to discriminate among two sites without using a third one as a reference. Technically speaking, this has the following three main implications:

1. The dimension  $s_g$  is independent from the site  $g \in G$ , and then there exists an integer  $s$  such that

$$\mathcal{H}_g \cong \mathbb{C}^s \quad \forall g \in G.$$

2. The cardinality  $|N_g|$  is independent on the site  $g \in G$ : this means that we can identify each  $S_g$  with a set  $S$ .
3. A path  $h_1 h_2 \cdots h_m$  of edges  $h_1, h_2, \dots, h_m \in S$  which is closed starting from a site  $g$  must be closed starting from any other site.
4. The set of transition matrices  $\{A_{gg'}\}_{g' \in N_g}$  is the same for every site  $g \in G$ .

**Remark 4.1.** Notice that our notion of homogeneity implies that the graph of the interactions itself is not represented by a state in the theory, since it encodes the evolution: the graph has the status of physical law and does not undergo dynamical changes. In other words, in order to describe general relativistic scenarios one would need either to find some homogeneous effects recovering Einstein's equations or to resort to some additional structure. However, we do not offer a treatment apt to recover GR in the present work.

**Isotropy.** An isotropic evolution can be intuitively stated as the universality of the physical law from the point of view of the network edges: evolution must not allow to discriminate among a minimal number of directions in one step. The minimality of these (in general more than one) sets  $S'_g \subseteq S_g$  of directions depends on the symmetries of the network, as explained in the following. This can be mathematically translated considering for  $g \in G$  some groups  $L_g$  of automorphisms of the graph of the interactions, along with some  $\Lambda_{gg'}$  groups of permutations of the elements of a subset  $S'_{g'} \subseteq S_{g'}$  depending on  $g$ , such that for  $l_g \in L_g$  one has

$$\exists \Lambda_{gg'} : l_g(g'h) = l_g(g')\lambda_{gg'}(h) \quad \lambda_g^{g'} \in \Lambda_{gg'}.$$

The qw is *isotropic on (a system)  $g \in G$*  with respect to a given subset  $S'_g \subseteq S_g$  requiring that:

1. There exists a group  $L_g$  (called the *isotropy group*) of automorphisms of the graph of the interactions whose action on  $g$  and  $gh$  is defined by

$$(g, gh) \mapsto (l_g(g), l_g(gh)) := (g, g\lambda_{gg}(h)), \quad (42)$$

where  $l_g \in L_g$  and  $h \in S_g$ . In addition, the action of  $\Lambda_{gg}$  is required to be transitive on  $S'_g$ .

2. We require that the transition matrices  $\{A_{gg'}\}_{g' \in N_g}$  are equivalent modulo some suitable unitary transformations on the left and on the right. The evolution operator of the walk is covariant under the action of  $L_{g'}$ , and there exist two unitary representations of  $L_g$ ,  $U$  over  $\mathbb{C}^{S_g}$  and  $V$  over  $\mathbb{C}^{S'_g}$ , such that

$$A_{g,l_g(gh)} = U_{l_g} A_{g,gh} V_{l_g}^\dagger \quad \forall l_g \in L_g, \forall h \in S_g. \tag{43}$$

#### 4.1.2 Consequences of the principles

The graphs of the interactions turns out to be defined as a Cayley graph of a group. Indeed, let us take a graph  $\Gamma$  satisfying our principles of reciprocity and homogeneity, and show that we can construct a group having  $\Gamma$  as a Cayley graph. First, let us choose an arbitrary element in the set of vertices  $G$  as the identity element  $e \in G$ . All the other  $g \in G$  can be reached by sequential composition of elements in  $S$ : the set  $G$  is closed under this operation, which can be applied to any element since each neighbourhood scheme is defined by the same set  $S$ ; moreover, it is associative by definition and there is a one-to-one correspondence between each string  $g = h_1 \cdots h_m$  and the element defined as

$$g^{-1} := h_m^{-1} \cdots h_1^{-1} \in G,$$

playing the role of the inverse of  $g$ . We have thus shown that  $G$ , endowed with the composition rule given by the connectivity of the graph  $\Gamma$ , satisfies the group axioms and is in fact a group.

We now show explicitly how to construct the group  $G$ . If there exists more than one string reaching  $g$  and starting from  $e$ , say

$$g = h_{i_1}^{(1)} \cdots h_{i_m}^{(1)} = \dots = h_{i_1}^{(l)} \cdots h_{i_m}^{(l)} = \dots,$$

these will play the role of the relators  $R$  of the group. Since the closed paths are the same starting from every site of the network, this means that we can define, in the free group on  $S$ , the normal closure  $N_R$ , which is represented as the identity in  $G$ . Any other element in  $G$  admits a representation as a decomposition  $fN_R$  for  $f \in F_S$ . By

this argument,  $G$  is built up as the quotient  $F_S/N_R$  and the graph  $\Gamma$  is thus the Cayley graph  $\Gamma(G, S)$ . By locality, the group is finitely generated.

Our notion of homogeneity shall also affect the isotropy requirement. For each  $h \in S$ , we define

$$A_h := A_{gg'} \quad g' = gh, \quad \forall g \in G$$

as the transition matrix associated to the edge  $h$ . By the calculation performed in Section 3.1, the evolution defined in Eq. (40) can be represented as a qw on an arbitrary Cayley graph  $\Gamma(G, S)$  as defined in Definition 3.1. In particular, the evolution operator is given by

$$A = \sum_{h \in S} T_h \otimes A_h,$$

where  $T$  is the right-regular representation of  $G$  on  $\ell^2(G)$ .

To respect homogeneity, we finally require that there exists a unique group  $\Lambda$  of permutations of the elements of  $S$  such that  $\forall g, g' \in G$  one has  $\Lambda_{gg'} \cong \Lambda$ . Accordingly, by Eq. (42), there exists a unique isotropy group  $L$  such that  $L \cong L_g$  for every  $g \in G$ . This amounts to demanding that the walk is *isotropic* (on all the systems  $g \in G$ ) with respect to some subsets  $S' \subseteq S$ . Moreover, the two representations of the isotropy group in Eq. (43) shall coincide. We now give a characterization result for the isotropy group  $L$ .

**Lemma 4.1** ([ME94]). *Let  $L$  be a group of automorphisms of a Cayley graph  $\Gamma(G, S_+)$  such that there exists a group  $\Lambda$  of permutation of the elements of  $S$  and whose action is defined as*

$$l(g'h) = l(g')\lambda(h), \quad \forall g' \in G \quad \forall h \in S, \lambda \in \Lambda,$$

and  $l(e) = e$ . Then  $L$  is a finite subgroup of  $\text{Aut}(G)$ .

*Proof.* Consider the action of an arbitrary element  $l \in L$  on the graph vertices. Since the graph automorphisms preserve the edges, by hypothesis we have

$$l(h) = l(eh) = l(e)\lambda(h) = e\lambda(h) = \lambda(h), \quad \forall h \in S. \quad (44)$$

Moreover

$$l(hh') = l(h)\lambda(h') \equiv l(h)l(h') \quad \forall h, h' \in S.$$



Iterating, in general we obtain

$$l(h_1 \cdots h_p) = l(h_1) \cdots l(h_p), \quad \forall h_1, \dots, h_p \in S, \tag{45}$$

and, being  $S$  a set of generators for  $G$ , this amounts to

$$l(gg') = l(g)l(g') \quad \forall g, g' \in G.$$

Accordingly,  $L$  is a group automorphism of  $G$ . By Eq. (44),  $L$  is isomorphic to  $\Lambda$ , hence  $L$  is finite. ■

The isotropy group must be transitive on some subsets  $S' \subseteq S$ : we now dermine the minimal choice for the sets  $S'$ . By reciprocity,  $S$  can be partitioned into two arbitrary sets  $S_+$  and  $S_-$ , where  $S_-$  contains the inverses of the elements in  $S_+$ . Furthermore, we can subdivide  $S_{\pm}$  into sets

$$S_{\pm}^n := \{h \in S_{\pm} \mid h \text{ has order } n\}.$$

Accordingly, one has the two partitions

$$S_{\pm} = \bigcup_{n=1}^{+\infty} S_{\pm}^n, \quad S = S_+ \cup S_-$$

provided that a numerable number of sets  $S_{\pm}^n$  is empty, since the group  $G$  is finitely generated. By Lemma 4.1,  $L \leq \text{Aut}(G)$ : automorphisms  $l \in L$  must preserve the order of the elements in  $S$  and, since the partitions  $S_{\pm}^n$  are arbitrary, the minimal requirement is to impose that the isotropy group is transitive on each  $S_{\pm}^n$ , meaning that any direction is equivalent compatibly with the group structure.

**Remark 4.2.** *Given a partition  $S^n = S_+^n \cup S_-^n$  for some  $n \in \mathbb{N}_+$ , then  $L$  is either transitive on  $S_{\pm}^n$  separately or on the whole  $S^n$ . Furthermore, two transition matrices associated to different generators must be distinct, otherwise the associated neighbouring sites are dynamically indistinguishable. Therefore one has to demand the following condition:*

$$[U_l, A_h] \neq 0 \quad \forall h \in S, \forall l \in L : l(h) \neq h. \tag{46}$$

In particular, the representation must be faithful, otherwise it will have a nontrivial kernel and condition (46) cannot be satisfied.

Finally, the above discussion means that there exists a unitary faithful representation  $U$  over  $\mathbb{C}^s$  of the isotropy group  $L$  such that one has the covariance condition

$$A = \sum_{h \in S} T_h \otimes A_h = \sum_{h \in S} T_{l(h)} \otimes U_l A_h U_l^\dagger \quad \forall l \in L. \quad (47)$$

**Remark 4.3.** We observe that one can always choose  $U_l \in \mathbf{SU}(2)$  for every  $l \in L$ , since the covariance condition (47) is not sensitive to this choice. Moreover, in Ref. [86] it is shown that one can classify isotropic walks imposing the condition

$$\sum_{h \in S} A_h = I_s \quad (48)$$

and then multiplying the transition matrices by a unitary commuting with the isotropy group.

## 4.2 THE WEYL QUANTUM WALKS

We here introduce the so-called three-dimensional Weyl qws, which recover the Weyl equations in the limit of small wave-vectors. The Weyl qws has been originally presented in the seminal Ref. [70], where it is pointed out that its transition matrices are a particular solution for the unitarity conditions (30) and (31) on the body-centered cubic (BCC) lattice. In the same work, the author conjecture the impossibility to solve the unitarity constraints on other three-dimensional lattices.

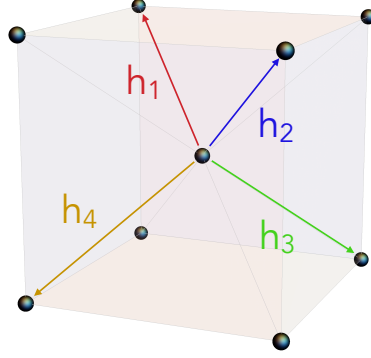


Figure 2: Primitive cell of the body-centered cubic (BCC) lattice, corresponding to the generating set  $S_+ = \{\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \mathbf{h}_4\}$  with the nontrivial relator  $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 + \mathbf{h}_4 = 0$ .

In Figure 2 one can find the neighbourhood scheme associated to the Cayley graphs of  $\mathbb{Z}^3$  on which the Weyl qw are defined. The transition matrices are given by

$$\begin{aligned}
 A_{\mathbf{h}_1} &= \begin{pmatrix} \eta^\pm & 0 \\ \eta^\pm & 0 \end{pmatrix}, & A_{-\mathbf{h}_1} &= \begin{pmatrix} 0 & -\eta^\mp \\ 0 & \eta^\mp \end{pmatrix}, \\
 A_{\mathbf{h}_2} &= \begin{pmatrix} 0 & \eta^\pm \\ 0 & \eta^\pm \end{pmatrix}, & A_{-\mathbf{h}_2} &= \begin{pmatrix} \eta^\mp & 0 \\ -\eta^\mp & 0 \end{pmatrix}, \\
 A_{\mathbf{h}_3} &= \begin{pmatrix} 0 & -\eta^\pm \\ 0 & \eta^\pm \end{pmatrix}, & A_{-\mathbf{h}_3} &= \begin{pmatrix} \eta^\mp & 0 \\ \eta^\mp & 0 \end{pmatrix}, \\
 A_{\mathbf{h}_4} &= \begin{pmatrix} \eta^\pm & 0 \\ -\eta^\pm & 0 \end{pmatrix}, & A_{-\mathbf{h}_4} &= \begin{pmatrix} 0 & \eta^\mp \\ 0 & \eta^\mp \end{pmatrix},
 \end{aligned} \tag{49}$$

where  $\eta^\pm = \frac{1 \pm i}{4}$  and  $S_+ = \{\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \mathbf{h}_4\}$  with the nontrivial relator  $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 + \mathbf{h}_4 = 0$ . In the Fourier representation, the qw evolution operator  $A_{\mathbf{k}}$  reads

$$A_{\mathbf{k}}^\pm = \sum_{\mathbf{h} \in S} e^{i\mathbf{k} \cdot \mathbf{h}} A_{\mathbf{h}}.$$

Defining

$$\mathbf{h}_x := \frac{\mathbf{h}_1 + \mathbf{h}_2}{2}, \quad \mathbf{h}_y := \frac{\mathbf{h}_1 + \mathbf{h}_3}{2}, \quad \mathbf{h}_z := \frac{\mathbf{h}_1 + \mathbf{h}_4}{2},$$

one obtains

$$A_{\mathbf{k}}^{\pm} = d_{\mathbf{k}}^{\pm} I - i \mathbf{a}_{\mathbf{k}}^{\pm} \cdot \boldsymbol{\sigma} \quad (50)$$

with

$$d_{\mathbf{k}}^{\pm} := c_x c_y c_z \pm s_x s_y s_z, \quad (51)$$

$$(a_{\mathbf{k}}^{\pm})_x := s_x c_y c_z \mp c_x s_y s_z, \quad (52)$$

$$(a_{\mathbf{k}}^{\pm})_y := \pm c_x s_y c_z + s_x c_y s_z, \quad (53)$$

$$(a_{\mathbf{k}}^{\pm})_z := c_x c_y s_z \mp s_x s_y c_z, \quad (54)$$

having posed  $c_i, s_i := \cos \frac{k_i}{\sqrt{3}}, \sin \frac{k_i}{\sqrt{3}}$ . Following the method of the interpolating Hamiltonian exposed in Chapter 3, one obtains the differential equation

$$i \partial_t \psi(\mathbf{k}, t) = \left( \frac{1}{\sqrt{3}} \boldsymbol{\alpha}^{\pm} \cdot \mathbf{k} \right) \psi(\mathbf{k}, t) \quad (55)$$

for narrowband states  $\psi(\mathbf{k}, t)$ , where  $\alpha_x^{\pm} = \sigma_x, \alpha_y^{\pm} = \pm \sigma_y, \alpha_z^{\pm} = \sigma_z$ . Eqs. (55) are three-dimensional Weyl equations upon a rescaling of a factor  $\frac{1}{\sqrt{3}}$  for the momentum.

#### 4.3 THE DIRAC QUANTUM WALK

Finding a solution of the unitarity conditions (31) for  $s = 4$  and for arbitrary graphs is in general a hard computational problem. One can use the Weyl qws as building blocks to construct walks with coin system of dimension  $s > 2$ . In particular, two Weyl walks can be coupled: it turns out [86] that there exists a unique way to do it preserving locality and unitarity. The only possible walk of this sort is given by

$$D_{\mathbf{k}} = \begin{pmatrix} nW_{\mathbf{k}} & imI \\ imI & nW_{\mathbf{k}}^{\dagger} \end{pmatrix},$$

where  $n, m \in \mathbb{R}$  such that  $n^2 + m^2 = 1$  and  $W_{\mathbf{k}}$  is the Weyl qw with the plus sign given in Eq. (50). The Dirac qw can be written as

$$D_{\mathbf{k}} = nd_{\mathbf{k}} I - i \gamma^0 (n \mathbf{a}_{\mathbf{k}} \cdot \boldsymbol{\gamma} - mI),$$

where the coefficients  $d_{\mathbf{k}}, \mathbf{a}_{\mathbf{k}}$  are those defined in Eq. (51) for the Weyl qw. The differential equation for narrowband states is

$$i\partial_t\psi(\mathbf{k}, t) = \gamma^0 \left( \frac{n}{\sqrt{3}}\boldsymbol{\gamma} \cdot \mathbf{k} + mI \right) \psi(\mathbf{k}, t),$$

which, in the limit of small masses  $n \simeq 1$ , reads

$$i\gamma^0\partial_t\psi(\mathbf{k}, t) = \left( \frac{1}{\sqrt{3}}\boldsymbol{\gamma} \cdot \mathbf{k} + mI \right) \psi(\mathbf{k}, t). \quad (56)$$

Eq. (56) is the Dirac equation with a rescaling of a factor  $\frac{1}{\sqrt{3}}$  for the momentum.



Part II

COARSE-GRAINING AND STRUCTURE RESULTS





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## COARSE-GRAINING OF QUANTUM WALKS ON CAYLEY GRAPHS

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In Chapters 2 and 3 we have shown how Abelianity for qws allows one to conveniently represent them in the Fourier domain. We developed a rigorous mathematical formalization based on Proposition 2.1, which implies that the finite-dimensional irreps of an Abelian group over  $\mathbb{C}$  are one-dimensional. As a consequence, whenever a qw is defined on the Cayley graph of an Abelian group, one can resort to the decomposition of the (right-regular representation of the) translations  $T_{h_i}$  into the one-dimensional unitary irreps, whose form is a phase factor  $e^{ik_i}$ . One can thus interpret the factor  $k_i$ , which labels the irreps, as the momentum of the walk, and then extract kinematical information from the spectrum of evolution operator. Moreover, adopting the method of the interpolating Hamiltonian, one can also perform an analysis of the dynamics of the qw, deriving a differential equation in the Fourier space and thus passing to the continuum limit.

However, the abovementioned procedure is not admitted in non-Abelian cases, since the irreps are in general of dimension greater than one. This is one of the main reasons why it is standard in the literature to focus qws defined on lattices, namely graphs of Abelian groups embedded in Euclidean spaces. There exist very few cases where non-Abelian qws have been considered, e.g. in Refs. [93, 112], and yet a procedure to study their kinematics and dynamics were still lacking.

In Refs. [ME95, ME96], the authors developed a unitary tiling procedure, which applies in general to any qw on a Cayley graph of a group  $G$ , in order to represent

the walk on an arbitrary subgroup  $H \leq G$ . This is done by partitioning  $G$  into cosets of  $H$  and enlarging the dimension of the original coin system in such a way that the translational information of  $G$  is encoded in the new coin-system. Specializing this procedure to the case of virtually Abelian groups, one realizes that, for every virtually Abelian qw, there exists an Abelian walk which is unitarily equivalent. We shall now revisit the tiling procedure in a detailed way, and then show how one can use it in order to represent a virtually Abelian qw in the Fourier space. This analysis will be generalized further in Chapters 8 and 9, also providing a general method to construct virtually Abelian groups and qws on them.

### 5.1 TILING OF QWS ON GROUPS

Consider an arbitrary qw on the Cayley graph of a group  $G$ . Our aim is to define a coarse-graining for the qw exploiting a subgroup  $H \leq G$ . To do so, we shall define a tiling procedure resorting to a coset partition of  $G$  with respect to a proper subgroup  $H$ —namely  $H \notin \{\{e\}, G\}$ , otherwise the coarse-graining either is trivial or completely loses all the information about the walk. Accordingly, in the present section we will restrict to the study of quantum walks on Cayley graphs of groups  $G$  with a proper subgroup  $H$ . Groups having no proper subgroups are characterized by the following results.

**Theorem 5.1** (Lagrange [138]). *Let  $G$  be a finite group and  $H \leq G$ . Then  $|H|$  divides  $|G|$ .*

**Lemma 5.1.** *Let  $G$  be group without proper subgroups. Then  $G$  is cyclic of prime order.*

*Proof.* Suppose that  $G$  has no proper subgroup, namely the only subgroups in  $G$  are the trivial one  $\{e\}$  and  $G$  itself. Take an arbitrary element  $g \in G$  and consider the subgroup  $H = \langle g \rangle$  generated by  $g$ . By definition, the subgroup  $H$  is cyclic and by hypothesis coincides either with  $\{e\}$  (this is the case if  $g = e$ ) or with  $G$ . In either case,  $G$  is cyclic. Furthermore,  $G$  must be finite, since if it was infinite cyclic this would contradict the hypothesis. Then by Theorem 5.1 it must be  $|G| = p$  with  $p = 1$  or  $p$  a prime number. ■

By Lemma 5.1, the tiling procedure we are going to define excludes the case of cyclic groups of prime order. However, our general case of interest throughout the present work is that of finitely generated and *infinite* groups. Accordingly we can safely neglect this case. Nevertheless, for the sake of completeness we remark that we shall treat this

special instance in the context of qws on Cayley graphs of arbitrary finite cyclic groups with a one-dimensional coin system in Chapter 6.

The core idea stems from the existence of a nontrivial partition of  $G$  into cosets of an arbitrary subgroup  $H$ , denoting the cosets by a set of labels whose cardinality can be in principle either finite or infinite. In the following we will consider right cosets without loss of generality. Since the cosets are disjoint objects, each elements of  $G$  is univocally assigned to one and only one coset. This also defines a partition of the vertices of the Cayley graph of  $G$ , which are thus grouped into clusters whose cardinality precisely amounts to  $|G/H|$ . In this way a tessellation of the Cayley graph is induced, where each tile contains one vertex from each coset.

We now provide a formal definition of this intuitive notion of “regular tiling of a Cayley graph”  $\Gamma(G, S_+)$ . Firstly we shall need to define the translations on the coarse-grained graph. Denoting the coset representatives of  $H$  in  $G$  by  $c_j$  (with  $j = 1, \dots, l$  and  $c_1 \in H$ ), then for every  $x \in H$ ,  $h_i \in S_+$  and  $j \in G/H$

$$\exists x' \in H, \tau(i, j) \in G/H : xc_j h_i^{-1} = x' c_{\tau(i, j)} \quad (57)$$

by definition of quotient set. Intuitively, relation (57) states how the generators  $h_i \in S_+$  of  $G$  “translates along the cosets” of  $H$ .

**Definition 5.1** (Regular tiling of a Cayley graph). *Let  $G$  be a group with a proper subgroup  $H$  of arbitrary index  $l$  and let  $\Gamma(G, S_+)$  be a Cayley graph of  $G$ . We call a regular tiling  $\mathcal{C}$  of  $\Gamma$  with respect to  $H$  a choice of representatives  $c_j \in G$  for the following right-coset partition of  $G$ :*

$$\bigcup_{j=1}^l Hc_j = G.$$

*In addition, we say that  $\mathcal{C}$  has order  $l$  and generating set:*

$$\tilde{S}_+ := \{c_{\tau(i, j)} h_i c_j^{-1} \mid h_i \in S_+, j \in G/H\}. \quad (58)$$

Notice that the coarse-grained generators  $\tilde{h}_i \in \tilde{S}_+$  belongs to the subgroup  $H$  by Eq. (57). In the following proposition, we prove that, if  $S_+$  is a generating set for  $G$ , then also the set  $\tilde{S}_+$  is a generating set for  $H$ .

**Proposition 5.1.** *Let  $G$  be a group,  $S_+$  a generating set for  $G$  and  $H$  a subgroup of  $G$ . Given a regular tiling  $\mathcal{C}$  of the Cayley graph  $\Gamma(G, S_+)$ , then  $\tilde{S}_+ = \{c_{\tau(i,j)}h_i c_j^{-1} \mid h_i \in S_+, j \in G/H\}$  is a generating set for  $H$ .*

*Proof.* For every arbitrary generator  $\tilde{h} \in S_H$  of  $H$ , by definition there exist  $h_{i_1}, h_{i_2}, \dots, h_{i_n} \in S \equiv S_+ \cup S_-$  such that

$$\tilde{h} = h_{i_1} h_{i_2} \cdots h_{i_n}.$$

By composition of the elements of  $\tilde{S}_+$  we can now recursively construct the element

$$c_{\tau(i_1, \tau(\tau(\dots)))} \tilde{h} c_1^{-1} = c_{\tau(i_1), \tau(\tau(\dots))} h_{i_1} \cdots h_{i_{n-1}} c_{\tau(i_{n,1})}^{-1} c_{\tau(i_{n,1})} h_{i_n} c_1^{-1},$$

which is contained in  $H$  by construction (since  $c_{\tau(m,j)} h_m c_j^{-1} \in H$  for every  $j \in G/N$ ). Moreover, since  $c_1 \in H$ , it must also be  $c_{\tau(i_1, \tau(\tau(\dots)))} \in H$ , meaning that  $\tau(i_1, \tau(\tau(\dots))) = 1$ . We thus constructed  $c_1 \tilde{h} c_1^{-1}$  for every generator  $\tilde{h} \in S_H$  using the elements of  $\tilde{S}_+$ . Hence the thesis follows noticing that, on the other hand, the set  $\{c_1 \tilde{h} c_1^{-1}\}_{\tilde{h} \in S_H}$  generates the whole group  $H$ . ■

Proposition 5.1 guarantees that Definition 5.1 of a regular tiling of a Cayley graphs is well-posed. Notice that, given a Cayley graph  $\Gamma(G, S_+)$  and a subgroup  $H \leq G$ , there exists in general more than one regular tiling of  $\Gamma$  with respect to  $H$ : the choice of the coset representatives is not unique. Nevertheless, for every regular tiling  $\mathcal{C}$  we can now provide the right-regular representation  $T$  on  $\ell^2(G)$  in terms of the right-regular representation  $\tilde{T}$  on  $\ell^2(H)$ . We first define

$$\tilde{h}_{ij} := c_{\tau(i,j)} h_i c_j^{-1} \quad h_i \in S_+, c_j \in G/H.$$

We can then define the coarse-graining map from  $\ell^2(G)$  to  $\ell^2(H) \otimes \mathbf{C}^l$  as follows

$$\begin{aligned} U_{\mathcal{C}} : \ell^2(G) &\longrightarrow \ell^2(H) \otimes \mathbf{C}^l, \\ |xc_j\rangle &\longmapsto |x\rangle |j\rangle. \end{aligned}$$

$U_{\mathcal{C}}$  is unitary by definition, since the decomposition of each  $g \in G$  as an element  $x_g c_{j_g}$  of  $G/H$  is unique. We are now ready to explicitly calculate the coarse-grained generators

$$\mathcal{C}[T_h] := U_{\mathcal{C}} T_h U_{\mathcal{C}}^\dagger \quad h \in S_+.$$

We obtain

$$\begin{aligned}
 \mathcal{C}[T_h] &= \sum_{x \in H} \sum_{j \in G/H} U_{\mathcal{C}} \left| xc_j h^{-1} \right\rangle \left\langle xc_j \right| U_{\mathcal{C}}^\dagger = \\
 &= \sum_{x \in H} \sum_{j \in G/H} U_{\mathcal{C}} \left| x \left( c_{\tau(h,j)} h c_j^{-1} \right)^{-1} c_{\tau(h,j)} \right\rangle \left\langle xc_j \right| U_{\mathcal{C}}^\dagger = \\
 &= \sum_{x \in H} \sum_{j \in G/H} \left| x \left( c_{\tau(h,j)} h c_j^{-1} \right)^{-1} \right\rangle \left\langle x \right| \otimes |\tau(h,j)\rangle \langle j| = \\
 &= \sum_{j \in G/H} \tilde{T}_{\tilde{h}_{h,j}} \otimes |\tau(h,j)\rangle \langle j|.
 \end{aligned} \tag{59}$$

Correspondingly, given a qw on  $\Gamma(G, S_+)$

$$A := \sum_{h \in S} T_h \otimes A_h, \quad (A : \ell^2(G) \otimes \mathbb{C}^s \rightarrow \ell^2(G) \otimes \mathbb{C}^s),$$

one can find an equivalent walk in terms of the generators of  $H$ , designating the coset labels as additional internal degrees of freedom. With a slight abuse of notation, we denote also  $\mathcal{C}[A] = (U_{\mathcal{C}} \otimes I_s) A (U_{\mathcal{C}} \otimes I_s)^\dagger$ , reading

$$\begin{aligned}
 \mathcal{C}[A] &= \sum_{h \in S} \sum_{j \in G/H} \tilde{T}_{\tilde{h}_{h,j}} \otimes |\tau(h,j)\rangle \langle j| \otimes A_h = \\
 &= \sum_{\tilde{h} \in \tilde{S}} \tilde{T}_{\tilde{h}} \otimes \left( \sum_{h,j: \tilde{h}_{h,j} = \tilde{h}} |\tau(h,j)\rangle \langle j| \otimes A_h \right) =: \\
 &=: \sum_{\tilde{h} \in \tilde{S}} \tilde{T}_{\tilde{h}} \otimes A_{\tilde{h}},
 \end{aligned} \tag{60}$$

where  $\tilde{S} = \tilde{S}_+ \cup \tilde{S}_-$  with  $\tilde{S}_+$  defined in Definition 5.1.

**Remark 5.1.** In Proposition 5.1 we proved that the set  $\tilde{S} = \{c_{\tau(i,j)} h_i c_j^{-1} \mid h_i \in S, j \in G/H\}$  is a set of generators for  $H$ . The transition matrices of  $\mathcal{C}[A]$  are denoted by  $A_{\tilde{h}}$ , for fixed  $\tilde{h} = c_{\tau(h,j)} h c_j^{-1}$ . We notice that, in general, the map  $\tau$  is not an injective function from  $S \times G/H$  to  $\tilde{S}$ , and so is not the mapping  $(h, j) \mapsto \tilde{h}_{h,j}$ .

The coarse-grained walk  $\mathcal{C}[A]$  is a qw on the Cayley graph  $\Gamma(H, \tilde{S})$  defined on  $\ell^2(H) \times \mathbb{C}^{s \cdot l}$ . Correspondingly, the coin system is enlarged to dimension  $s \cdot l$ , according to the cardinality of  $G/H$ . Clearly, our case of interest shall be for  $l < \infty$ . The coarse-graining procedure groups the sites of  $\Gamma(G, S_+)$  in tiles tessellating the graph and

whose elements are in a bijective correspondence with the elements of  $G/H$ . While the elements of the tiles becomes extra degrees of freedom for the coarse-grained walk, the tiles are in a bijective correspondence with the elements of  $H$  and can be regarded as the nodes of the new, coarse-grained graph  $\Gamma(H, \tilde{S}_+)$ . We have thus proved the following result.

**Proposition 5.2.** *Let  $P$  a group property,  $G$  a group and  $H \leq G$  satisfying  $P$ . A virtually  $P$  QW on a Cayley graph  $\Gamma(G, S_+)$  is equivalent to a  $P$  QW on  $\Gamma(H, \tilde{S}_+)$ .*

**Corollary 5.1.** *A QW on the Cayley graph of a finite group is equivalent to a QW on a point.*

**Remark 5.2.** *One could ask whether the opposite of Proposition 5.2 is also true. In Chapter 6 we will give a (negative) answer to this question, presenting a counterexample.*

**Remark 5.3.** *Notice that any two coarse-grainings of a QW corresponding to two different regular tilings are unitarily equivalent. Let  $\mathcal{C}_1, \mathcal{C}_2$  be two regular tilings of a Cayley graph  $\Gamma(G, S_+)$  with respect to the subgroups  $H_1, H_2 \leq G$ , respectively. Then, for a QW  $A$  on  $\Gamma(G, S_+)$ , the relation*

$$\mathcal{C}_2[A] = \left( U_{\mathcal{C}_2} U_{\mathcal{C}_1}^\dagger \otimes I \right) \mathcal{C}_1[A] \left( U_{\mathcal{C}_2} U_{\mathcal{C}_1}^\dagger \otimes I \right)^\dagger$$

holds. The operator  $U_{\mathcal{C}_2} U_{\mathcal{C}_1}^\dagger$  reads

$$\begin{aligned} U_{\mathcal{C}_2} U_{\mathcal{C}_1}^\dagger &= \sum_{x_2 \in H_2} \sum_{j_2 \in G/H_2} \sum_{x_1 \in H_1} \sum_{j_1 \in G/H_1} |x_2\rangle |j_2\rangle \langle x_2 c_{j_2}^{(2)} | x_1 c_{j_1}^{(1)} \rangle \langle x_1 | \langle j_1 | = \\ &= \sum_{\substack{(j_1, j_2) : \\ G/H_1 \cap G/H_2 \neq \{\emptyset\}}} \left( \sum_{x_1 \in H_1} \left| x_1 \left( c_{j_2}^{(2)} c_{j_1}^{(1)-1} \right)^{-1} \right\rangle \langle x_1 \right) \otimes |j_2\rangle \langle j_1| = \\ &= \sum_{\substack{(j_1, j_2) : \\ G/H_1 \cap G/H_2 \neq \{\emptyset\}}} \tilde{T}_{c_{j_2}^{(2)} c_{j_1}^{(1)-1}} \otimes |j_2\rangle \langle j_1|. \end{aligned} \quad (61)$$

In Chapter 8 we shall specialize the above analysis to the case where the quotient  $G/H$  is a group, namely  $H$  is normal in  $G$ , while in Section 5.2 we are going to show an application of the general procedure to case of virtually Abelian QWs.

## 5.2 FOURIER REPRESENTATION OF VIRTUALLY ABELIAN QWS

Consider an infinite virtually Abelian group  $G$ . The analysis conducted in Chapter 2 shows that  $G$  contains a subgroup  $H \cong \mathbb{Z}^d$ , with  $d > 1$ , of finite index  $l$ . Then, for every Cayley graph  $\Gamma(G, S_+)$ , we can choose an arbitrary regular tiling  $\mathcal{C}$  with respect to  $H$ . We now show how a virtually Abelian qw  $A$  on  $\Gamma(G, S_+)$  with a  $s$ -dimensional coin can be regarded as an Abelian qw on  $\Gamma(H, \tilde{S}_+)$  with  $(s \cdot l)$ -dimensional coin. This shall allow to diagonalize  $A$  on  $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^{s \cdot l}$  via its representation in the Fourier domain.

As done in Chapter 3, in the following we will write the elements of  $H$  as  $d$ -dimensional vectors and we will adopt the additive notation for the composition in  $H$ , keeping the multiplicative notation for the general group composition in  $G$ . This slightly idiosyncratic notation is necessary to define the Fourier transform on the coarse-grained walk. Thus by  $\mathbf{x}c_j$  for  $\mathbf{x} \in H, c_j \in G$  we will denote the element equal to the left-composition of  $\mathbf{x}$  with  $c_j$  in  $G$ .

As in the previous section, we define the unitary mapping realising the coarse-graining according to the regular tiling  $\mathcal{C}$ :

$$U_c : \ell^2(G) \longrightarrow \ell^2(H) \otimes \mathbb{C}^l, \\ |\mathbf{x}c_j\rangle \longmapsto |\mathbf{x}\rangle|j\rangle.$$

The plane waves on cosets are defined as

$$|\mathbf{k}\rangle_j := \frac{1}{(2\pi)^{d/2}} \sum_{\mathbf{x} \in H} e^{i\mathbf{k} \cdot \mathbf{x}} |\mathbf{x}c_j\rangle.$$

The action of the coarse-graining operator  $U_c$  on the  $|\mathbf{k}\rangle_j$  decouples the plane waves on  $H$  from the degree of freedom assigned to the cosets as follows

$$U_c |\mathbf{k}\rangle_j = \frac{1}{(2\pi)^{d/2}} \sum_{\mathbf{x} \in H} e^{i\mathbf{k} \cdot \mathbf{x}} U_c |\mathbf{x}c_j\rangle = \frac{1}{(2\pi)^{d/2}} \sum_{\mathbf{x} \in H} e^{i\mathbf{k} \cdot \mathbf{x}} |\mathbf{x}\rangle|j\rangle =: \\ =: |\mathbf{k}\rangle_H |j\rangle.$$

We have that  $\forall h \in S, \forall \mathbf{x} \in H$  and  $\forall j \in G/H$  there exists  $\mathbf{x}' \in H$  and  $\tau(h, j) \in G/H$  such that

$$\mathbf{x}c_j h^{-1} = \mathbf{x}' c_{\tau(h, j)}, \quad \tilde{\mathbf{h}}_{h, j} := \mathbf{x} - \mathbf{x}' = c_{\tau(h, j)} h c_j^{-1} \in H.$$

Thus the action of the translation  $T_h$  for an arbitrary generator  $h \in S$  of  $G$  on the coset plane waves

$$\begin{aligned} T_h |\mathbf{k}\rangle_j &= \frac{1}{(2\pi)^{d/2}} \sum_{\mathbf{x} \in H} e^{i\mathbf{k} \cdot \mathbf{x}} |\mathbf{x}c_j h^{-1}\rangle = \\ &= \frac{1}{(2\pi)^{d/2}} \sum_{\mathbf{x}' \in H} e^{i\mathbf{k} \cdot (\tilde{\mathbf{h}}_{h,j} + \mathbf{x}')} |\mathbf{x}'c_{\tau(h,j)}\rangle = \\ &= e^{i\mathbf{k} \cdot \tilde{\mathbf{h}}_{h,j}} |\mathbf{k}\rangle_{\tau(h,j)}, \end{aligned} \quad (62)$$

is, up to a phase factor, a permutation of the  $|\mathbf{k}\rangle_j$ . Accordingly, from Eq. (62) we obtain

$$\begin{aligned} \mathcal{C}[T_h] |\mathbf{k}\rangle_H |j\rangle &= \mathcal{C}[T_h] U_{\mathcal{C}} |\mathbf{k}\rangle_j = U_H T_h |\mathbf{k}\rangle_j = \\ &= e^{i\mathbf{k} \cdot \tilde{\mathbf{h}}_{h,j}} |\mathbf{k}\rangle_H |\tau(h,j)\rangle. \end{aligned} \quad (63)$$

Eq. (63) shows that  $|\mathbf{k}\rangle_H$  is an invariant space of the coarse-grained generators  $\mathcal{C}[T_h]$ .

This allows to diagonalize the qw  $\sum_{h \in S} T_h \otimes A_h$  on  $\Gamma(G, S_+)$  over the wave-vector space of  $\ell^2(H) \otimes \mathbb{C}^l$  exploiting the additional degrees of freedom. Evaluating the matrix elements for the translations  $\tilde{T}_h$  one gets

$$\langle \mathbf{k}|_H \langle j_1 | \mathcal{C}[T_h] |\mathbf{k}\rangle_H |j_2\rangle = e^{i\mathbf{k} \cdot \tilde{\mathbf{h}}_{h,j}} \delta_{j_1, \tau(h,j_2)} \quad j_1, j_2 = 1, \dots, l.$$

We can finally obtain the wave-vector representation  $\tilde{A}_{\mathbf{k}}$  of the qw on  $\Gamma(H, \tilde{S}_+)$ , which has a block form in terms of the “old” transition matrices  $A_h$ , with the  $j_1 j_2$ -block given by

$$(\tilde{A}_{\mathbf{k}})_{j_1 j_2} = \sum_{h: \tau(h,j_2)=j_1} e^{i\mathbf{k} \cdot \tilde{\mathbf{h}}_{h,j_2}} A_h. \quad (64)$$

We have thus the following corollary of Proposition 5.2.

**Corollary 5.2.** *A virtually Abelian qw on  $\Gamma(G, S_+)$  is equivalent to an Abelian qw.*

**Remark 5.4.** *By Remark 5.3, in the virtually Abelian case two different regular tilings  $\mathcal{C}_1, \mathcal{C}_2$  with respect to two subgroups  $H_1, H_2 \leq G$ , respectively, do not affect the dispersion relation of*



a QW. When  $H_1 = H_2$ , namely when  $\mathcal{C}_1$  and  $\mathcal{C}_2$  can be different just for the choice of the coset representatives, the operator switching between the two coarse-grainings in Eq. (61) becomes

$$\begin{aligned} U_{\mathcal{C}_2} U_{\mathcal{C}_1}^\dagger &= \sum_{j \in G/H} \sum_{x \in H} \left( \left| x \left( c_j^{(2)} c_j^{(1)-1} \right)^{-1} \right\rangle \left\langle x \right| \right) \otimes |j\rangle \langle j| = \\ &= \sum_{j \in G/H} \tilde{T}_{c_j^{(2)} c_j^{(1)-1}} \otimes |j\rangle \langle j|. \end{aligned}$$

Then, since

$$\mathcal{C}_2[A] = \left( U_{\mathcal{C}_2} U_{\mathcal{C}_1}^\dagger \otimes I \right) \mathcal{C}_1[A] \left( U_{\mathcal{C}_2} U_{\mathcal{C}_1}^\dagger \otimes I \right)^\dagger,$$

$\mathcal{C}_2[A]$  is equal to  $\mathcal{C}_1[A]$  up to a translation  $c_{\tau(h,j)}^{(2)} c_{\tau(h,j)}^{(1)-1} c_j^{(1)} c_j^{(2)-1}$  on the generator  $\tilde{\mathbf{h}}_{h,j}^{(1)}$  for each  $j = 1, \dots, l$ .

### 5.3 EXAMPLE OF A MASSLESS VIRTUALLY ABELIAN QW

We now consider the virtually Abelian group quasi-isometric to  $\mathbb{R}^2$ :

$$G = \langle a, b \mid a^2 b^{-2} \rangle,$$

whose corresponding Cayley graph is depicted in Fig. 3. We shall derive the most general isotropic qws

$$A = \sum_{g \in S_+} T_g \otimes A_g$$

on the Cayley graph of  $G$  solving the unitarity constraints on the transition matrices, which are the following:

$$A_i A_{j-1}^\dagger = A_i^\dagger A_{j-1} = 0, \tag{65}$$

$$\begin{aligned} A_i A_j^\dagger + A_{i-1} A_{j-1}^\dagger &= A_i^\dagger A_j + A_{i-1}^\dagger A_{j-1} = \\ &= A_i A_{i-1}^\dagger + A_j A_{j-1}^\dagger = A_i^\dagger A_{i-1} + A_j^\dagger A_{j-1} = 0, \end{aligned} \tag{66}$$

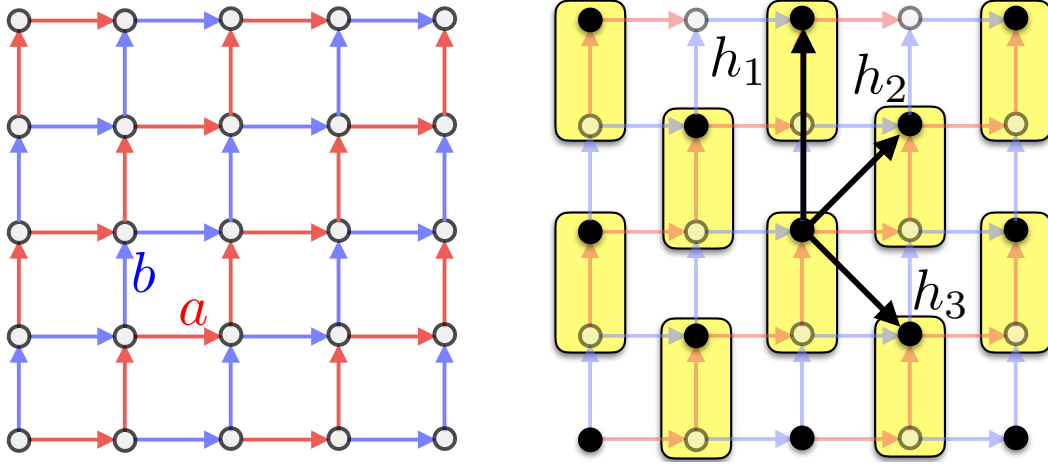


Figure 3: (Left) The Cayley graph of  $G = \langle a, b \mid a^2 b^{-2} \rangle$ . The group is a non-Abelian virtually Abelian group. (Right) A regular tiling of the Cayley graph of  $G$  with commuting generators  $h_1 = ba$  and  $h_2 = a^2$ . The subgroup has index two and we chose  $\{e, a\}$  as a set of coset representatives.

for  $i \neq j \in \{a, b\}$ . The normalization constraint gives

$$\begin{aligned} A_a A_a^\dagger + A_b A_b^\dagger + A_{a^{-1}} A_{a^{-1}}^\dagger + A_{b^{-1}} A_{b^{-1}}^\dagger &= \\ &= A_a^\dagger A_a + A_b^\dagger A_b + A_{a^{-1}}^\dagger A_{a^{-1}} + A_{b^{-1}}^\dagger A_{b^{-1}} = I_s. \end{aligned} \quad (67)$$

From Eqs. (65) it is easy to see that for coin system of dimension  $s = 1$  it is impossible to solve the unitarity conditions. In fact, in Chapter 6 we shall introduce a necessary condition for Cayley graphs to implement qws with a one-dimensional coin system. It is easy to see that the constraints (65) and (66) contains those of the 2D Weyl qw of Ref. [86] up to a swap  $a^{-1} \Leftrightarrow b^{-1}$ , namely those arising from an Abelian simple square lattice. One can then check that the transition matrices are the same of the 2D Weyl qw, divided into two classes, and given by

$$\begin{aligned} A_a^I &= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, & A_b^I &= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \\ A_{a^{-1}}^I &= \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, & A_{b^{-1}}^I &= \frac{1}{2} \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}, \\ A_g^{\text{II}} &= Y (A_g^I)^t Y^\dagger, & Y &= \frac{1}{\sqrt{2}} (I_2 + i\sigma_y), \end{aligned}$$

which are anti-unitarily equivalent.

We choose now the Abelian subgroup  $H \cong \mathbb{Z}^2$  of index 2 generated by  $\mathbf{h}_1 = ba$ ,  $\mathbf{h}_2 = a^2$  and  $\mathbf{h}_3 = a^{-1}b$  and the following regular tiling of  $\Gamma(G, S_+)$

$$G = H \cup Hc, \quad c = a^{-1}.$$

The corresponding presentation of the coarse-grained graph is

$$H = \langle \mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3 \mid \mathbf{h}_1 - (\mathbf{h}_2 - \mathbf{h}_3) \rangle. \quad (68)$$

The wave-vector on the cosets, namely the invariant spaces under the  $T_{\mathbf{h}_i}$  for  $i = 1, 2, 3$ , are given by

$$|\mathbf{k}\rangle_0 := \frac{1}{2\pi} \sum_{\mathbf{x} \in H} e^{-i\mathbf{k} \cdot \mathbf{x}} |\mathbf{x}\rangle, \quad |\mathbf{k}\rangle_1 := \frac{1}{2\pi} \sum_{\mathbf{x} \in H} e^{-i\mathbf{k} \cdot \mathbf{x}} |\mathbf{x}a^{-1}\rangle.$$

Evaluating the action of the generator of  $G$  on the  $|\mathbf{k}\rangle_j$ , one can reconstruct the coarse-grained walk  $\mathcal{C}[A]$ , which will be written in terms of the generators of  $H$  and their inverses. First we evaluate the action of the generators of  $G$  on the coset wave-vectors:

$$\begin{aligned} T_a |\mathbf{k}\rangle_0 &= |\mathbf{k}\rangle_1, & T_a |\mathbf{k}\rangle_1 &= e^{-ik_2} |\mathbf{k}\rangle_0, \\ T_b |\mathbf{k}\rangle_0 &= e^{-ik_3} |\mathbf{k}\rangle_1, & T_b |\mathbf{k}\rangle_1 &= e^{-ik_1} |\mathbf{k}\rangle_0, \\ T_{a^{-1}} |\mathbf{k}\rangle_0 &= e^{ik_2} |\mathbf{k}\rangle_1, & T_{a^{-1}} |\mathbf{k}\rangle_1 &= |\mathbf{k}\rangle_0, \\ T_{b^{-1}} |\mathbf{k}\rangle_0 &= e^{ik_1} |\mathbf{k}\rangle_1, & T_{b^{-1}} |\mathbf{k}\rangle_1 &= e^{ik_3} |\mathbf{k}\rangle_0. \end{aligned}$$

It follows the off-diagonal expression for the coarse-grained walk:

$$\begin{aligned} \mathcal{C}[A]_{\mathbf{k}} &= \begin{pmatrix} 0 & A_{\mathbf{k}} \\ A'_{\mathbf{k}} & 0 \end{pmatrix}, \\ A_{\mathbf{k}} &= e^{-ik_2} A_a + e^{-ik_1} A_b + A_{a^{-1}} + e^{ik_3} A_{b^{-1}}, \\ A'_{\mathbf{k}} &= A_a + e^{-ik_3} A_b + e^{ik_2} A_{a^{-1}} + e^{ik_2} A_{b^{-1}}. \end{aligned} \quad (69)$$

Exploiting the relators in (68), Eqs. (69) become

$$\begin{aligned} A_{\mathbf{k}} &= e^{-i\frac{k_y}{2}} B_{\mathbf{k}}, & A'_{\mathbf{k}} &= e^{i\frac{k_y}{2}} \sigma_z B_{\mathbf{k}} \sigma_z, \\ B_{\mathbf{k}} &:= \left( e^{-i\frac{k_x}{2}} A_a + e^{-i\frac{k_y}{2}} A_b + e^{i\frac{k_y}{2}} A_{a-1} + e^{i\frac{k_x}{2}} A_{b-1} \right), \end{aligned}$$

where  $k_x := k_2 + k_3$  and  $k_y := k_1$ . Defining

$$V := \begin{pmatrix} I & 0 \\ 0 & e^{i\frac{k_y}{2}} \sigma_z \end{pmatrix}, \quad R := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

one has

$$\mathcal{C}[A]_{\mathbf{k}} = V(R \otimes I) (\sigma_z \otimes B_{\mathbf{k}} \sigma_z) (R^\dagger \otimes I) V^\dagger. \quad (70)$$

Accordingly  $\mathcal{C}[A]_{\mathbf{k}}$  is unitarily equivalent to  $\sigma_z \otimes B_{\mathbf{k}} \sigma_z$  whose four eigenvalues  $e^{-i\omega_r^\pm(k_x, k_y)}$  for  $r = 1, 2$  are expressed in terms of the walk dispersion relations

$$\begin{aligned} \omega_1^\pm &:= \pm \arccos \alpha(k_x, k_y) + \pi/2, & \omega_2^\pm &:= \omega_1^\pm + \pi, \\ \alpha(k_x, k_y) &:= \frac{1}{2} \left( \sin \frac{k_x}{2} + \sin \frac{k_y}{2} \right). \end{aligned}$$

We notice that this dispersion relations are equivalent, up to shifts in wave-vectors, to those of the 2D Weyl QW. The dispersion relation close to its minimum (for wave-vectors close to  $(\pi, \pi)$ ) becomes linear in  $\mathbf{k}$ . In this sense, the non-Abelianity of the original graph does not induce relevant effects on the dynamics of the coarse-grained QW.

We conclude analysing the relation between the coarse-graining of the two solutions obtained in this section, namely  $\mathcal{C}[A^I]_{\mathbf{k}}$  and  $\mathcal{C}[A^{II}]_{\mathbf{k}}$ . Through a block diagonal change of basis matrix, we saw that  $\mathcal{C}[A^I]_{\mathbf{k}}$  is unitarily equivalent to  $\sigma_z \otimes B_{\mathbf{k}} \sigma_z$ . Since two solutions  $A^I$  and  $A^{II}$  are connected by a local anti-unitary transformation,  $\mathcal{C}[A^{II}]_{\mathbf{k}}$  is, by linearity, unitarily equivalent to  $\sigma_z \otimes \sigma_z B_{\mathbf{k}}^T$ , which is just  $\mathcal{C}[A^I]_{-\mathbf{k}}^\dagger$  (up to a change of basis). This means that the two coarse-grained QWs are connected by PT symmetry, with parity and time-reversal maps given by  $P : \mathbf{k} \mapsto -\mathbf{k}$  and  $T : A \mapsto A^\dagger$ .

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## ON THE SCALAR QUANTUM WALKS ON CAYLEY GRAPHS

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In Chapter 3 we presented a general framework to treat qws on Cayley graphs of arbitrary groups and with a finite-dimensional coin system. A suitable representation for the evolution operator has been studied, along with a general existence condition based on the unitarity of the evolution (i.e. the unitarity constraints on the transition matrices).

The most elementary case is that of qws with a one-dimensional coin system, which are called *scalar*. In Chapter 5 we developed a method to connect a qw on  $G$  with  $s$ -dimensional coin with an equivalent qw on a subgroup  $H \leq G$  with a  $(s \cdot l)$ -dimensional coin, where  $l$  is the index of  $H$  in  $G$ . A natural question that may arise is: which spinorial qws are derivable from a scalar one? Of course, some restrictions are necessary in order to try to give an at least partial answer.

As we have discussed in Chapter 2, requiring that a group  $G$  is quasi-isometric to  $\mathbb{R}^d$  implies that  $G$  contains a finite-index subgroup  $H \cong \mathbb{Z}^d$ . In the present chapter we shall restrict the analysis to the case of Abelian scalar qws. We will classify them, finding that their evolution is trivial. Our result states that nontrivial scalar qws on Cayley graphs quasi-isometric to  $\mathbb{R}^d$  have to be defined on groups which are virtually  $\mathbb{Z}^d$  but also non Abelian.

We will then classify the scalar non-Abelian qws admitting a coarse graining on  $\mathbb{Z}$  with a two-dimensional coin. In this context, the difficulty is the construction of abstract groups and their Cayley graphs (in principle there are infinitely many of

them for each group). In Chapter 9 we will undertake this investigation starting from the case of index 2 up to space-dimension  $d = 3$  and requiring isotropy.

Scalar qws on  $\mathbb{Z}^d$  have been first studied in Ref. [98], where a no-go theorem has been given in the case of a hypercubic lattice in  $d$  dimensions. Scalar qws on Cayley graphs of arbitrary groups have been explored in Ref. [112]. The authors gave a necessary existence condition for scalar qws on general Cayley graphs, called *quadrangularity* condition, and characterized scalar qws on groups presented with two and three generators. We notice that their definition of qw on a Cayley graph  $\Gamma(G, S_+)$  does not assume that the generating set  $S_+$  is symmetric. This Chapter mainly presents a detailed discussion of Ref. [ME97].

### 6.1 THE QUADRANGULARITY CONDITION

We report and prove a necessary condition for the existence of a scalar qw on an arbitrary Cayley graph Ref. [112].

**Proposition 6.1.** *Let  $\Gamma(G, S_+)$  a Cayley graph and suppose that there exists a scalar qw  $A = \sum_{h \in S_+} z_h T_h$  on  $\Gamma$ . Then*

$$\forall (h_1, h_2) \in S_+ \times S_+ : h_1 \neq h_2 \exists (h_3, h_4) \neq (h_1, h_2) : h_1 h_2^{-1} = h_3 h_4^{-1}. \quad (71)$$

*Proof.* By unitarity of  $A = \sum_{h \in S_+} z_h T_h$ , the conditions in Eqs. (30) and (31) are satisfied. In particular, in this case Eq. (31) reads:

$$\sum_{hh'^{-1}=h''} z_h z_{h'}^* = \sum_{h^{-1}h'=h''} z_h^* z_{h'} = 0, \quad (72)$$

where  $h'' \in \{g \in G \mid g = hh'^{-1} \neq e : h, h' \in S_+\}$  and for  $z_h \neq 0 \forall h \in S_+$ . Now, by contradiction, suppose that there exists a pair  $(h_1, h_2)$  not satisfying the condition in (71). Then by Eq. (72) the relation  $z_{h_1} z_{h_2}^* = 0$  must hold. This is absurd, since it implies either  $z_{h_1} = 0$  or  $z_{h_2} = 0$ . ■

The condition stated in Eq. (71) is called *quadrangularity condition*. If the generating set  $S_+$  is symmetric, the quadrangularity condition is equivalent to the existence, for every nontrivial path of length two on a Cayley graphs, of at least two words on the generating set which realizes it. If  $S_+$  is not symmetric, the paths of length two of

the form  $h_1 h_2$  for  $(h_1, h_2) \in S_+ \times S_-$  must have at least two different realizations. We notice that this condition is not necessary for spinorial walks.

**Remark 6.1.** *We observe that requiring a symmetric generating set  $S_+ \equiv S$  is a stronger condition, and yet it account for the more general case of non-symmetric  $S_+$ , in the following sense. Indeed, the existence of a family of QWS on a Cayley graph with symmetric generating set can admit the existence of a family of monoidal QWS on the same graph, provided that the edges assigned to elements in  $S_-$  are removed from the graph and the corresponding transition matrices are set to zero (if allowed by the unitarity conditions). Vice versa, finding the general family of monoidal QWS on a graph gives no information on the existence of a QW with symmetric generating set on the corresponding graph.*

### 6.2 CLASSIFICATION OF THE ABELIAN SCALAR QWS

We shall now characterize the scalar QWS on Cayley graphs of finitely generated Abelian groups. By the fundamental theorem of finitely generated Abelian groups (Theorem 2.3), every finitely generated and infinite Abelian group  $G$  is of the form  $G \cong \mathbb{Z}_{i_1} \times \dots \times \mathbb{Z}_{i_n} \times \mathbb{Z}^d$ , for  $d \geq 0$  and  $0 \leq n < \infty$ .

As anticipated in Chapter 3, the right-regular representation of a finite Abelian group admits a decomposition into one-dimensional unitary irreducible representations. This allows to study QWS on finite Abelian groups in the (discrete) Fourier space, as it has been done in the case of  $\mathbb{Z}$ . Let  $F \cong \mathbb{Z}_m$  be a finite cyclic group of order  $m$ , and let  $C_m$  denote the right-regular representation of its generator on  $\mathbb{C}^m$ . Then  $C_m$  is diagonalized as

$$C_m = \sum_{j=1}^m |j\rangle\langle j| e^{ik_j} := \sum_{j=1}^m |j\rangle\langle j| e^{2\pi i \frac{j}{m}},$$

where the  $k_j$  are the wave-vectors and play the role of the discrete momenta.

We are now ready to derive a full characterization of general Abelian scalar QWS, giving the general structure of the evolution operator.

**Theorem 6.1.** *Let  $A$  be a scalar QW on an arbitrary Cayley graph of  $G \cong \mathbb{Z}_{i_1} \times \dots \times \mathbb{Z}_{i_n} \times \mathbb{Z}^d$  for  $1 \leq d < \infty$ , and  $0 \leq n < \infty$ . Then  $A$  splits into the direct sum of one-dimensional monoidal QWS, namely*

$$A = \bigoplus_{j \in I} e^{-i\theta_j} T_j, \quad I := \{1, \dots, i_1 \times i_2 \times \dots \times i_n\}$$

where the  $T_j$  are shift operators over  $\ell^2(\mathbb{Z}^d)$ . In particular, the dispersion relations are linear in the wave-vectors.

*Proof.* Let  $A$  be a scalar qw on an arbitrary Cayley graph  $\Gamma(G, S_+)$  of a group  $G \cong \mathbb{Z}_{i_1} \times \dots \times \mathbb{Z}_{i_n} \times \mathbb{Z}^d$ , for  $d \geq 1$ . Posing

$$F := \mathbb{Z}_{i_1} \times \dots \times \mathbb{Z}_{i_n}, \quad Z := \mathbb{Z}^d,$$

we can write every element of  $G$  as pairs contained in  $F \times Z$ . Accordingly, we can suitably decompose the generating set  $S_+$  into the following union

$$S_+ = \bigcup_{h \in S_+^Z} R(h) \times \{h\},$$

where the  $R(h)$  are sets contained in  $F$  and  $S_+^Z$  is a generating set for  $Z$ . Let  $T_{(f,h)}$  denote the right-regular representation of the generic element of  $S_+$  and  $C_l$  the right-regular representation of the generator of  $\mathbb{Z}_{i_l}$ . Then we can define the product representation  $T_f$  of every  $f \in \bigcup_{h \in S_+^Z} R(h)$ : there exist some integers  $m_l(f) \in \{1, \dots, i_l\}$  such that  $T_f = C_{i_1}^{m_{i_1}(f)} \otimes \dots \otimes C_{i_n}^{m_{i_n}(f)}$ . Denoting with  $T_h$  the right-regular representation of the generic element of  $S_+^Z$ , the diagonalization of the qw operator

$$A = \sum_{(f,h) \in S_+} T_{(f,h)} z_{(f,h)}$$

on  $\ell^2(G) \otimes \mathbb{C}$  thus reads

$$\begin{aligned} A &= \sum_{h \in S_+^Z} \sum_{f \in R(h)} (T_f \otimes T_h) z_{(f,h)} = \\ &= \sum_{j_1=1}^{i_1} \dots \sum_{j_n=1}^{i_n} |j_1\rangle \langle j_1| \otimes \dots \otimes |j_n\rangle \langle j_n| \otimes \sum_{h \in S_+^Z} T_h z_h(\mathbf{j}), \end{aligned} \quad (73)$$

where

$$z_h(\mathbf{j}) := \sum_{f \in R(h)} z_{(f,h)} e^{2\pi i \left( j_1 \frac{m_{i_1}(f)}{i_1} + \dots + j_n \frac{m_{i_n}(f)}{i_n} \right)}, \quad \mathbf{j} := (j_1, \dots, j_n). \quad (74)$$

Now, if  $d = 0$ , namely  $G = F$  is finite, this means that  $S_+^Z = \{e\}$  and the walk (73) consists in a diagonal matrix (with phase factors as entries). Accordingly, the thesis fol-



lows. In the case  $d \geq 1$ , the evolution operator in Eq. (73) is now block-diagonalizable in the (continuous) Fourier space as

$$\int_B d\mathbf{k} |\mathbf{k}\rangle \langle \mathbf{k}| A_{\mathbf{k}}(\mathbf{j}) := \int_B d\mathbf{k} |\mathbf{k}\rangle \langle \mathbf{k}| \left( \sum_{\mathbf{h}} e^{-i\mathbf{k} \cdot \mathbf{h}} z_{\mathbf{h}}(\mathbf{j}) \right) \quad \forall \mathbf{j}, \quad (75)$$

where the walk operator  $A_{\mathbf{k}}(\mathbf{j})$  is unitary (a phase factor) by construction for every  $\mathbf{j}$ . Then the scalars  $z_{\mathbf{h}}(\mathbf{j})$  must satisfy the unitarity constraints of Eq. (72). Notice that in Eq. (75) we passed to the vector notation for the generators of  $Z$ . Now define for every  $\mathbf{h}_i, \mathbf{h}_j \in S_+^Z$  the collection  $M$  of all the vectors  $\mathbf{v} = \mathbf{h}_i - \mathbf{h}_j \in \mathbb{Z}^d$  such that

$$\|\mathbf{v}\| = \max_{\mathbf{h}_i, \mathbf{h}_j \in S_+^Z} \|\mathbf{h}_i - \mathbf{h}_j\|. \quad (76)$$

Suppose that the quadrangularity condition (71) is satisfied for  $S_+^Z$ : namely for every nonvanishing  $\mathbf{v}' \in M$  there exist two distinct pairs  $(\mathbf{h}_1, \mathbf{h}_2)$  and  $(\mathbf{h}_3, \mathbf{h}_4)$  such that

$$\mathbf{v}' = \mathbf{h}_1 - \mathbf{h}_2 = \mathbf{h}_3 - \mathbf{h}_4 \neq 0. \quad (77)$$

The set  $M$  contains at least one nonvanishing element by hypothesis, since otherwise  $d = 0$ , namely  $Z \cong \{e\}$ . Then define  $\mathbf{d}_{ij} := \mathbf{h}_i - \mathbf{h}_j$ : being  $2\mathbf{v}' = \mathbf{d}_{14} + \mathbf{d}_{32}$ , then one has

$$\begin{aligned} 2\|\mathbf{v}'\| &= \|\mathbf{d}_{14} + \mathbf{d}_{32}\| \leq \|\mathbf{d}_{14}\| + \|\mathbf{d}_{32}\| \leq \\ &\leq \|\mathbf{v}'\| + \|\mathbf{v}'\| = 2\|\mathbf{v}'\|, \end{aligned}$$

where we used the triangle inequality and the definition (76) of  $\mathbf{v}'$ . This implies that  $\mathbf{d}_{14} \propto \mathbf{d}_{32}$  and  $\|\mathbf{v}'\| = \|\mathbf{d}_{14}\| = \|\mathbf{d}_{32}\|$ , in turn implying  $\mathbf{d}_{14} = \pm \mathbf{d}_{32}$ . The latter relation, substituted in Eq. (77), finally gives

$$\mathbf{h}_1 = \mathbf{h}_3, \quad \mathbf{h}_2 = \mathbf{h}_4$$

i.e. the pair is unique. From Eqs. (72) one then gets the unitarity condition

$$z_{\mathbf{h}_1}(\mathbf{j}) z_{\mathbf{h}_2}^*(\mathbf{j}) = 0,$$

namely  $z_{\mathbf{h}_1}(\mathbf{j}) = 0$  or  $z_{\mathbf{h}_2}(\mathbf{j}) = 0$ . Thus we must remove  $\mathbf{h}_1$  or  $\mathbf{h}_2$  from  $S_+^Z$ . Iterating the above argument, we finally conclude that for every  $\mathbf{j}$  there exists  $\tilde{\mathbf{h}}(\mathbf{j}) \in S_+^Z$  such that

$$A_{\mathbf{k}}(\mathbf{j}) = \sum_{\mathbf{h} \in S_+^Z} \delta_{\tilde{\mathbf{h}}(\mathbf{j}), \mathbf{h}} z_{\mathbf{h}}(\mathbf{j}) e^{-i\mathbf{k} \cdot \mathbf{h}} = z_{\tilde{\mathbf{h}}(\mathbf{j})}(\mathbf{j}) e^{-i\mathbf{k} \cdot \tilde{\mathbf{h}}(\mathbf{j})}.$$

Conveniently defining  $e^{-i\theta_j} := z_{\tilde{\mathbf{h}}(\mathbf{j})}(\mathbf{j})$  (by unitarity of  $A_{\mathbf{k}}(\mathbf{j})$ ) and  $\mathbf{h}_j := \tilde{\mathbf{h}}(\mathbf{j})$ , and substituting into Eq. (73), we can write any infinite Abelian scalar qw as the direct sum of scalar qws on the line:

$$A = \bigoplus_{j \in I} e^{-i\theta_j} T_j, \quad I := \{1, \dots, i_1 \times i_2 \times \dots \times i_n\}.$$

Else, in the Fourier representation the evolution operator reads

$$A = \int_B d\mathbf{k} \bigoplus_{j \in I} e^{-i(\mathbf{k} \cdot \mathbf{h}_j + \theta_j)} \otimes |\mathbf{k}\rangle \langle \mathbf{k}|,$$

with  $\mathbf{h}_j \in S_+^Z$ . This finally proves that the dispersion relations are linear in  $\mathbf{k}$ . ■

The structure result of Theorem 6.1 generalizes the no-go theorem of Ref. [98], since it accounts for general Abelian groups and arbitrary presentations, namely any first-neighbours scheme.

### 6.3 SCALAR QWS ON THE INFINITE DIHEDRAL GROUP

In this section we classify all the spinorial qws on the line with a two-dimensional coin system which are derivable as coarse-grainings of scalar qws. By the classification of Theorem 6.1, we can focus on non-Abelian scalar qws on Cayley graphs of some virtually Abelian groups  $G$ . The groups  $G$  shall contain a subgroup  $H \cong \mathbb{Z}$  of index 2. As a standard choice, we impose the generating set  $\tilde{S}_+ = \{a\}$  for the coarse-grained qw on  $H \cong \mathbb{Z}$  (namely the integer lattice with the usual first-neighbours scheme). We will show that the admissible  $G$  and  $\Gamma(G, S)$  are unique and define an infinite family of qws parametrized by two continuous parameters.

6.3.1 Derivation of the group and its Cayley graph

We now aim to derive all the admissible non-Abelian groups of the form  $G \cong \mathbb{Z} \cup \mathbb{Z}r$ , along with their Cayley graphs satisfying the quadrangularity condition (71). First, we prove a simple lemma which will be handy for the derivation.

**Lemma 6.1.** *Let  $G$  be a group and  $H$  a subgroup of index 2 in  $G$ . Then  $H$  is normal in  $G$ .*

*Proof.* By contradiction, let  $H$  be a subgroup of index 2 which is not normal in  $G \cong \mathbb{Z} \cup \mathbb{Z}r$ . Accordingly,

$$\exists x_1, x_2 \in H : rx_1r^{-1} = x_2r.$$

The above relation implies  $rx_1 = x_2r^2$ . Suppose that  $r^2 \in H$ : the last equation reads  $r \in H$ , which is absurd. Then it must be

$$\exists x \in H : r^2 = xr.$$

On the other hand, last relation reads  $r = x \in H$ , which is again absurd by hypothesis.

■

As a consequence of Lemma 6.1, left- and right-cosets of an index-2 subgroup coincide. Without loss of generality, we will conventionally choose the right-cosets to perform the coarse-graining.

**Proposition 6.2.** *Let  $G$  be a non-Abelian group with a subgroup  $H \cong \mathbb{Z}$  of index 2. Then  $G \cong D_\infty$ , where  $D_\infty$  is the infinite dihedral group.*

*Proof.* Let us define

$$G \cong H \cup Hr, \quad H \cong \mathbb{Z}, \quad H = \langle a \rangle.$$

By Lemma 6.1,  $H$  is normal in  $G$ , and then

$$\exists m, l \in \mathbb{Z} : rar^{-1} = a^m \wedge r^{-1}ar = a^l$$

with  $m, l \notin \{0, 1\}$ , since  $G$  is non-Abelian by hypothesis. Accordingly  $a = r^{-1}a^m r = (r^{-1}ar)^m = a^{lm}$ , implying  $l = \frac{1}{m}$ : it must then be  $m = -1$ . Thus we have

$$\varphi(a) := rar^{-1} = a^{-1}. \tag{78}$$

On the other hand, it must be  $r^2 \in H$ , since otherwise one has  $r^2 = a^q r$  for some integer  $q$ , which, being equivalent to  $r \in H$ , is absurd. Suppose that  $r^2 = a^p$  for some integer  $p$ . Using Eq. (78), the relation  $r = r^{-1} a^p = a^p r^{-1} = r^{-1} a^{-p}$  holds, implying  $p = 0$  and finally  $r^2 = e$ . Posing  $C = \langle r | r^2 \rangle$ , one has  $G = HC$  and  $H \cap C = \{e\}$ , meaning that

$$G = H \rtimes_{\varphi} C \cong \mathbb{Z} \rtimes_{\varphi} \mathbb{Z}_2 \equiv D_{\infty}.$$

■

Thus, we have shown that the inverse map  $\varphi$  is the only nontrivial automorphism of  $\mathbb{Z}$  achieving the semidirect product with  $\mathbb{Z}_2$ . In Chapters 8 and 9 we shall generalize the construction of the proof of Proposition 6.2 in the context of *group extensions*.

Since the cosets are mutually disjoint, the set of every Cayley graph of  $D_{\infty}$  can be partitioned into two distinct subsets, corresponding to the cosets  $H, Hr$ . The elements of  $H$  are in one-to-one correspondence with those of  $Hr$  via composition by elements of the form  $a^m r$ . We shall translate these observations into statements on the possible Cayley graphs of the infinite dihedral group in order to derive the only Cayley graph satisfying quadrangularity and admitting a regular tiling with coarsened-grained set of generators  $\tilde{S} = \{a, -a, e\}$ .

**Proposition 6.3.** *Let  $\Gamma(D_{\infty}, S_+)$  be a Cayley graph of  $D_{\infty}$  satisfying quadrangularity and admitting a regular tiling which gives rise to the Cayley graph  $\Gamma(\mathbb{Z}, \{a, e\})$ . Then  $\Gamma(D_{\infty}, S_+)$  is unique and corresponds to the presentation*

$$D_{\infty} = \langle e, a, a^{-1}, b, c, d \mid b^2, c^2, bda^{-1}, cda, baba, caca, bca^{-2} \rangle \quad (79)$$

(as shown in Figure 4).

*Proof.* Our strategy is to start with a generic set of generators for  $D_{\infty}$ , written in terms of the generator  $a$  of the subgroup  $H \cong \mathbb{Z}$ , and then impose for the coarse-grained generators  $\tilde{h}$  the condition

$$\tilde{h} \in \{a, e\}. \quad (80)$$

We have to explicitly compute the set  $S_+$  in Eq. (58), given by

$$\tilde{S}_+ = \{c_{\tau(i,j)} h_i c_j^{-1} \mid h_i \in S_+, j \in D_{\infty}/H\} = \{a, e\}. \quad (81)$$

We notice the the case of symmetric  $S_+$  is already accounted: considering the inverses  $\left(c_{\tau(i,j)}h_i c_j^{-1}\right)^{-1} = c_j h_i^{-1} c_{\tau(i,j)}^{-1}$ , one simply conclude that this amounts to consider also  $\tilde{S}_+$  symmetric. In general, the  $\tilde{h}$  depend on the coset representatives: accordingly, we shall pose

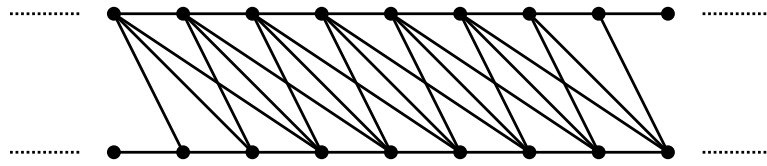
$$c_1 = a^m, \quad c_2 = a^{m'} r \tag{82}$$

as a general form. We shall exclude the case  $a^l \in S_+$  for  $|l| \geq 2$ , since choosing  $j = 1$  in Eq. (81) one would end up with  $\tilde{h} = a^l \in \tilde{S}_+$ , which is in contrast with condition (80). Moreover, we could also include  $e$  in  $S_+$ , since the identity element is invariant under coarse-graining. Accordingly, we are left with just the two following cases.

- 1) **Case  $a \in S_+$ .** Except for  $a$  and  $e$ , all the possible element in  $S_+$  are contained in the coset we pose  $Hr: a^n r$  as their general form. Combining (81) with Eqs. (80) and (82), we get  $|n - (m' - m)| \leq 1$ , namely the elements of the set

$$\tilde{S}' := \{a^{(m'-m)} r, a^{(m'-m)+1} r, a^{(m'-m)-1} r\}$$

are admissible generators for  $D_\infty$ . By quadrangularity, there must exist some  $h, h' \in \tilde{S}'$  such that  $a^2 = hh'^{-1}$ : this implies  $a^{(m'-m)\pm 1} r \in S_+$ . Moreover, from the relation  $h'h^{-1} = a^{-2}$ , by quadrangularity it must be also  $a^{-1} \in S_+$ . Including  $a^{(m'-m)} r$  in  $S_+$  one has  $e$  as coarse-grained generator. Now, it is easy to check that  $\forall m, m'$  the set  $\tilde{S}'$  gives rise to topologically equivalent Cayley graphs: the only graphical difference is a constant left-translation  $a^{(m'-m)}$ . Here it follows an example for the choice  $m' - m = 2$ :



The horizontal translations correspond to  $a^{\pm 1}$ , while the diagonal ones to  $r, ar, a^{-1}r$ . Accordingly, one can just set  $m = m' = 0$ , corresponding to the following uncoloured graph:

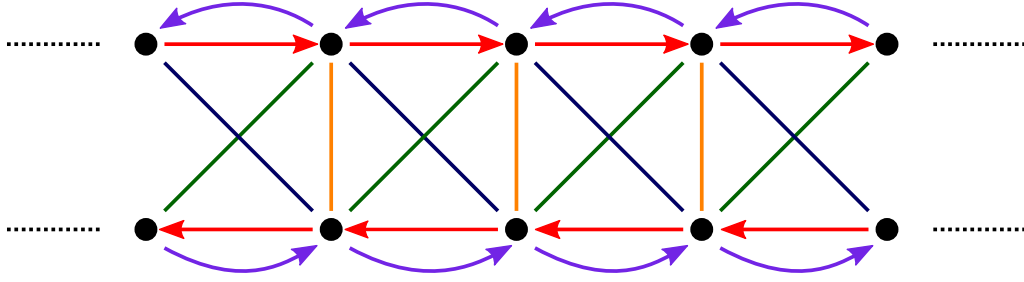
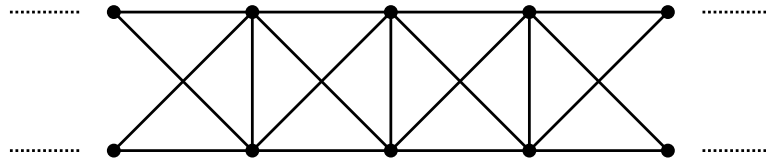


Figure 4: The most general Cayley graph of the infinite dihedral group which admits a scalar QW with coarse-graining on  $\mathbb{Z}$  with coordination number two. The group presentation is given in Eq. (79). The generators—namely  $a$  (red),  $a^{-1}$  (violet),  $b$  (dark blue),  $c$  (green) and  $d$  (orange)—are associated to edges of the graph, each corresponding to a transition scalar of the walk. Another Cayley graph of  $D_\infty$  with the same properties can be obtained by dropping  $d$  and the relators containing it. Moreover, one can include  $e$  in the generating set, which would correspond to a loop at each site.



2) **Case  $a \notin S_+$ .** In the previous case we have shown that

$$a \in S_+ \iff a^{-1} \in S_+.$$

It clearly follows that  $a \notin S_+ \Rightarrow a^{-1} \notin S_+$ : and then  $S_+ \subseteq \{e, \tilde{S}^l\}$ . However, it suffices to check that path of length 2 corresponding to the element  $a^2$  to show that this generating set violates quadrangularity. Therefore the case  $a \notin S_+$  is ruled out.

Assigning a consistent colouring to the uncoloured graph derived in case 1), one finds the unique admissible Cayley graph of  $D_\infty$ , shown in Fig. 4. ■

In Figure 5 we show the Cayley graph of the subgroup  $H \cong \mathbb{Z}$  of  $D_\infty$  corresponding to the regular tiling with coarsed-grained set of generators  $\tilde{S} = \{a, -a, e\}$ . In the next

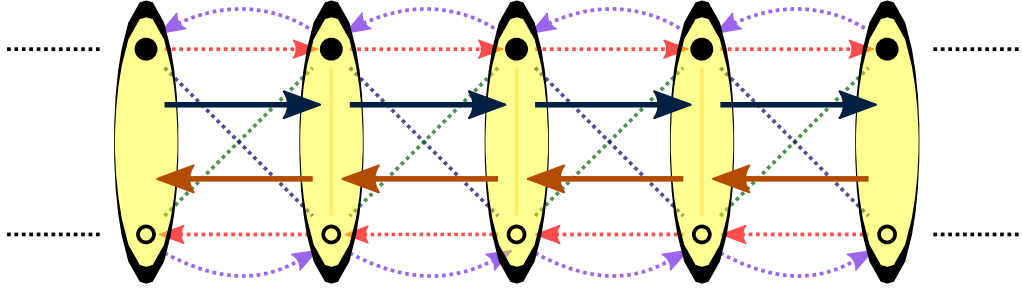


Figure 5: Realisation of the scalar qw in Fig. 4 as a quantum walk on  $\mathbb{Z} = \langle a, a^{-1} \mid \rangle$  with a two-dimensional coin system. The original vertexes are grouped into pairs, realizing an additional helicity degree of freedom, and each edge—namely  $a$  (dark blue) and  $a^{-1}$  (brown)—is associated to a transition matrix. The cosets are associated to an element of a basis for  $\mathbb{C}^2$ : we choose the canonical basis, that is  $c_1 \rightarrow (1, 0)$  (full circles) and  $c_2 \rightarrow (0, 1)$  (empty circles). We omitted the loops corresponding to  $e$ .

subsection we derive the family of scalar qws on the infinite dihedral group presented as in Figure 4.

### 6.3.2 Derivation of the scalar qws on $D_\infty$

We recall the unitarity conditions

$$\sum_{h \in S} |z_h|^2 = 1, \quad (83)$$

$$\sum_{hh'^{-1}=h''} z_h z_{h'}^* = \sum_{h^{-1}h'=h''} z_h^* z_{h'} = 0, \quad (84)$$

where  $h'' \in \{g \in D_\infty \mid g = hh'^{-1} \neq e : h, h' \in S\}$ , for the qw operator

$$A = \sum_{h \in S} z_h T_h$$

on  $\ell^2(D_\infty)$ . We shall now solve the set of conditions (84) on the Cayley graph  $\Gamma(D_\infty, S)$  given in Figure 4. Consider the polar representation  $z_h = |z_h|e^{i\theta_h}$  for the transition scalars. The paths of length 2 corresponds to the elements

$$a^2, \quad ab, \quad ac, \quad ad$$

and their inverses. Then unitarity constraints (possibly with  $z_d$  or  $z_e$  vanishing) are given by:

$$z_{a\pm 1}z_{a\mp 1}^* + z_gz_f^* = 0, \quad (85)$$

$$z_{a\pm 1}z_g^* + z_gz_{a\pm 1}^* = 0, \quad (86)$$

$$z_dz_e^* + z_ez_d^* + z_{a\pm 1}z_b^* + z_bz_{a\pm 1}^* + z_{a\mp 1}z_c^* + z_cz_{a\mp 1}^* = 0, \quad (87)$$

$$z_gz_e^* + z_ez_g^* + z_dz_{a\pm 1}^* + z_{a\pm 1}z_d^* = 0, \quad (88)$$

$$z_{a\pm 1}z_e^* + z_ez_{a\pm 1}^* + z_dz_g^* + z_gz_d^* = 0, \quad (89)$$

with  $g, f \in \{b, c\}$  and  $g \neq f$ . From Eqs. (86), it follows

$$e^{i\theta_b} = t_1ie^{i\theta_{a-1}}, \quad e^{i\theta_c} = t_2ie^{i\theta_a}, \quad t_{1,2} \text{ arbitrary signs.}$$

From (85) one has

$$|z_a||z_{a-1}| = |z_b||z_c|, \quad s_1 := t_1 = -t_2, \quad e^{i\phi} := e^{i\theta_a} = s_2e^{i\theta_{a-1}},$$

which are consistent with all of the (86).

Therefore, we can satisfy Eqs. (84) and the normalization constraint (83) defining the transition scalars as follows:

$$\begin{aligned} z_a &= \nu\sqrt{p}\sqrt{q}e^{i\phi}, & z_{a-1} &= s_2\nu\sqrt{1-p}\sqrt{1-q}e^{i\phi}, \\ z_b &= s_2s_1i\nu\sqrt{p}\sqrt{1-q}e^{i\phi}, & z_c &= -s_1i\nu\sqrt{1-p}\sqrt{q}e^{i\phi}, \\ z_e &= \mu\alpha e^{i\theta_e}, & z_d &= \mu\beta e^{i\theta_d}, \end{aligned}$$

where  $p, q \in (0, 1)$ ,  $\mu \in [0, 1)$ ,  $\alpha \in [0, 1]$  and  $\nu := \sqrt{1-\mu^2}$ ,  $\beta := \sqrt{1-\alpha^2}$ . Then, we conveniently split the continuation of the general derivation through the following four cases.



- **Case**  $z_d = z_e = 0$  ( $\mu = 0$ ). Eqs. (87) are satisfied, while Eqs. (88) and (89) are trivial. Accordingly, in this case the transition scalars are given by:

$$\begin{aligned} z_a &= \sqrt{p}\sqrt{q}e^{i\phi}, \quad z_{a^{-1}} = s_2\sqrt{1-p}\sqrt{1-q}e^{i\phi}, \\ z_b &= s_2s_1i\sqrt{p}\sqrt{1-q}e^{i\phi}, \quad z_c = -s_1i\sqrt{1-p}\sqrt{q}e^{i\phi}. \end{aligned}$$

- **Case**  $z_e = 0$  ( $\alpha = 0$ ). Again, Eqs. (87) are already satisfied. From Eqs. (88) one gets  $e^{i\theta_d} = s_3ie^{i\phi}$  for  $s_3$  an arbitrary sign, while from Eqs. (89) we have

$$\begin{aligned} e^{2i\theta_d} &= -s_2e^{2i\phi} \Rightarrow s_2 = +1, \\ |z_b| &= |z_c|. \end{aligned}$$

We conclude that the transition scalars are given by:

$$\begin{aligned} z_a &= \nu p, \quad z_{a^{-1}} = \nu(1-p), \\ z_b &= s_1i\nu\sqrt{p}\sqrt{1-p}, \quad z_c = -s_1i\nu\sqrt{p}\sqrt{1-p}, \\ z_d &= s_3i\mu, \end{aligned}$$

for  $p, \mu \in (0, 1)$ .

- **Case**  $z_d = 0$  ( $\beta = 0$ ). Again, Eqs. (87) are already satisfied. From Eqs. (88) one has  $e^{i\theta_e} = s'_3e^{i\phi} := -s_1s_3e^{i\phi}$ . From Eqs. (89) one gets

$$\begin{aligned} e^{2i\theta_e} &= -s_2e^{2i\phi} \Rightarrow s_2 = -1, \\ |z_a| &= |z_{a^{-1}}|. \end{aligned}$$

We thus conclude that the transition scalars are (up to a global phase factor)

$$\begin{aligned} z_a &= \nu\sqrt{p}\sqrt{1-p}, \quad z_{a^{-1}} = -\nu\sqrt{p}\sqrt{1-p}, \\ z_b &= -s_1i\nu p, \quad z_c = -s_1i\nu(1-p), \quad z_e = -s_1s_3\mu \end{aligned}$$

for  $p, \mu \in (0, 1)$ .

- **Case**  $z_e, z_d \neq 0$  ( $\mu, \alpha, \beta \neq 0$ ). Eqs. (87) read

$$z_d z_e^* + z_e z_d^* = 0 \Rightarrow e^{i\theta_e} = s_4 i e^{i\theta_d},$$

for  $s_4$  a sign. Substituting into Eqs. (88), one gets

$$\begin{aligned} s_1 s_2 s_4 |z_b| |z_e| \cos(\theta_d - \phi) &= -|z_d| |z_a| \cos(\theta_d - \phi), \\ s_1 s_2 s_4 |z_c| |z_e| \cos(\theta_d - \phi) &= |z_d| |z_{a-1}| \cos(\theta_d - \phi), \end{aligned}$$

which can be satisfied if and only if  $\cos(\theta_d - \phi) = 0$ , implying  $e^{i\theta_d} = s_3 i e^{i\phi}$ . From Eqs. (89) we have

$$s_1 |z_e| (|z_a| + s_2 |z_{a-1}|) = s_4 |z_d| (s_2 |z_b| - |z_c|). \quad (90)$$

Notice that a change of the sign  $s_1 s_4$  affects last equation just by a relabeling  $|z_a| \leftrightarrow |z_{a-1}|$  (if  $s_2 = -1$ ) or  $|z_b| \leftrightarrow |z_c|$  (if  $s_2 = +1$ ), yet the unitarity conditions are invariant: without loss of generality we set  $s_1 s_4 = +1$ . Depending on the positivity or negativity of  $s_2$ , by Eq. (90) one has to impose respectively the condition  $|z_b| > |z_c|$  or  $|z_{a-1}| > |z_a|$ . These last conditions affect the domain of  $p, q$ . Finally, from Eq. (90) one can also find  $\alpha$  in terms of  $p, q, s_2$ .

We conclude that in the general case the transition scalars (up to a global phase factor) are given by:

$$\begin{aligned} z_a &= v \sqrt{p} \sqrt{q}, & z_{a-1} &= s_2 v \sqrt{1-p} \sqrt{1-q}, \\ z_b &= s_2 s_1 i v \sqrt{p} \sqrt{1-q}, & z_c &= -s_1 i v \sqrt{1-p} \sqrt{q}, \\ z_e &= -s_1 s_3 \mu \alpha, & z_d &= s_3 i \mu \beta, \end{aligned} \quad (91)$$

where  $\alpha = \sqrt{p} \sqrt{1-q} - s_2 \sqrt{1-p} \sqrt{q}$  and  $p, q, \mu \in (0, 1)$ , while  $p > q$  if  $s_2 = +1$ ,  $(1-q) > p$  if  $s_2 = -1$ .

### 6.3.3 Scalar qws on $D_\infty$

We now use the transition scalars of the qws on  $D_\infty$ , which we derived in the previous subsection, to represent the coarse-grained family of qws on the subgroup  $H \leq \mathbb{Z}$  of  $D_\infty$ . In order to compute the transition matrices we make use of the formula in Eq. (60),

recalling that the regular tiling that we chose (without loss of generality, as proved in Subsection 6.3.1) is the one shown in Figure 5.

The transition matrices of the coarse-grained qws, computed choosing  $\{|1\rangle, |2\rangle\}$  as the canonical basis of  $\mathbb{C}^2$  and using Eq. (60), are:

$$A_{+a} = \begin{pmatrix} z_a & z_b \\ z_c & z_{a-1} \end{pmatrix}, \quad A_{-a} = \begin{pmatrix} z_{a-1} & z_c \\ z_b & z_a \end{pmatrix}, \quad A_e = \begin{pmatrix} z_e & z_d \\ z_d & z_e \end{pmatrix}.$$

In Figure 5 one also finds the graphical interpretation of the coarse-graining in terms of qw on the integer lattice. With reference to the transition scalars in (91) derived in the previous subsection, we pose

$$\cos \theta := \sqrt{p}, \quad \sin \theta := -s_1 \sqrt{1-p}, \quad \cos \theta' := \sqrt{q}, \quad \sin \theta' = s_1 s_2 \sqrt{1-q}, \quad s := s_2 s_3.$$

Thus, defining  $A_k := e^{-ik} A_{+a} + e^{ik} A_{-a} + A_e$ , the coarse-grained scalar qws in the Fourier representation are given by

$$A_k = e^{i\theta\sigma_x} A_k^D e^{i\theta'\sigma_x}, \quad (92)$$

where  $\theta, \theta' \in (-\pi/2, 0) \cup (0, \pi/2)$  and  $A_k^D$  is the Dirac qw in one space-dimension derived in Ref. [136]:

$$A_k^D = \begin{pmatrix} v e^{-ik} & i s \mu \\ i s \mu & v e^{ik} \end{pmatrix}, \quad v^2 + \mu^2 = 1, \quad s = \pm 1.$$

Let us now consider parity invariant qws  $\int_B dk |k\rangle\langle k| \otimes A_k^P$  on  $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ , i.e.

$$P A_k^P P^\dagger = A_{-k}, \quad P = P^\dagger = P^{-1},$$

where  $P$  represent the parity transformation on  $\mathbb{C}^2$ . We observe that the coarse-grained qw  $A_k$  is parity invariant with  $P = \sigma_x$ .

**Remark 6.2.** We notice that the parity symmetry is inherited via the coarse-graining procedure: the automorphism  $\varphi$  realizing the semidirect product  $D_\infty = \mathbb{Z} \rtimes_\varphi \mathbb{Z}_2$  is just the inverse map. It is immediate to see that the Hadamard walk, introduced in Chapter 1, is not parity invariant.

Then, by the results of the present section and by the classification of Abelian scalar QWs (Theorem 6.1), it follows that the Hadamard walk cannot be represented as the coarse-graining of a scalar QW on a Cayley graph. This provides a negative answer to the conjecture made in Remark 5.2: that is, given a group property  $P$ , if a QW is virtually  $P$  then it is also  $P$  (on an extended coin system), but the vice versa does not hold true.

We conclude the present chapter studying the spectrum of the family of walks (92). Defining

$$\delta := z_a + z_{a-1}, \quad \gamma := z_e,$$

the dispersion relations of (92) are given by:

$$\pm\omega(k) = \arccos(\delta \cos k + \gamma), \quad |\delta \pm \gamma| \leq 1, \quad \delta, \gamma \in \mathbb{R}. \quad (93)$$

For every  $\delta$  and  $\gamma$ , the minimum of  $\omega(k)$  is attained at  $k_0 = 0$ . Around  $k_0$  the behaviour can be either flat, or  $\pm|k|$  plus a constant, or smooth. For  $\gamma = 0$  we recover (up to a local change of basis) the 1D Dirac QW  $A_k^D$ , while for  $\delta = 1$  we get the 1D Weyl QW  $A_k = \exp(-ik\sigma_z)$ , which describes the dynamics of massless particles with a dispersion relation which is linear in  $k$  (see Chapter 1). We observe that when  $\delta + \gamma = 1$  the QW exhibits a non-dispersive behaviour for  $|k| \approx 0$  and a dispersive behaviour for greater values of  $|k|$ . The dispersion relations are plotted for some values of the parameters  $\delta, \gamma$  in Figures 6 and 7. Notice that the dispersion relations in Figure 7 are the same as those in Figure 6, apart from a transformation  $\omega(k) \rightarrow \pi - \omega(k + \pi)$ .

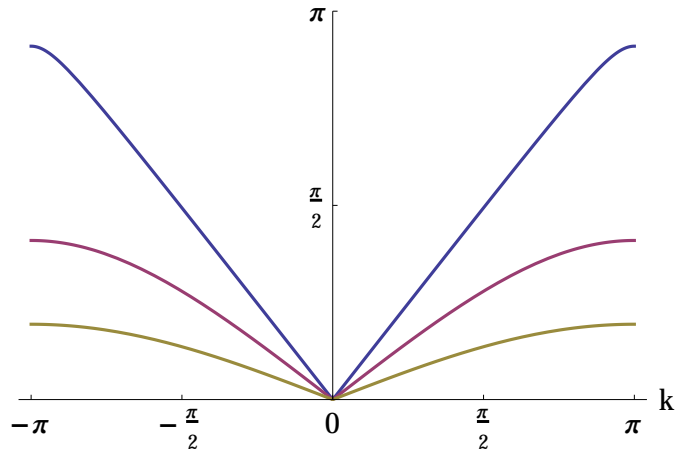


Figure 6: Plot of  $\omega(k) = \arccos(\delta \cos k + \gamma)$ , for (from top to bottom)  $\delta = 0.98, 0.36, 0.09$  and  $\delta + \gamma = 1$ . This class of qws exhibits, for  $|k| \approx 0$  and positive  $\delta$ , a massless (Weyl) dispersion relation (up to a rescaling of  $k$ ):  $\omega(k) \approx \delta|k|$ . For  $|k| \approx \pi$ ,  $\omega(k)$  becomes dispersive (massive).

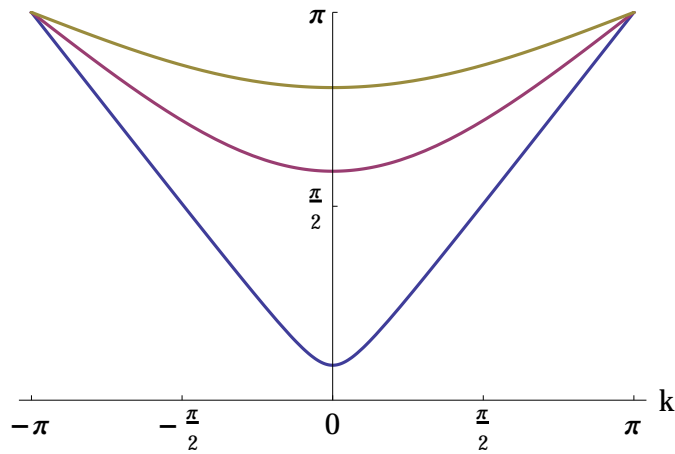


Figure 7: Plot of  $\omega(k) = \arccos(\delta \cos k + \gamma)$ , for (from bottom to top)  $\delta = 0.98, 0.36, 0.09$  and  $\delta - \gamma = 1$ . This class of qws exhibits a massive dispersion relation for  $|k| \approx 0$ , and a massless one for  $|k| \approx \pi$ . The Dirac dispersion relation is recovered for  $|k| \approx 0$  and  $\delta \approx 1$ .



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## ISOTROPIC QUANTUM WALKS AND THE WEYL EQUATION

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In Chapter 4 we proved Lemma 4.1, stating that the isotropy group of a qw on the Cayley graph of a finitely generated group  $G$  is a finite subgroup of  $\text{Aut}(G)$ . In the present section we investigate how the isotropy assumption affects the possible presentations of a group  $G$  for a Cayley graph of  $G$  to admit an isotropic qw. We shall pay a particular attention to the case  $G \cong \mathbb{Z}^d$ , as a consequence of Corollary 5.2, since we wish to classify the qws on a Cayley graph admitting a quasi-isometry to Euclidean spaces. In the following of this work, we will refer to qws on Cayley graphs of groups quasi-isometric to  $\mathbb{R}^d$  as *Euclidean* qws. This case will be instructive on the general non-Abelian one.

### 7.1 GENERALITIES ON ISOTROPY FOR QWS ON CAYLEY GRAPHS

Recalling that the action of the isotropy group  $L$  is transitive on the generating set  $S_+$ , by definition  $S_+$  can be constructed as the orbit of an arbitrary element  $h \in S_+$  under the action of  $L$ . The following proposition states that  $L$  can always be faithfully embedded in a finite orthogonal matrix group.

**Proposition 7.1.** *Let  $L$  be a finite group, admitting a faithful representation in  $\text{GL}(m, \mathbb{Z})$  for some integer  $m$ . Then there exists an integer  $n \leq m$  such that  $L$  admits a faithful representation in  $\text{O}(n, \mathbb{R})$ .*

*Proof.* Let  $M$  be a finite-dimensional faithful representation on integers of a finite group  $L$ . Such a representation  $M$  always exists by Cayley Theorem 2.2, since every finite group can be faithfully represented as a group of finite-dimensional permutation matrices containing exactly one 1 in each row and column (with remaining elements which are zeros). Let us define the matrix:

$$P := \sum_{l \in L} M_l^T M_l.$$

For every  $f \in L$  we have the following relation

$$\begin{aligned} PM_f &= \sum_{l \in L} M_l^T M_{lf} = \sum_{l' \in L} M_{l'f^{-1}}^T M_{l'} = \\ &= \sum_{l' \in L} \left( M_{l'} M_{f^{-1}} \right)^T M_{l'} = M_{f^{-1}}^T P. \end{aligned} \tag{94}$$

Moreover,  $P$  is positive, since it is a sum of positive operators by definition. Accordingly, for  $|\eta\rangle \in \ker P$ , we have

$$\langle \eta | P | \eta \rangle = \sum_{l \in L} \langle \eta | M_l^T M_l | \eta \rangle = 0 \implies M_l | \eta \rangle = 0, \quad \forall l \in L.$$

This implies  $|\eta\rangle = 0$ , since all the  $M_l$  are invertible. Thus  $P$  is also invertible and we can define the following change of representation:

$$\tilde{M}_l := P^{1/2} M_l P^{-1/2}. \tag{95}$$

Exploiting the definition of  $P$  and property (94), we finally obtain

$$\begin{aligned} \tilde{M}_l^T \tilde{M}_l &= P^{-1/2} M_l^T P M_l P^{-1/2} = \\ &= P^{-1/2} M_l^T M_{l^{-1}}^T P P^{-1/2} = I. \end{aligned} \tag{96}$$

We observe that it may be the case that  $M$  is reducible on the integers: in this case, the reduced sector of  $M$  are defined on a space with a lower dimension than the original one. Indeed, by definition (95), the reduced sectors of  $\tilde{M}$  are defined in general on  $\mathbb{R}$ . Assuming  $\tilde{M}$  having minimal dimension, we conclude that relation (96) means that  $\{\tilde{M}_l^i\}_{l \in L} \subset \mathcal{O}(n, \mathbb{R})$ . ■



**Corollary 7.1.** *Let  $L$  be a finite subgroup of  $\text{Aut}(\mathbb{Z}^d)$ . Then there exists a faithful representation of  $L$  in  $\mathcal{O}(d, \mathbb{R})$ .*

*Proof.* It suffices to use the fact that, by Theorem 2.1,  $\text{Aut}(\mathbb{Z}^d) \cong \text{GL}(d, \mathbb{Z})$  and apply Proposition 7.1. ■

We now consider the qws on Cayley graphs of groups quasi-isometric to  $\mathbb{R}^d$  in full generality. By Theorem 2.4, these groups are virtually  $\mathbb{Z}^d$ . On the other hand, we know from Corollary 5.2 that every virtually- $\mathbb{Z}^d$  qw admits a representation as a qw on  $\mathbb{Z}^d$  with an enlarged coin system. Therefore, without loss of generality we shall now study the qws on  $\mathbb{Z}^d$  as the paradigmatic case of Euclidean qws on Cayley graphs. The simplest case from the point of view of the coin system is the scalar one. In the previous Chapter, we classified the Abelian scalar qws (Theorem 6.1), finding that these are mere direct sums of shifts times a global phase factor. Accordingly, the next simplest case to analyse is that of qws on  $\mathbb{Z}^d$  with a two-dimensional coin system. For the sake of convenience, we will restrict to the cases of physical interest  $d = 1, 2, 3$ .

We now aim to construct all the admissible Cayley graphs of  $\mathbb{Z}^d$  satisfying isotropy. The possible isotropy groups  $L$  are the finite subgroups of  $\text{Aut}(\mathbb{Z}^d) \cong \text{GL}(d, \mathbb{Z})$ . Corollary 7.1 implies that we can construct the desired generating sets  $S_+$  for  $\mathbb{Z}^d$  as the orbit of an arbitrary vector  $\mathbf{v} \in \mathbb{R}^d$  under the action of a finite subgroup  $L < \text{GL}(d, \mathbb{Z})$  represented in  $\mathcal{O}(d, \mathbb{R})$  (from now on we denote it just as  $\mathcal{O}(d)$ ). Accordingly, for every generating set of  $\mathbb{Z}^d$ , if the associated Cayley graph satisfies isotropy then one can represent the generators having all the same Euclidean norm: they lie on a sphere centred at the origin.

Using the results of Refs. [139–141], the finite subgroups of  $\text{GL}(d, \mathbb{Z})$  are classified and are isomorphic to the following abstract groups:

- $d = 3$ :  $\mathbb{Z}_n$  and  $D_n$  with  $n \in \{1, 2, 3, 4, 6\}$ ,  $A_4$ ,  $S_4$ , along with the direct products of all the previous groups with  $\mathbb{Z}_2$ ;
- $d = 2$ :  $\mathbb{Z}_n$  and  $D_n$  with  $n \in \{1, 2, 3, 4, 6\}$ ;
- $d = 1$ :  $\{e\}$  and  $\mathbb{Z}_2$ .

$D_n$  denotes the dihedral groups of order  $2n$ , while  $S_4$  and  $A_4 \triangleleft S_4$  are respectively the symmetric group of all the permutations of 4 elements and the alternating group of order 12, which is the subgroup of the even permutations.

We observe that for  $d = 1, 2$  the finite subgroups of  $\text{GL}(d, \mathbb{Z})$  coincide with those of  $\mathcal{O}(d)$ , while for  $d = 3$  this is not the case. It is immediate to see that we can treat our

cases of interest  $d = 1, 2, 3$  jointly, constructing the generating sets  $S_+$  just for  $d = 3$  and thus recovering  $d = 1, 2$  as special instances.

Our strategy to construct the generating sets  $S_+$  for  $\mathbb{Z}^d$  satisfying isotropy is to consider the representations of the aforementioned finite subgroups in  $\mathcal{O}(3)$ , construct the orbits of an arbitrary vector in  $\mathbb{R}^3$  under them, and finally study the unitarity conditions for the sets  $S_+$  thus obtained. In Appendix A we shall study the orbits of a vector  $\mathbf{v} \in \mathbb{R}^3$  under the real, orthogonal and three-dimensional faithful representations of the isotropy groups  $L < \mathcal{O}(3)$ . This choice is not arbitrary and we can safely assume it, as justified via the following argument.

Suppose that we took into account also the unfaithful representations of  $L$ : by definition, these would have a nontrivial kernel. Kernels of groups homomorphisms are by Proposition 2.2 normal subgroups, and thus the effective action of the unfaithful representations of  $L$  on  $\mathbf{v}$  would be given by a faithful representation of the quotient group. Now, inspecting the subgroup structure of the isotropy groups  $L \in \mathcal{S}$  where

$$\mathcal{S} := \left\{ \mathbb{Z}_n, D_n, A_4, S_4, \mathbb{Z}_n \times \mathbb{Z}_2, D_n \times \mathbb{Z}_2, A_4 \times \mathbb{Z}_2, S_4 \times \mathbb{Z}_2 \mid n \in \{1, 2, 3, 4, 6\} \right\}, \quad (97)$$

it is easy to find the normal subgroups and consider the quotient groups. This is straightforward as for  $\mathbb{Z}_n$  and  $D_n$ , while in the case of  $A_4$  and  $S_4$  one can directly verify—e.g. considering their faithful representations given in Appendix A.1—that  $V_4 := \mathbb{Z}_2 \times \mathbb{Z}_2$  is normal in  $A_4$  and  $V_4, A_4$  are normal in  $S_4$ . We have the following quotient groups:

$$A_4/V_4 \cong \mathbb{Z}_3, \quad S_4/A_4 \cong \mathbb{Z}_2, \quad S_4/V_4 \cong D_3.$$

One can then easily realise all the quotient groups built up with the groups in  $\mathcal{S}$  are themselves contained in  $\mathcal{S}$ , and then are finite subgroups of  $\mathrm{GL}(3, \mathbb{Z})$ . Finally, we conclude that the case of unfaithful representations can be excluded taking into account the faithful ones.

## 7.2 UNITARITY CONDITIONS AND ISOTROPY

In the previous section we saw how the isotropy assumption affects the admissible Cayley graphs for a qw. Here we connect isotropy with the unitarity conditions, which we report here for the reader's convenience:

$$\sum_{h \in S} A_h A_h^\dagger = \sum_{h \in S} A_h^\dagger A_h = I_s, \quad (98)$$

$$\sum_{hh'^{-1}=h''} A_h A_{h'}^\dagger = \sum_{h^{-1}h'=h''} A_h^\dagger A_{h'} = 0, \quad (99)$$

where  $h'' \in \{g \in G \mid g = hh'^{-1} \neq e : h, h' \in S\}$  and the  $A_h$  are the  $s \times s$  transition matrices of the qw on  $\Gamma(G, S)$ . The case under analysis here is  $s = 2$ , namely the transition matrices are  $2 \times 2$  complex matrices. Our aim is to use the unitarity constraints in order to establish some criteria to rule out some classes of presentations based on their relators. We introduce here a simple computational technique, generalizing the calculations performed in the scalar case (Chapter 6), to derive the transition matrices of a qw. This method is extensively used in the Appendices.

Since  $G \cong \mathbb{Z}^d$  for  $d = 1, 2, 3$ , we adopt the vector notation for the generators. Given a matrix  $O$ , it always admits a *polar decomposition*  $O = V|O|$ , where  $|O| := \sqrt{O^\dagger O}$  is positive (the modulus of  $O$ ), and  $V$  is unitary. Thus the transition matrices can be written as:

$$A_{\mathbf{h}} = V_{\mathbf{h}} |A_{\mathbf{h}}|. \quad (100)$$

Being  $S_+$  the orbit of a  $d$ -dimensional real vector under elements of  $\mathcal{O}(d)$ , the generators lie on a sphere and then for every  $\mathbf{h} \in S_+$  there is a unique way to express  $\mathbf{h}'' = 2\mathbf{h}$  with elements of  $S$ . Accordingly, from the set of constraints (99) one derives:

$$A_{\mathbf{h}} A_{-\mathbf{h}}^\dagger = 0, \quad (101)$$

$$A_{\mathbf{h}}^\dagger A_{-\mathbf{h}} = 0. \quad (102)$$

Eqs. (101) are equivalent to  $|A_{\mathbf{h}}| |A_{-\mathbf{h}}| = 0$  for every  $\mathbf{h} \in S_+$ . By definition, the transition matrices are nonvanishing, hence  $|A_{\mathbf{h}}|$  and  $|A_{-\mathbf{h}}|$  must be rank-one and must have orthogonal supports. Thus the following form

$$A_{\mathbf{h}} =: \alpha_{\mathbf{h}} V_{\mathbf{h}} |\eta_{\mathbf{h}}\rangle \langle \eta_{\mathbf{h}}|, \quad A_{-\mathbf{h}} =: \alpha_{-\mathbf{h}} V_{-\mathbf{h}} |\eta_{-\mathbf{h}}\rangle \langle \eta_{-\mathbf{h}}|, \quad (103)$$

holds, where  $\{|\eta_{+\mathbf{h}}\rangle, |\eta_{-\mathbf{h}}\rangle\}$  is an orthonormal basis and  $\alpha_{\mathbf{h}} > 0$  for every  $\mathbf{h} \in S_+$ . The isotropy requirement demands that the  $A_{\mathbf{h}}$  are unitarily equivalent (the same holds for the  $A_{-\mathbf{h}}$ ), and then  $\alpha_{\pm} := \alpha_{\pm\mathbf{h}} = \alpha_{\pm\mathbf{h}'}$ . Furthermore, we follow the argument of Ref. [ME96] to easily show that we can always choose  $V_{\mathbf{h}} = V_{-\mathbf{h}}$ . The conditions (102) imply that  $V_{\mathbf{h}}V_{-\mathbf{h}}^\dagger$  is diagonal in the basis  $\{|\eta_{+\mathbf{h}}\rangle, |\eta_{-\mathbf{h}}\rangle\}$ . Since the transition matrices are not full-rank, their polar decomposition is not unique: taking  $V_{\mathbf{h}}(|\eta_{+\mathbf{h}}\rangle\langle\eta_{+\mathbf{h}}| + e^{i\theta_{\mathbf{h}}}|\eta_{-\mathbf{h}}\rangle\langle\eta_{-\mathbf{h}}|)$  gives the same polar decomposition as  $V_{\mathbf{h}}$  for every  $\mathbf{h} \in S$ . Accordingly, one can tune the phases  $\theta_{\pm\mathbf{h}}$  to safely choose  $V_{\mathbf{h}}V_{-\mathbf{h}}^\dagger = I_s \forall \mathbf{h} \in S$ .

Suppose now that there exists a subgroup  $K \leq L$  such that for some  $\mathbf{h}_1 \in S_+$  the condition

$$\begin{aligned} \mathbf{h}_l, \mathbf{h}_m \in \{\mathbf{0}, \mathcal{O}_L(\mathbf{h}_1)\}, \forall \mathbf{h}_i, \mathbf{h}_j \in \mathcal{O}_K(\mathbf{h}_1) : \mathbf{h}_i \neq \mathbf{h}_j \\ \mathbf{h}_i - \mathbf{h}_j = \mathbf{h}_l - \mathbf{h}_m \iff (\mathbf{h}_i = \mathbf{h}_l) \vee (\mathbf{h}_i = -\mathbf{h}_m) \end{aligned} \quad (104)$$

holds. In this case, the set of equations

$$A_{\mathbf{h}_1}A_{\mathbf{h}_j}^\dagger + A_{-\mathbf{h}_j}A_{-\mathbf{h}_1}^\dagger = 0, \quad (105)$$

$$A_{\mathbf{h}_1}^\dagger A_{\mathbf{h}_j} + A_{-\mathbf{h}_j}^\dagger A_{-\mathbf{h}_1} = 0, \quad (106)$$

is derived from conditions (99) for every  $\mathbf{h}_j \in \mathcal{O}_K(\mathbf{h}_1)$ . Multiplying Eq. (105) by  $A_{\mathbf{h}_j}^\dagger$  on the left or by  $A_{\mathbf{h}_1}$  on the right, and using the form (103), we obtain

$$A_{\mathbf{h}_j}^\dagger A_{\mathbf{h}_1} A_{\mathbf{h}_j}^\dagger = A_{\mathbf{h}_1} A_{\mathbf{h}_j}^\dagger A_{\mathbf{h}_1} = 0.$$

Let  $U$  be a representation of  $L$  on  $\mathbb{U}(2)$ . Posing  $A_{\mathbf{h}_j} = U_k A_{\mathbf{h}_1} U_k^\dagger$  for some  $k \in K$  by isotropy, last relation reads

$$U_k A_{\mathbf{h}_1}^\dagger U_k^\dagger A_{\mathbf{h}_1} U_k A_{\mathbf{h}_1}^\dagger U_k^\dagger = A_{\mathbf{h}_1} U_k A_{\mathbf{h}_1}^\dagger U_k^\dagger A_{\mathbf{h}_1} = 0.$$

Exploiting again Eq. (103), the previous equation becomes

$$\langle \eta_{\mathbf{h}_1} | V_{\mathbf{h}_1}^\dagger U_k^\dagger V_{\mathbf{h}_1} | \eta_{\mathbf{h}_1} \rangle \langle \eta_{\mathbf{h}_1} | U_k | \eta_{\mathbf{h}_1} \rangle = 0.$$

Then, at least one among

$$\langle \eta_{\mathbf{h}_1} | V_{\mathbf{h}_1}^\dagger U_k^\dagger V_{\mathbf{h}_1} | \eta_{\mathbf{h}_1} \rangle = 0, \quad (107)$$

$$\langle \eta_{\mathbf{h}_1} | U_k | \eta_{\mathbf{h}_1} \rangle = 0, \quad (108)$$

must be satisfied. Furthermore, we remind that in Remark 4.3 we showed that the representation  $U$  can be always chosen with unit determinant: for  $s = 2$  this amounts to have

$$U_l = \cos \theta I_2 + i \sin \theta \mathbf{n}_l \cdot \boldsymbol{\sigma} \quad \forall l \in L,$$

where  $|\mathbf{n}_l| = 1$ . From either Eqs. (107) and (108) one has that

$$U_k = i \mathbf{n}_k \cdot \boldsymbol{\sigma} \quad \forall k \in K.$$

Making use of the identity

$$U_k U_{k'} = -\mathbf{n}_k \cdot \mathbf{n}_{k'} I_2 - i(\mathbf{n}_k \times \mathbf{n}_{k'}) \cdot \boldsymbol{\sigma},$$

it follows that all the  $\mathbf{n}_k$  must be mutually orthogonal and then  $|K| \leq 4$ . The case  $K \cong \mathbb{Z}_3$  cannot obey Eqs. (107) or (108) with  $U_K := \text{Rng}_K(U)$  faithful. We finally end up with  $K \in \{e, \mathbb{Z}_2, \mathbb{Z}_2 \times \mathbb{Z}_2, \mathbb{Z}_4\}$ .

Notice that, up to a change of basis, one can always choose  $|\eta_{\pm \mathbf{h}_1}\rangle$  to be the eigenstates of  $\sigma_z$  without loss of generality. Then, from Eqs. (107) and (108) and up to a change of basis, it must be:

$$U_K \in \{I_2, J_1, J_2, H\},$$

$$J_1 := \{I_2, i\sigma_x\}, \quad J_2 := \{I_2, -V_{\mathbf{h}_1}(i\sigma_x)V_{\mathbf{h}_1}^\dagger\}, \quad H := \{I_2, i\sigma_x, i\sigma_y, i\sigma_z\}.$$

We observe that  $H$  is a projective faithful representation of  $\mathbb{Z}_2 \times \mathbb{Z}_2$ , while  $J$  is a projective faithful representation of either  $\mathbb{Z}_4$  or  $\mathbb{Z}_2$ . We have thus proved the following lemma.

**Lemma 7.1.** *If the isotropy group  $L$  contains a subgroup  $K$  such that there exists  $\mathbf{h}_1 \in S_+$  such that  $\mathcal{O}_K(\mathbf{h}_1)$  satisfies condition (104), then  $U_K \in \{I_2, J_1, J_2, H\}$ .*

**Corollary 7.2.** *If  $L$  contains a ternary subgroup  $K \cong \mathbb{Z}_3$  such that there exists  $\mathbf{h}_1 \in S_+$  such that  $\mathcal{O}_K(\mathbf{h}_1)$  satisfies condition (104), then the set of vertices  $\mathcal{O}_L(\mathbf{h}_1)$  cannot satisfy the necessary conditions (105) and (106) for unitarity.*

**Proof.** By Prop. 7.1  $K$  has to be, up to a change of basis and a sign, a subgroup of the Heisenberg group  $H$ . However  $H$  does not contain ternary subgroups. ■

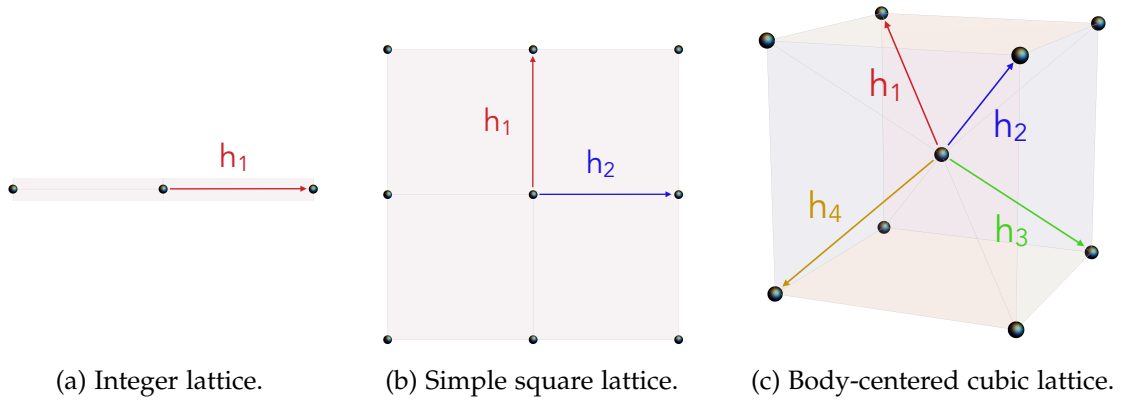


Figure 8: We report here the primitive cells of the unique graphs admitting isotropic QWs in dimensions  $d = 1, 2, 3$ . Figure 8(a): the isotropy groups can be  $U_L = \{I\}$  and  $U_L = \{I, i\sigma_X\}$ , corresponding respectively to  $S_+ = \{\mathbf{h}_1\}$  and  $S_+ \equiv S_- = \{\mathbf{h}_1, -\mathbf{h}_1\}$ . Figure 8(b): the isotropy groups can be  $U_L = \{I, i\sigma_X\}, \{I, i\sigma_Z\}$  and  $U_L = \{I, i\sigma_X, i\sigma_Y, i\sigma_Z\}$ , corresponding respectively to  $S_+ = \{\mathbf{h}_1, \mathbf{h}_2\}$  and  $S_+ \equiv S_- = \{\mathbf{h}_1, \mathbf{h}_2, -\mathbf{h}_1, -\mathbf{h}_2\}$ . Figure 8(c): the only possible isotropy group is  $U_L = \{I, i\sigma_X, i\sigma_Y, i\sigma_Z\}$ , corresponding to  $S_+ = \{\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \mathbf{h}_4\}$  with the nontrivial relator  $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 + \mathbf{h}_4 = 0$ . We notice that the case  $d = 1$  is the only one supporting the self-interaction, namely such that  $A_e \neq 0$ .

### 7.3 THE EUCLIDEAN ISOTROPIC QWS WITH MINIMAL COMPLEXITY: THE WEYL QUANTUM WALKS

Throughout the present section, we solve the unitarity conditions in dimension  $d = 1, 2, 3$  for the Cayley graphs associated to the primitive cells shown in Fig. 8, and for all the possible isotropy groups. We remind that in general each isotropy group gives rise to a distinct presentation for  $\mathbb{Z}^d$ , possibly with the same first-neighbours structure. As discussed in Fig. 8, different presentations can be in general associated to the same primitive cell (one can include in  $S_+$  the inverses or not). We will now prove our main result, which is stated in Prop. 7.1 after the following derivation.

**Theorem 7.1** (Classification of the isotropic QWs on lattices of dimension  $d = 1, 2, 3$  for cell dimension  $s = 2$ ). *Let  $S = S_+ \cup S_- \cup \{e\}$  denote a set of generators for  $\mathbb{Z}^d$  and let  $\{A_{\mathbf{h}}\}_{\mathbf{h} \in S}$  denote the set of transition matrices of a QW on  $\mathbb{Z}^d$  with cell dimension  $s = 2$  and isotropic on  $S_+$ . Then for each  $d = 1, 2, 3$  the admissible graphs are unique (see Fig. 8) and one has the following:*

a) Case  $d = 1$ :

$$A_{\mathbf{h}_1} = V \begin{pmatrix} n & 0 \\ 0 & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = V \begin{pmatrix} 0 & 0 \\ 0 & n \end{pmatrix},$$

$$A_e = V \begin{pmatrix} 0 & im \\ im & 0 \end{pmatrix},$$

where  $n, m$  are real such that  $n^2 + m^2 = 1$ , and  $V$  is an arbitrary unitary if  $S_+ = \{\mathbf{h}_1\}$  or  $V$  is a unitary commuting with  $\sigma_X$  if  $S_+ = \{\mathbf{h}_1, -\mathbf{h}_1\}$ .

b) Case  $d = 2$ : one has  $A_e = 0$  and

$$A_{\mathbf{h}_1} = \frac{1}{2}V \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = \frac{1}{2}V \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix},$$

$$A_{\mathbf{h}_2} = \frac{1}{2}V \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \quad A_{-\mathbf{h}_2} = \frac{1}{2}V \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix},$$

where  $V$  is a unitary commuting with  $\sigma_X$  if  $S_+ = \{\mathbf{h}_1, \mathbf{h}_2\}$  or  $V = I$  if  $S_+ = \{\mathbf{h}_1, \mathbf{h}_2, -\mathbf{h}_1, -\mathbf{h}_2\}$ .

c) Case  $d = 3$ : one has  $A_e = 0$  and

$$A_{\mathbf{h}_1} = \begin{pmatrix} \eta^\pm & 0 \\ \eta^\pm & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = \begin{pmatrix} 0 & -\eta^\mp \\ 0 & \eta^\mp \end{pmatrix},$$

$$A_{\mathbf{h}_2} = \begin{pmatrix} 0 & \eta^\pm \\ 0 & \eta^\pm \end{pmatrix}, \quad A_{-\mathbf{h}_2} = \begin{pmatrix} \eta^\mp & 0 \\ -\eta^\mp & 0 \end{pmatrix},$$

$$A_{\mathbf{h}_3} = \begin{pmatrix} 0 & -\eta^\pm \\ 0 & \eta^\pm \end{pmatrix}, \quad A_{-\mathbf{h}_3} = \begin{pmatrix} \eta^\mp & 0 \\ \eta^\mp & 0 \end{pmatrix},$$

$$A_{\mathbf{h}_4} = \begin{pmatrix} \eta^\pm & 0 \\ -\eta^\pm & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_4} = \begin{pmatrix} 0 & \eta^\mp \\ 0 & \eta^\mp \end{pmatrix}.$$

where  $\eta^\pm = \frac{1 \pm i}{4}$  and  $S_+ = \{\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \mathbf{h}_4\}$  with the nontrivial relator  $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 + \mathbf{h}_4 = 0$ .

*Proof.* In Appendix A we make use of Proposition 7.1 along with the unitarity constraints to exclude an infinite set of Cayley graphs arising from the finite subgroups of  $O(3)$  enumerated in (97). The remaining admissible graphs are those presented in Fig. 8).

Before starting the derivation, we remind that in each case we can choose  $|\eta_{\pm\mathbf{h}_1}\rangle$  to be the eigenstates of  $\sigma_Z$ . Moreover, we will make use of Eq. (103) to represent the transition matrices, reminding that  $V_{\mathbf{h}} = V_{-\mathbf{h}}$ . Finally, we recall that in Remark. 4.3 we showed that one can always impose condition (48) and then multiply the transition matrices on the left by an arbitrary unitary commuting with the elements of the representation  $U_L$ .

**Case  $d = 1$ .** We can write the transition matrices associated to  $\pm\mathbf{h}_1$  as

$$A_{\mathbf{h}_1} = \alpha_+ V |\eta_{\mathbf{h}_1}\rangle \langle \eta_{\mathbf{h}_1}|, \quad A_{-\mathbf{h}_1} = \alpha_- V |\eta_{-\mathbf{h}_1}\rangle \langle \eta_{-\mathbf{h}_1}|.$$

Multiplying on the right respectively by  $A_{\mathbf{h}_1}$  and  $A_{-\mathbf{h}_1}^\dagger$  the unitarity conditions

$$\begin{aligned} A_{\mathbf{h}_1} A_e^\dagger + A_e A_{-\mathbf{h}_1}^\dagger &= 0, \\ A_e^\dagger A_{\mathbf{h}_1} + A_{-\mathbf{h}_1}^\dagger A_e &= 0, \end{aligned} \tag{109}$$

one obtains

$$A_{\pm\mathbf{h}_1} A_e^\dagger A_{\pm\mathbf{h}_1} = 0,$$

which implies  $A_e = VW$ , where  $W$  has vanishing diagonal elements in the basis  $\{|\eta_{+\mathbf{h}_1}\rangle, |\eta_{-\mathbf{h}_1}\rangle\}$ . Substituting into Eqs. (109), one derives  $\alpha_+ = \alpha_- =: n$  and, up to a change of basis,  $A_e = imV\sigma_X$  with  $m \geq 0$ . Imposing the normalization condition (30) amounts to the relation  $n^2 + m^2 = 1$ . The admissible isotropy groups are  $I$  and, up to a change of basis,  $J_1$ . Then, for  $U_L = \{I\}$ , the transition matrices are given by:

$$\begin{aligned} A_{\mathbf{h}_1} &= V \begin{pmatrix} n & 0 \\ 0 & 0 \end{pmatrix}, & A_{-\mathbf{h}_1} &= V \begin{pmatrix} 0 & 0 \\ 0 & n \end{pmatrix}, \\ A_e &= V \begin{pmatrix} 0 & im \\ im & 0 \end{pmatrix}, \end{aligned}$$

where  $V$  is an arbitrary unitary. For  $U_L = \{I, i\sigma_X\}$ , we impose condition (48) and then  $V$  can be taken as an arbitrary unitary commuting with  $\sigma_X$ .



**Case  $d = 2$ .** The form of the transition matrices is:

$$\begin{aligned} A_{\pm\mathbf{h}_1} &= \alpha_{\pm} V_{\mathbf{h}_1} |\eta_{\pm\mathbf{h}_1}\rangle \langle \eta_{\pm\mathbf{h}_1}|, \\ A_{\pm\mathbf{h}_2} &= \alpha_{\pm} V_{\mathbf{h}_2} |\eta_{\pm\mathbf{h}_2}\rangle \langle \eta_{\pm\mathbf{h}_2}|. \end{aligned}$$

Multiplying on the right by  $A_{\mathbf{h}_1}$  the unitarity conditions

$$A_{\mathbf{h}_1} A_{\pm\mathbf{h}_2}^{\dagger} + A_{\mp\mathbf{h}_2} A_{-\mathbf{h}_1}^{\dagger} = 0, \quad (110)$$

one obtains

$$A_{\mathbf{h}_1} A_{\pm\mathbf{h}_2}^{\dagger} A_{\mathbf{h}_1} = 0.$$

The latter implies either i)  $|\eta_{\pm\mathbf{h}_1}\rangle = |\eta_{\pm\mathbf{h}_2}\rangle$  or ii)  $|\eta_{\pm\mathbf{h}_1}\rangle = |\eta_{\mp\mathbf{h}_2}\rangle$  and that, in both cases, one can choose  $V_{\mathbf{h}_1} = V_{\mathbf{h}_2}(i\sigma_Y)$  up to a change of basis. In either cases, substituting into Eqs. (110) one derives  $\alpha_+ = \alpha_- =: \alpha$  and, from the normalization condition (30),  $\alpha = \frac{1}{\sqrt{2}}$ . Redefining  $V := V_{\mathbf{h}_2}$ , in case i) one obtains the following family of transition matrices:

$$\begin{aligned} A_{\pm\mathbf{h}_1} &= \pm\alpha V |\eta_{\mp\mathbf{h}_1}\rangle \langle \eta_{\pm\mathbf{h}_1}|, \\ A_{\pm\mathbf{h}_2} &= \alpha V |\eta_{\pm\mathbf{h}_1}\rangle \langle \eta_{\pm\mathbf{h}_1}|. \end{aligned} \quad (111)$$

The second family, namely case ii), is connected to the first one via the exchange  $\mathbf{h}_2 \leftrightarrow -\mathbf{h}_2$ . One can check that the self-interaction term  $T_e \otimes A_e$  is not supported by the unitarity conditions

$$A_{\mathbf{h}} A_e^{\dagger} + A_e A_{-\mathbf{h}}^{\dagger} = A_{\mathbf{h}}^{\dagger} A_e + A_e^{\dagger} A_{-\mathbf{h}} = 0 \quad \forall \mathbf{h} \in S,$$

namely  $A_e = 0$ . Imposing condition (48), one can choose

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

and then multiply the transition matrices by a unitary commuting with the representation  $U_L$ . The isotropy group can be either  $J_2 \equiv \{I, i\sigma_Z\}$  or  $H$  for the first family of

walks, while either  $J_1 = \{I, i\sigma_X\}$  or  $H$  for the second one. Thus the first family is given by

$$\begin{aligned} A_{\mathbf{h}_1} &= \frac{1}{2}V \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, & A_{-\mathbf{h}_1} &= \frac{1}{2}V \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}, \\ A_{\mathbf{h}_2} &= \frac{1}{2}V \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, & A_{-\mathbf{h}_2} &= \frac{1}{2}V \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \end{aligned}$$

where  $V$  is either an arbitrary unitary commuting with  $\sigma_Z$  or  $V = I$ , while the second family of transition matrices is obtained exchanging  $\mathbf{h}_2 \leftrightarrow -\mathbf{h}_2$  and taking  $V$  as either an arbitrary unitary commuting with  $\sigma_X$  or  $V = I$ .

**Case  $d = 3$ .** The isotropy requirement can be fulfilled with  $U_L = H$ . At least one of the two conditions of Eqs. (107) or (108) must be fulfilled for any nontrivial  $l \in L$ . Since Eq. (108) cannot be satisfied for  $U_l = i\sigma_Z$ , then it must be  $\langle \eta_{\mathbf{h}_1} | V_{\mathbf{h}_1}^\dagger \sigma_Z V_{\mathbf{h}_1} | \eta_{\mathbf{h}_1} \rangle = 0$ . This implies

$$\text{Tr}[V_{\mathbf{h}_1}^\dagger \sigma_Z V_{\mathbf{h}_1} \sigma_Z] = 0. \quad (112)$$

Writing  $V_{\mathbf{h}_1}$  in the general unitary form

$$V_{\mathbf{h}_1} = \theta \begin{pmatrix} \mu & -\nu^* \\ \nu & \mu^* \end{pmatrix},$$

where  $|\theta|^2 = |\mu|^2 + |\nu|^2 = 1$ , the condition in Eq. (112) implies  $|\mu| = |\nu| = 2^{-1/2}$ , and using the polar decomposition (103) of  $A_{\pm\mathbf{h}_1}$  we obtain

$$A_{\mathbf{h}_1} = \frac{\alpha_+}{\sqrt{2}} \begin{pmatrix} \phi & 0 \\ \psi & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = \frac{\alpha_-}{\sqrt{2}} \begin{pmatrix} 0 & -\psi^* \\ 0 & \phi^* \end{pmatrix}, \quad (113)$$

with  $\phi, \psi$  phase factors. Using isotropy, namely considering the orbit of the above matrices under conjugation with  $H$ , we obtain

$$\begin{aligned} A_{\mathbf{h}_2} &= \frac{\alpha_+}{\sqrt{2}} \begin{pmatrix} 0 & \psi \\ 0 & \phi \end{pmatrix}, & A_{-\mathbf{h}_2} &= \frac{\alpha_-}{\sqrt{2}} \begin{pmatrix} \phi^* & 0 \\ -\psi^* & 0 \end{pmatrix}, \\ A_{\mathbf{h}_3} &= \frac{\alpha_+}{\sqrt{2}} \begin{pmatrix} 0 & -\psi \\ 0 & \phi \end{pmatrix}, & A_{-\mathbf{h}_3} &= \frac{\alpha_-}{\sqrt{2}} \begin{pmatrix} \phi^* & 0 \\ \psi^* & 0 \end{pmatrix}, \\ A_{\mathbf{h}_4} &= \frac{\alpha_+}{\sqrt{2}} \begin{pmatrix} \phi & 0 \\ -\psi & 0 \end{pmatrix}, & A_{-\mathbf{h}_4} &= \frac{\alpha_-}{\sqrt{2}} \begin{pmatrix} 0 & \psi^* \\ 0 & \phi^* \end{pmatrix}. \end{aligned} \quad (114)$$

Also in this case, the self-interaction term is not supported by the unitarity conditions. Finally, we can write the matrix  $A_{\mathbf{k}}$  in Eq. (3.2.1) as

$$A_{\mathbf{k}} = \sum_{i=1}^4 (A_{\mathbf{h}_i} e^{ik_i} + A_{-\mathbf{h}_i} e^{-ik_i})$$

and imposing unitarity of  $A_{\mathbf{k}}$  for every  $\mathbf{k}$ , one obtains the following conditions

$$\alpha_+^2 = \alpha_-^2 = \frac{1}{4}, \quad \phi^{*2} + \phi^2 = \psi^{*2} + \psi^2 = 0,$$

namely

$$\phi, \psi \in \left\{ \pm \zeta^+ := \pm \frac{1+i}{\sqrt{2}}, \pm \zeta^- := \pm \frac{1-i}{\sqrt{2}} \right\}.$$

The different choices of the overall signs for  $\phi, \psi$  are connected to each other by an overall phase factor and by unitary conjugation by  $\sigma_Z$ . Then we can fix them choosing the plus signs. The choices  $\phi = \zeta^\pm, \psi = \zeta^\mp$  are equivalent to  $\phi = \psi = \zeta^\pm$  via conjugation of the former by  $e^{\pm i \frac{\pi}{4} \sigma_Z}$  and an exchange  $\mathbf{h}_1 \leftrightarrow \mathbf{h}_4$ . Accordingly, the QWs found are given by the transition matrices of Eqs. (113) and (114) with  $\psi = \phi = \zeta^\pm$ , namely the two Weyl QWs presented in Ref. [86]. ■

Confronting the one-dimensional space with the QWs on the infinite dihedral group derived in Chapter 6, we thus also proved the following result.

**Corollary 7.3.** *The set of scalar QWs on  $D_\infty$  admitting a coarse-grained on the line coincides with the set of parity-invariant QWs on  $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ .*



Part III

EUCLIDEAN QUANTUM WALKS AND BEYOND



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## THE GROUP EXTENSION PROBLEM

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### 8.1 CONSTRUCTING EXTENSIONS OF GROUPS

We wish to characterize the groups which can be built up starting from two groups  $N, Q$  and such that  $N$  is a normal subgroup of  $G$  and  $G/N \cong Q$ . Technically speaking, this characterization is called *group extension problem*.

**Definition 8.1** (Extension of groups). *Let  $N$  and  $Q$  be two groups. A group  $G$  is said to be an extension of  $N$  by  $Q$  if  $G$  contains a normal subgroup  $N$  such that the quotient group  $G/N$  is isomorphic to  $Q$ .*

We recall that, by Definition 2.23,  $G$  is an extension of  $N$  by  $Q$  if and only if  $G$  is a  $N$ -by- $Q$  group. We warn the reader that it is not rare to find in the literature the nomenclature “extension of  $Q$  by  $N$ ” to indicate a  $N$ -by- $Q$  group. In our opinion this terminology can be misleading, since the quotient  $Q$  can fail to be a subgroup of the  $N$ -by- $Q$  extension  $G$ . In the present section we shall not make further assumptions on  $N$  (or  $Q$ ), while in the following we will restrict to the case of interest  $N \cong \mathbb{Z}^d$ . We now characterize the extension problem in full generality.

Let  $G$  be an arbitrary extension of  $N$  by  $Q$ . The cardinality  $|Q|$  (i.e. the order of the group  $Q$ ) is precisely the index of  $N$  in  $G$ . The identity of  $Q$  will be denoted by  $\tilde{e}$ . The elements  $q \in Q$  are in a bijective correspondence with the cosets representatives  $c_q$ ,

which (by normality of  $N$ ) follow the same composition rules of the elements  $q$  up to a multiplication by elements of  $N$ , namely one has

$$c_{q_1}c_{q_2}c_{q_1q_2}^{-1} \in N \quad \forall q_1, q_2 \in Q. \quad (115)$$

Now we shall show how to construct the extensions  $G$  of  $N$  by  $Q$ . By definition, any element  $g \in G$  can be decomposed in a unique fashion as  $g = nc_q$ , where  $n \in N$  and  $c_q$  is the representative of the coset corresponding to  $q \in Q$ . The group composition law can be obtained as follows

$$n_1c_{q_1}n_2c_{q_2} = n_1c_{q_1}n_2c_{q_1}^{-1}c_{q_1}c_{q_2} =: n_1\varphi_{q_1}(n_2)f(q_1, q_2)c_{q_1q_2},$$

where

$$\varphi_q(n) = c_qnc_q^{-1}, \quad f(q_1, q_2) = c_{q_1}c_{q_2}c_{q_1q_2}^{-1}$$

and clearly

$$\varphi_q \in \text{Aut}(N), \quad f(q_1, q_2) \in N \quad \forall q, q_1, q_2 \in Q.$$

Hence, a piece of information we need in order to construct the extension  $G$  is the assignment of a composition rule for the coset representatives: this observation motivates the following definition.

**Definition 8.2** (2-cocycle). *Let  $G$  be an extension of  $N$  by  $Q$  and  $c_q$  the representatives of the cosets of  $N$  in  $G$ . The map  $f : Q \times Q \rightarrow N$  defined by*

$$f(q_1, q_2) := c_{q_1}c_{q_2}c_{q_1q_2}^{-1} \quad \forall q_1, q_2 \in Q$$

*is called a 2-cocycle.*

From Definition 8.2 it follows that the element  $f(\bar{e}, q) = c_{\bar{e}}$  is independent from  $q$  for every  $q \in Q$ . Accordingly, the composition rule of the coset representatives does not change for any choice of  $c_{\bar{e}}$ : this means that two extensions of  $N$  by  $Q$ , differing just by a choice of  $c_{\bar{e}}$ , result to be isomorphic. Thus, one can just pose  $c_{\bar{e}} \equiv e$ . From relation (115) one has that

$$\varphi_{q_1} \circ \varphi_{q_2} \circ \varphi_{q_1q_2}^{-1} \in \text{Inn}(N)$$



and indeed, for  $n \in N$ ,

$$\varphi_{q_1} \circ \varphi_{q_2}(n) = (c_{q_1} c_{q_2}) n (c_{q_1} c_{q_2})^{-1} =: \varphi_{f(q_1, q_2)} \circ \varphi_{q_1 q_2}(n) \quad \forall q_1, q_2 \in Q, \quad (116)$$

where for every  $m \in N$  we defined the inner automorphism of  $N$

$$\phi_m(\cdot) = m \cdot m^{-1}. \quad (117)$$

Then  $\{\varphi_q\}_{q \in Q}$  can be identified as a family of outer automorphisms. Since  $\text{Inn}(N) \leq \text{Aut}(N)$  and  $\text{Out}(N) = \text{Aut}(N)/\text{Inn}(N)$  (see Remark 2.1), relation (116) induces a homomorphism from  $q \in Q$  to  $\text{Out}(N)$  via the following maps:

$$\begin{aligned} \varphi: Q &\longrightarrow \text{Aut}(N) \\ q &\longmapsto \varphi_q \end{aligned}$$

and

$$\begin{aligned} \pi: \text{Aut}(N) &\longrightarrow \text{Out}(N) \\ \varphi_q &\longmapsto \pi(\varphi_q), \end{aligned}$$

such that their composition  $\tilde{\varphi} := \pi \circ \varphi$  is a group homomorphism. We remind that, in general, the elements of  $\text{Out}(N)$  are not outer automorphisms of  $N$ . The outer automorphism  $\varphi_q$  is a coset representative corresponding to the element  $\tilde{\varphi}_q$ . Therefore, in order to identify a group extension one need to choose a family of outer automorphisms of  $N$  and a 2-cocycle, i.e. a pair  $(\varphi, f)$  such that Eq. (116) is satisfied.

We now provide necessary and sufficient conditions on  $\varphi, f$  to give rise to a group extension. Before this, we give a convenient definition.

**Definition 8.3** (Centre of a group). *Let  $G$  be a group. The center of  $G$  is the subset  $Z(G) \subseteq G$  of elements commuting with every element of  $G$ , namely*

$$Z(G) := \{z \in G \mid zg = gz \quad \forall g \in G\}.$$

**Lemma 8.1.** *Let  $N$  and  $Q$  be two groups. Then there exists an extension  $G$  of  $N$  by  $Q$  if and only if there exist two maps,  $\varphi : Q \rightarrow \text{Aut}(N)$  and  $f : Q \times Q \rightarrow N$ , obeying relation (116) and with  $f$  satisfying the following two properties:*

$$f(q, \tilde{e}) = f(\tilde{e}, q) = e \quad \forall q \in Q, \quad (118)$$

$$f(q_1, q_2)f(q_1q_2, q_3) = \varphi_{q_1}(f(q_2, q_3))f(q_1, q_2q_3) \quad \forall q_1, q_2, q_3 \in Q. \quad (119)$$

**Proof.** ( $\Rightarrow$ ) Eq. (118) follows from the definition of 2-cocycle along with the choice  $c_{\tilde{e}} = e$ . Let us now prove relation (119) imposing associativity to the product of the coset representatives. On the one hand, one has

$$(c_{q_1}c_{q_2})c_{q_3} = f(q_1, q_2)c_{q_1q_2}c_{q_3} = f(q_1, q_2)f(q_1q_2, q_3)c_{q_1q_2q_3}, \quad \forall q_1, q_2, q_3 \in Q.$$

On the other hand, also

$$\begin{aligned} c_{q_1}(c_{q_2}c_{q_3}) &= c_{q_1}f(q_2, q_3)c_{q_2q_3} = \varphi_{q_1}(f(q_2, q_3))c_{q_1}c_{q_2q_3} = \\ &= \varphi_{q_1}(f(q_2, q_3))f(q_1, q_2q_3)c_{q_1q_2q_3}, \quad \forall q_1, q_2, q_3 \in Q. \end{aligned}$$

holds. Relation (119) follows confronting the last two equation.

( $\Leftarrow$ ) Let  $N$  and  $Q$  be two groups. Define  $G$  as the set of the ordered pairs  $(n, q) \in N \times Q$  equipped with the composition law

$$(n_1, q_1)(n_2, q_2) := (n_1\varphi_{q_1}(n_2)f(q_1, q_2), q_1q_2),$$

where the maps  $\varphi : Q \rightarrow \text{Aut}(N)$  and  $f : Q \times Q \rightarrow N$  obey relation (116) and  $f$  satisfies the properties (118) and (119). Let us now show that  $G$  is an extension of  $N$  by  $Q$ . From the above composition law and using the properties of  $\varphi$  and  $f$ , one can verify that  $G$  is a group with  $e = (e_N, \tilde{e})$  and inverses given by

$$(n, q)^{-1} = \left( \varphi_q^{-1}(n^{-1}f(q, q^{-1})^{-1}), q^{-1} \right).$$

One can also check that the pairs  $(n, \tilde{e})$  form a normal subgroup isomorphic to  $N$ . For consistency we finally need to check that, upon defining

$$\varphi'_q((n, \tilde{e})) := c_q(n, \tilde{e})c_q^{-1} \quad \forall q \in Q, \forall n \in N, \forall c_q \in G, \quad (120)$$

one has  $\varphi'_q((n, \tilde{e})) = (\varphi_q(n), \tilde{e})$  for every  $q \in Q$  and every  $n \in N$ . Indeed, denoting  $c_q = (n_q, q)$ , Eq. (120) reads

$$(\varphi_q(n), \tilde{e}) = (n_q, q)(n, \tilde{e})(\varphi_q^{-1}(n_q^{-1}f(q, q^{-1})^{-1}), q^{-1}),$$

obtaining

$$(\varphi_q(n), \tilde{e}) = (n_q \varphi_q(n) n_q^{-1}, \tilde{e}).$$

Then one can just choose  $n_q \in Z(N)$  for every  $q \in Q$ , obtaining the extension corresponding to fixed  $\varphi$  and  $f$ . ■

For two given fixed groups  $N$  and  $Q$ , in order to construct an extension of  $N$  by  $Q$  one then has to choose a map  $\varphi$  and a 2-cocycle  $f$ . Nevertheless, two extensions with different choices of  $\varphi$  and  $f$  may still be isomorphic.

**Definition 8.4** (Pseudo-congruence). *Let  $G$  and  $G'$  be two extensions of  $N$  by  $Q$ , and  $\alpha \in \text{Aut}(N)$  and  $\beta \in \text{Aut}(Q)$ .  $G$  and  $G'$  are called pseudo-congruent extensions if there exists an isomorphism  $\psi : G \rightarrow G'$  such that*

$$\psi(nc_q) = \alpha(n)c'_{\beta(q)} \quad \forall n \in N, \forall q \in Q. \quad (121)$$

**Lemma 8.2.** *Let  $G$  be an extension of  $N$  by  $Q$  with assigned outer automorphisms  $\{\varphi_q\}_{q \in Q}$ . Then there exists a pseudo-congruent extension  $G'$  with associated outer automorphisms  $\{\varphi'_q\}_{q \in Q}$  if and only if there exist  $\alpha \in \text{Aut}(N)$  and  $\beta \in \text{Aut}(Q)$  such that*

$$\varphi_q = \alpha^{-1} \circ \varphi'_{\beta(q)} \circ \alpha \quad \forall q \in Q. \quad (122)$$

**Proof.** ( $\Rightarrow$ ) By definition, there exists an isomorphism  $\psi : G \rightarrow G'$  satisfying Eq. (121) for some  $\alpha \in \text{Aut}(N)$  and  $\beta \in \text{Aut}(Q)$ . Clearly, the condition

$$\alpha(f(q_1, q_2)) = \psi(c_{q_1}c_{q_2}c_{q_1q_2}^{-1}) = c'_{\beta(q_1)}c'_{\beta(q_2)}c'^{-1}_{\beta(q_1q_2)} = f'(\beta(q_1), \beta(q_2)) \quad (123)$$

must hold  $\forall q_1, q_2 \in Q$ . Moreover, one has  $n_1\varphi_{q_1}(n_2)f(q_1, q_2)c_{q_1q_2} = n_1c_{q_1}n_2c_{q_2}$  and then, letting  $\psi$  act on both sides, one obtains

$$\begin{aligned} \alpha(n_1)\alpha \circ \varphi_{q_1}(n_2)\alpha(f(q_1, q_2))c'_{\beta(q_1q_2)} &= \\ &= \alpha(n_1)c'_{\beta(q_2)}\alpha(n_2)c'_{\beta(q_2)} = \alpha(n_1)\varphi'_{\beta(q_1)} \circ \alpha(n_2)f'(\beta(q_1), \beta(q_2))c'_{\beta(q_1q_2)}. \end{aligned} \quad (124)$$

Using condition (123), Eq. (124) finally gives Eq. (122).

( $\Leftarrow$ ) Let  $\alpha, \beta, \varphi'_q$  satisfy Eq. (122). Then one has

$$\begin{aligned}\varphi'_{q_1} \circ \varphi'_{q_2} &= \alpha \circ \varphi_{\beta^{-1}(q_1)} \circ \varphi_{\beta^{-1}(q_2)} \circ \alpha^{-1} = \alpha \circ \phi_{f(\beta^{-1}(q_1), \beta^{-1}(q_2))} \circ \varphi_{\beta^{-1}(q_1 q_2)} \circ \alpha^{-1} \\ &= \alpha \circ \phi_{f(\beta^{-1}(q_1), \beta^{-1}(q_2))} \circ \alpha^{-1} \circ \varphi'_{q_1 q_2},\end{aligned}$$

where we used the definition 117. Since  $\text{Inn}(N) \subseteq \text{Aut}(N)$ , there exists  $f'(q_1, q_2) \in N$  such that

$$\alpha \circ \phi_{f(\beta^{-1}(q_1), \beta^{-1}(q_2))} \circ \alpha^{-1} = \phi_{f'(q_1, q_2)}.$$

In particular, one can easily check that

$$f'(q_1, q_2) = \alpha(f(\beta^{-1}(q_1), \beta^{-1}(q_2))),$$

which is a 2-cocycle: it satisfies the properties of Lemma 8.1 since  $\alpha$  is an automorphism. Then  $\varphi'$  satisfies Eq. (116) and it thus defines, along with  $f'$ , an extension  $G'$  pseudo-congruent to  $G$  via the automorphisms  $\alpha$  and  $\beta$ . ■

**Lemma 8.3.** *Let  $G$  be an extension of  $N$  by  $Q$  with outer automorphisms  $\{\varphi_q\}_{q \in Q}$ . Then any extension  $G'$  with  $\{\varphi'_q\}_{q \in Q}$  differs from  $G$  for a change of cosets representatives if and only if there exist a family  $\{\phi_{n_q}\}_{q \in Q}$  of inner automorphisms such that*

$$\varphi'_q = \phi_{n_q} \circ \varphi_q \quad \forall q \in Q \tag{125}$$

with  $n_{\bar{e}} = e$ .

**Proof.** ( $\Rightarrow$ ) A change of cosets representatives  $c_q \mapsto n_q c_q$  leads to

$$\varphi_q(\cdot) = c_q \cdot c_q^{-1} \mapsto (n_q c_q) \cdot (n_q c_q)^{-1} = n_q (c_q \cdot c_q^{-1}) n_q^{-1} \equiv \phi_{n_q} \circ \varphi_q(\cdot)$$

and Eq. (125) holds. One can always choose  $e = n_{\bar{e}} c_{\bar{e}} = n_{\bar{e}}$ .

( $\Leftarrow$ ) Given  $\varphi'_q = \phi_{n_q} \circ \varphi_q$  for every  $q \in Q$  with  $n_{\bar{e}} = e$ , one can construct an extension  $G'$  as follows: take  $c'_q = h_q n_q c_q$ , with  $h_q \in Z(N)$  and  $h_{\bar{e}} = e$ ; this is the most general

choice satisfying Eq. (125) posing  $\varphi'_q(\cdot) := c'_q \cdot c'_q{}^{-1}$ . We have to check that the quantity defined as

$$f'(q_1, q_2) := c'_{q_1} c'_{q_2} c'_{q_1 q_2}{}^{-1} = h_1 \varphi_{q_1}(h_2) h_{12}^{-1} n_1 \varphi_{q_1}(n_2) f(q_1, q_2) n_{12}^{-1} \quad (126)$$

is a 2-cocycle. This can be done by direct computation, using the fact that  $f$  is a 2-cocycle and that every automorphism  $\varphi_q$  maps  $Z(N)$  to itself, thus verifying that both properties (118) and (119) hold. Finally, using Eq. (125), one has

$$\begin{aligned} \varphi'_{q_1} \circ \varphi'_{q_2} &\equiv \phi_{n_1} \circ \varphi_{q_1} \circ \phi_{n_2} \circ \varphi_{q_2} = \phi_{n_1} \circ \phi_{\varphi_{q_1}(n_2)} \circ \varphi_{q_1} \circ \varphi_{q_2} = \\ &= \phi_{n_1} \circ \phi_{\varphi_{q_1}(n_2)} \circ \phi_{f(q_1, q_2)} \circ \varphi_{q_1 q_2} \equiv \phi_{n_1 \varphi_{q_1}(n_2) f(q_1, q_2) n_{12}^{-1}} \circ \varphi'_{q_1 q_2} \end{aligned}$$

namely  $\varphi'$  satisfies Eq. (116) with  $f'$ . The extension we constructed differs from  $G$  for the change of coset representatives  $c_q \mapsto h_q n_q c_q$ . ■

Lemma 8.2 implies that in order to find the equivalence classes of pseudo-congruent extensions one can just consider the classes of homomorphisms  $\tilde{\varphi}$  up to pre-composition with arbitrary  $\beta \in \text{Aut}(Q)$  and conjugation with arbitrary  $\alpha \in \text{Aut}(N)$  (namely the conjugacy classes in  $\text{Aut}(N)$ ). Furthermore, for a fixed  $\tilde{\varphi}$ , different maps  $\varphi$  lead to equivalent extensions, since Lemma 8.3 implies that just the homomorphism  $\tilde{\varphi}$  is relevant in order to construct extensions (up to a change of the cosets representatives).

Finally, from Eq. (126) one has that, for a fixed homomorphism  $\tilde{\varphi}$ , two different 2-cocycles  $f, f'$  lead to the same extension up to a change of the cosets representatives if there exists  $\{n_i\}_{q_i \in Q}$  with  $n_i \in N \forall i$  such that

$$f'(q_1, q_2) = n_1 \varphi_{q_1}(n_2) f(q_1, q_2) n_{12}^{-1} \quad (127)$$

is satisfied  $\forall q_1, q_2 \in Q$ . Chosen  $f$ , one can find the families of  $f'$  and  $n_i \in N$  satisfying Eq. (127) and, for  $f$  fixed, the conjugacy classes of maps  $\tilde{\varphi}$  up to pre-composition with arbitrary automorphisms of  $Q$  classify the extensions up to pseudo-congruence. Unfortunately, it is not known a general criterion to classify and construct extension up to arbitrary isomorphisms, but this can possibly be done considering the particular groups  $N, Q$  under study.

## 8.2 INDUCED REPRESENTATIONS

The material of the present section is an application and expansion of the coarse-graining procedure presented in Chapter 5. Let  $G$  be a finitely generated group and  $N$  a subgroup of  $G$ . One can define a unitary mapping between  $\mathcal{H} = \ell^2(G)$  and  $\mathcal{K} = \ell^2(N) \otimes \ell^2(G/N)$  in the following way:

$$U_N: \mathcal{H} \longrightarrow \mathcal{K},$$

$$|nc_q\rangle \longmapsto |n\rangle\langle q|,$$

represented by the operator

$$U_N = \sum_{q \in G/N} \sum_{n \in N} |n\rangle\langle q| \langle nc_q|.$$

One has that

$$\exists n' \in N, q' \in G/N : nc_q h^{-1} = n' c_{q'(h,q)} \quad \forall n \in N, \forall h \in G, \forall q \in G/N$$

and  $c_{q'(h,q)} h c_q^{-1} \in N \quad \forall q \in G/N$ . Let  $T_h$  be the right-regular representation of elements  $h \in G$ . Then one can change the representation, providing a new one in terms of the right-regular representation of  $N$ :

$$\begin{aligned} \tilde{T} &= U_N T_h U_N = \sum_{q_1, q_2 \in G/N} \sum_{n, n' \in N} |n\rangle\langle n'| \otimes |q_1\rangle\langle q_2| \delta_{nc_{q_1}, n' c_{q_2} h^{-1}} = \\ &= \sum_{q \in G/N} T_{c_{q'(h,q)} h c_q^{-1}} \otimes |q'(h, q)\rangle\langle q|. \end{aligned}$$

This is just a change of representation for  $G$ . In Proposition 5.1 we proved that if  $S$  is a set of generators for  $G$ , then the set

$$\{c_{q'(h,q)} h c_q^{-1}\}_{h \in S}^{q \in G/N} \quad (128)$$

is a set of generators for  $N$ .

Now suppose to fix a given presentation of  $N$ , i.e. to choose some generators  $g_l$  for  $N$ . Does the generators of  $G$  reaching the given presentation of  $N$  with a change

of representation depends on the choice of the coset representatives? In the index-2 abelian case, the answer is no. We pose  $h_i = n_i c_{q(i)}$  and the generic coset representative  $x_q c_q$ , for  $x_q \in N$ . Then one has to impose

$$g_{l(i)} = x_1 c_{\bar{e}} h_i (x_{q(i)} c_{q(i)})^{-1} = x_1 n_i x_{q(i)}^{-1},$$

where the map  $l$  is injective, implying that every  $n_i$  is defined as  $x_1^{-1} g_{l(i)} x_{q(i)}$ . In the index-2 Abelian case,  $n_i := x_1^{-1} x_{q(i)} g_{l(i)}$ , therefore it is defined up to a fixed overall translation which does not change the resulting graph.

Now let  $G$  be an extension of  $N$  by  $Q$ . For an arbitrary  $h = x_h c_{q_h} \in G$ , one has

$$\tilde{T}_h = U_N T_h U_N^\dagger = \sum_{q_1, q_2 \in Q} \sum_{n, n' \in N} |n\rangle \langle n'| \otimes |q_1\rangle \langle q_2| \delta_{n c_{q_1}, n' c_{q_2} c_{q_h}^{-1} x_h^{-1}} \quad (129)$$

and, since according to the composition rule of the coset representatives it must be  $q_2 = q_1 q$ , one obtains  $n = n' c_{q_1 q} c_{q_h}^{-1} c_{q_1}^{-1} \varphi_{q_1}(x_h^{-1})$ . Accordingly Eq. (129) reads

$$\begin{aligned} \tilde{T}_h &= \sum_{q' \in Q} \sum_{n \in N} \left| n(\varphi_{q'}(x_h) c_{q'} c_{q_h} c_{q' q_h}^{-1})^{-1} \right\rangle \langle n | \otimes |q'\rangle \langle q' q_h| = \\ &= \sum_{q' \in Q} T_{\varphi_{q'}(x_h)} T_{f(q', q_h)} \otimes |q'\rangle \langle q'| T_{q_h}. \end{aligned}$$

Given a the evolution operator

$$A = \sum_{h \in S} z_h T_h$$

for a scalar qw, one can then give the following representation in terms of the right regular-representations of  $N$  and  $Q$ :

$$\tilde{A} = U_N A U_N^\dagger = \sum_{h \in S} \sum_{q' \in Q} z_h T_{\varphi_{q'}(x_h)} T_{f(q', q_h)} \otimes |q'\rangle \langle q'| T_{q_h}, \quad (130)$$

where  $h = x_h c_{q_h}$ . On the one hand, this change of representation is relevant in order to characterize scalar qws on an extension  $G$  manifestly in terms of  $N$  and  $Q$ ; on the other hand, it allows to investigate the isotropy group—if any—induced by the representation of the qw on  $\ell^2(N) \otimes \ell^2(Q)$  in terms of the action of  $Q$  on  $N$ .





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SCALAR EUCLIDEAN QUANTUM WALKS

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We wish now to characterize Euclidean qws from scratch, starting from the simplest cases. We will do the opposite of what we analysed in Chapter 7, that is to say that we here fix the dimension for the coin system and let the group vary. In particular, we shall assume minimal algorithmic complexity (one-dimensional coin system, i.e. scalar qws); in addition, by Theorem 6.1 a necessary condition for nontriviality of the evolution is non-Abelianity. Moreover, since quasi-isometry is an equivalence relation (Lemma 2.2) and  $\mathbb{R}^d$  is quasi-isometric to  $\mathbb{Z}^d$ , Theorem 2.4 implies that if a finitely generated group  $G$  is quasi-isometric to  $\mathbb{R}^d$ , then  $G$  is virtually  $\mathbb{Z}^d$ . In Corollary 2.3 we have proved that *virtually*  $\mathbb{Z}^d$  is equivalent to  $\mathbb{Z}^d$ -by-finite, whence restricting to groups quasi-isometric to  $\mathbb{R}^d$  is equivalent to restricting to  $\mathbb{Z}^d$ -by-finite groups. Correspondingly, we shall focus on non-Abelian  $\mathbb{Z}^d$ -by-finite groups, finding the extensions of  $\mathbb{Z}^d$ .

In this Chapter we address the problem of characterizing the extension of  $\mathbb{Z}^d$ . After proving a few general results, we will explicitly construct the (non-Abelian) extension of  $\mathbb{Z}^d$  with in index 2, namely non-Abelian  $\mathbb{Z}^d$ -by- $\mathbb{Z}_2$  groups, for  $d = 1, 2, 3$ . Then we shall find the form of their presentation making use of the quadrangularity condition of Proposition 6.1 and assuming that the coarse-grained qws satisfies the necessary condition for isotropy, namely the generating set is the orbit of an arbitrary vector  $\mathbf{v} \in \mathbb{R}^d$  under the action of a finite subgroup  $L < \text{GL}(d, \mathbb{Z})$  represented in  $\mathcal{O}(\mathbb{R})$ . Throughout the present chapter we will make use of the results, notations and nomenclature of Section 8.1 of Chapter 8.

9.1  $\mathbb{Z}^d$ -BY-FINITE GROUPS

We now want to characterize the extensions of  $\mathbb{Z}^d$  by some finite group  $Q$ . First, notice that if  $N$  is an Abelian group, then  $\text{Aut}(N) \cong \text{Out}(N)$ , since  $\text{Inn}(N) \cong \{e\}$ . Accordingly, we have that  $\varphi \equiv \tilde{\varphi}$ . The group of automorphisms of  $\mathbb{Z}^d$  is isomorphic to  $\text{GL}(d, \mathbb{Z})$  (Theorem 2.1): then, by Lemma 8.2, for each fixed finite group  $Q$  and homomorphism  $\varphi$  we can consider equivalence classes of extensions up to pre-composition of  $\varphi$  with an arbitrary  $\beta \in \text{Aut}(Q)$  and up to conjugation in  $\text{GL}(d, \mathbb{Z})$ , namely up to inner automorphisms<sup>1</sup>.

**Proposition 9.1.** *Every element  $q$  of a finite group  $Q$  has a finite order  $r_q$ .*

**Proof.** Since  $Q$  is finite,  $q^n$  can't be different for each integer  $n$ . Then there must exist at least two positive integers  $n', n''$  such that  $n' < n'' \leq |Q|$  and  $q^{n''} = q^{n'}$ . The thesis follows choosing the two integers such that  $r_q := n'' - n'$  is minimized. ■

Proposition 9.1, along with the definition of the homomorphism  $\varphi$ , imply that

$$\forall q \in Q \exists r_q \in \mathbb{N} : \varphi_q^{r_q}(n) = n \quad \forall n \in N.$$

Such an automorphism  $\varphi_q$  is called  *$r_q$ -involutory*. Since  $\varphi$  are groups of homomorphisms, in order to classify all the different  $\varphi$  we need the conjugacy classes of finite subgroups of  $\text{GL}(d, \mathbb{Z})$ : their elements will be  $r_q$ -involutory matrices. This fact can also help when finding solution to Eq. (127). Indeed, for two different choices of coset representatives  $\{c_q\}_{q \in Q}$  and  $\{c'_q\}_{q \in Q}$ , given  $(c_q)^{r_q} \in N$  one possible criterion could be looking for all the  $(c'_q)^{r_q} \in N$  such that  $\{c_q\}_{q \in Q}$  and  $\{c'_q\}_{q \in Q}$  gives rise to isomorphic groups up to a change of coset representatives; in order to do that, one needs to verify if

$$\forall q \in Q \exists n_q \in N : (c_q)^{r_q} = (n_q c'_q)^{r_q} = \prod_{j=0}^{r_q-1} \varphi_q^j(n_q) (c'_q)^{r_q}, \tag{131}$$

finding a family of solutions  $\{n_q\}_{q \in Q}$ .

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<sup>1</sup> Actually, a simple consequence of the Corollary 15 of Ref. [142] is that the outer automorphism group of  $\text{GL}_d(\mathbb{Z})$  is trivial. Therefore in the present case pseudo-congruence means that we are in fact considering equivalence classes of maps  $\varphi$  up to composition with arbitrary elements of  $\text{Aut}(\text{GL}(d, \mathbb{Z}))$ .

## 9.1.1 One-dimensional case

Let us pose  $\mathbb{Z} \cong N = \langle a \rangle$ . The (finite) subgroups of  $\mathrm{GL}(1, \mathbb{Z}) = \{1, -1\}$  are just the two following multiplicative groups:  $\{1\} \cong e$  and  $\{1, -1\} \cong \mathbb{Z}_2$ .

Choose now  $Q = \{\bar{e}, \bar{q}\} \cong \mathbb{Z}_2$  in order to construct all the  $\mathbb{Z}$ -by- $\mathbb{Z}_2$  groups  $G$ . We want to classify the homomorphisms  $\varphi$  from  $Q$  to  $\{1, -1\}$ :  $\varphi$  must be either the trivial map or an isomorphism. In the first case, one has  $\varphi_{\bar{q}} = \mathrm{id}$  and the resulting extension is Abelian, meaning that  $G$  is isomorphic to  $\mathbb{Z}$  or to  $\mathbb{Z} \times \mathbb{Z}_2$ . Since we have already classified the Abelian scalar qws with Theorem 6.1, we proceed with the non-Abelian case.

For  $\varphi_{\bar{q}} = -1$ , we have to choose some integer  $r$  such that  $c_{\bar{q}}^2 = ra$ . We have

$$ra = c_{\bar{q}}^2 = (c_{\bar{q}})c_{\bar{q}}^2(c_{\bar{q}})^{-1} = \varphi_{\bar{q}}(c_{\bar{q}}^2) = \varphi_{\bar{q}}(ra) = -ra,$$

which implies  $r = 0$ , namely  $G \cong \mathbb{Z} \rtimes_{\varphi} \mathbb{Z}_2 = D_{\infty}$ . We then recovered what we found in Chapter 6.

If we choose  $|Q|$  to be odd, by Theorem 5.1 the order  $r_q$  of each element of  $q \in Q$  must be odd. If we look for a nontrivial homomorphism  $\varphi: Q \rightarrow \{1, -1\}$ , with  $|Q|$  odd, then for some  $q$  we will have

$$\mathrm{id} = \varphi(\bar{e}) = \varphi(q^{r_q}) = \varphi(q)^{r_q} = (-1)^{r_q} = -\mathrm{id},$$

which is impossible. As a consequence, all the extensions of  $\mathbb{Z}$  by some  $Q$  of odd order must satisfy

$$\varphi_q \equiv \mathrm{id} \quad \forall q \in Q. \quad (132)$$

**Example 9.1** ( $\mathbb{Z}$ -by- $\mathbb{Z}_3$  groups). *Let us pose  $Q = \{\bar{e}, \bar{q}, \bar{q}^2\} \cong \mathbb{Z}_3$ : chosen a 2-cocycle  $f$ , one has*

$$f(\bar{q}, \bar{q})c_{\bar{q}^2} = c_{\bar{q}}^2 = (c_{\bar{q}})c_{\bar{q}}^2(c_{\bar{q}})^{-1} = \varphi_{\bar{q}}(f(\bar{q}, \bar{q}))c_{\bar{q}}c_{\bar{q}^2}c_{\bar{q}}^{-1} = f(\bar{q}, \bar{q})c_{\bar{q}}c_{\bar{q}^2}c_{\bar{q}}^{-1},$$

where we used Eq. (132). This implies

$$c_{\bar{q}^2} = c_{\bar{q}}c_{\bar{q}^2}c_{\bar{q}}^{-1} \implies c_{\bar{q}^2}c_{\bar{q}} = c_{\bar{q}}c_{\bar{q}^2},$$

however one also has

$$c_q n = n c_q, \quad mn = nm, \quad \forall n, m \in \mathbb{Z}, \quad \forall q \in \mathbb{Z}_3$$

whence follows that an extension of  $\mathbb{Z}$  by  $\mathbb{Z}_3$  must be abelian, meaning that it will be isomorphic to  $\mathbb{Z}$  or to  $\mathbb{Z} \times \mathbb{Z}_3$ .

## 9.2 2D AND 3D CASES WITH INDEX 2

In the following, the extensions in the cases  $d = 2, 3$  for index  $|Q| = 2$  will be discussed. The problem reduces to choose the only nontrivial value of the 2-cocycle  $f$ , namely  $f(\tilde{q}, \tilde{q}) = c^2 := c_{\tilde{q}}^2$ , which is clearly invariant under the automorphism  $\varphi := \varphi_{\tilde{q}}$ . Accordingly, one can calculate the invariant space of  $\varphi$ ; then one uses Eq. (131) to find all the equivalent 2-cocycle choices up to a change of the coset representative. In the present case, for a chosen  $c^2$ , one looks for a solution  $n \in \mathbb{Z}^d$  to the equation

$$c^2 = n + \varphi(n) + c'^2. \quad (133)$$

We will neglect the trivial homomorphisms  $\varphi$  (from  $Q \cong \mathbb{Z}_2$  to  $I_d$ ), since it gives rise to Abelian extensions.

**Proposition 9.2.** *Let  $G = N \cup Nc$  be a group, with  $N \cong \mathbb{Z}^d$  for  $d = 1, 2, 3$ ,  $\Gamma(G, S)$  a Cayley graph satisfying the quadrangularity condition (71) and  $\Gamma(N, \tilde{S})$  a coarse-graining satisfying isotropy. Then  $G$  is a split extension and for  $d = 2, 3$*

$$\exists g_1, g_2 \in \tilde{S} : S \supseteq \{g_1, g_1 c, g_1^{-1} c, g_2 c\}. \quad (134)$$

*Proof.* For  $d = 1$  we already proved the statement in Chapter 6. We now fix an arbitrary generating set  $\tilde{S}_+$  for  $N \cong \mathbb{Z}^d$  with  $d = 2, 3$ . Using equation (128), one can easily see that the following statements hold:

$$h_i \in S_+, N \implies h_i \in \tilde{S}_+ \wedge \varphi(h_i) \in \tilde{S}_+ \quad (135)$$

$$h_i = g_i c \in S_+, Nc \implies g_i \in \tilde{S}_+ \wedge \varphi(g_i) + c^2 \in \tilde{S}_+. \quad (136)$$

The generating set  $S_+$ , generating the whole group  $G$ , must contain at least one element from the coset  $Nc$ ; besides,  $|S_+| \geq 2$  also holds, since  $G$  contains a subgroup  $N \cong \mathbb{Z}^d$  of rank at least  $d = 2$ . We thus have two mutually exclusive cases:

- i)  $\nexists g \in \tilde{S} : g \in S$  and the elements of  $S_+$  has the form  $gc$  for  $g \in \tilde{S}$  (by condition (136));
- ii)  $\exists g_1, g_2 \in \tilde{S} : \{g_1, g_2c\} \subseteq S_+$ .

In case i), take  $g_1c, g_2c \in S_+$  such that  $g_1c(g_2c)^{-1} = g_1g_2^{-1}$  has maximal length. Following the same argument of the proof of Theorem 6.1, the combination must be unique in  $\tilde{S}$ , and to satisfy quadrangularity we have to find  $g_l c, g_p c \in S$  such that  $g_1g_2^{-1} = g_l g_p^{-1}$ . Then it must be  $g_l = g_2^{-1}$  and  $g_p = g_1^{-1}$ , implying  $g_i^{\pm 1}c \in S$  for  $i = 1, 2$ . One then also has the length-2 paths given by  $g_i c (g_i^{-1}c)^{-1} = g_i^2$ , which are unique in  $\tilde{S}$  and again by quadrangularity it must be  $g_i \in S$ , which is absurd. In case ii), as in case i) by quadrangularity it must be  $g_1^{\pm 1}c \in S$ . Thus by conditions 135 and 136 one has

$$\varphi(g_1^{\pm 1}), \varphi(g_i^{\pm 1}) + c^2 \in \tilde{S}.$$

By Corollary 7.1 we know that the elements in  $\tilde{S}$  can be represented in  $\mathbb{R}^d$  having the same length, then posing  $\mathbf{v}_1$  and  $\mathbf{w}$  as the vectors representing respectively  $\varphi(g_1)$  and  $c^2$  embedded in  $\mathbb{R}^d$ , we obtain

$$\|\mathbf{v}_1 + \mathbf{w}\| = \|-\mathbf{v}_1 + \mathbf{w}\| = \|\mathbf{v}_1\|.$$

This implies  $\mathbf{w} = 0$  or, equivalently,  $c^2 = e$ : thus  $G$  is a split extension and condition (134) holds. ■

In the following, we shall construct all the non-Abelian  $\mathbb{Z}^d$ -by- $\mathbb{Z}_2$  extensions for  $d = 2, 3$ . In the two-dimensional case we denote the canonical basis by

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

and in the three-dimensional case by

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

In [140, 141, 143] one can find a complete classification of the finite subgroup of  $\text{GL}(2, \mathbb{Z})$  and  $\text{GL}(2, \mathbb{Z})$  up to conjugation. By Lemma 8.2, conjugation in  $\text{GL}(d, \mathbb{Z})$  gives rise to isomorphic extensions, then it is enough to consider the conjugacy classes of finite subgroups of  $\text{GL}(d, \mathbb{Z})$ .

The subgroups of order 2 are three, clearly isomorphic to  $\mathbb{Z}_2 = \{\tilde{e}, \tilde{q}\}$ , and are respectively generated by:

$$-I_2, \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

**Lemma 9.1.** *Let  $G$  be a non-Abelian  $\mathbb{Z}^2$ -by- $\mathbb{Z}_2$  group. Then  $G$  is isomorphic to one of the following groups:*

1.  $G_1 = \langle a, b, c \mid aba^{-1}b^{-1}, c^2, cac^{-1}a, cbc^{-1}b \rangle \cong \mathbb{Z}^2 \rtimes_{-\text{id}} \mathbb{Z}_2,$
2.  $G_2 = \langle a, b, c \mid aba^{-1}b^{-1}, c^2, cac^{-1}b^{-1}, cbc^{-1}a^{-1} \rangle \cong \mathbb{Z}^2 \rtimes_{\sigma_x} \mathbb{Z}_2,$
3.  $G_3 = \langle a, b, c \mid aba^{-1}b^{-1}, c^2, cac^{-1}a^{-1}, cbc^{-1}b \rangle \cong \mathbb{Z}^2 \rtimes_{\sigma_z} \mathbb{Z}_2,$
4.  $G_4 = \langle a, b, c \mid aba^{-1}b^{-1}, c^2a^{-1}, cac^{-1}a^{-1}, cbc^{-1}b \rangle.$

*Proof.* Regardless of the homomorphism  $\varphi$  is chosen, one has that  $c_{\tilde{q}}^2 \in \mathbb{Z}^2$  will be invariant under  $\varphi_{\tilde{q}}$ . For each automorphism, then, one has to choose the only nontrivial 2-cocycle value  $f(\tilde{q}, \tilde{q}) = c_{\tilde{q}}^2$  among the invariant vectors of the particular automorphism chosen:

- For  $\varphi_{\tilde{q}} = -\mathbb{1}$ , the only invariant element of  $\mathbb{Z}^2$  is the zero vector. Then the only possibility is  $G \cong \mathbb{Z}^2 \rtimes_{-\text{id}} \mathbb{Z}_2$ .
- For  $\varphi_{\tilde{q}} = \sigma_x$ , the invariant elements of  $\mathbb{Z}^2$  are the ones of the form  $r_x(|0\rangle + |1\rangle)$ , with  $r_x \in \mathbb{Z}$ . Let us choose  $r_x = 0$ : using Eq. (133), we have

$$(\mathbb{1} + \sigma_x)(n_{\tilde{q},0} |0\rangle + n_{\tilde{q},1} |1\rangle) + r'_x(|0\rangle + |1\rangle) = (n_{\tilde{q},0} + n_{\tilde{q},1} + r'_x)(|0\rangle + |1\rangle) = 0,$$

namely  $\forall r'_x \exists n_{\bar{q},0}, n_{\bar{q},1} \in \mathbb{Z}$  such that such that the extension with  $c_{\bar{q}}'^2 = r'_x(|0\rangle + |1\rangle)$  differs from that with  $c_{\bar{q}}^2 = 0$  for a coset representatives. Then the only possibility is again  $G \cong \mathbb{Z}^2 \rtimes_{\sigma_x} \mathbb{Z}_2$ .

- For  $\varphi_{\bar{q}} = \sigma_z$ , the invariant space is  $r_z|0\rangle$ , with  $r_z \in \mathbb{Z}$ . Choosing  $r_z = 0$ , again from Eq. (133) we have

$$(\mathbb{1} + \sigma_z)(n_{\bar{q},0}|0\rangle + n_{\bar{q},1}|1\rangle) + r'_z|0\rangle = (2n_{\bar{q},0} + r'_z)|0\rangle = \mathbf{0},$$

namely  $\forall r'_z$  even  $\exists n_{\bar{q},0}, n_{\bar{q},1} \in \mathbb{Z}$  such that such that the extension with  $c_{\bar{q}}'^2 = r'_z|0\rangle$  differs from that with  $c_{\bar{q}}^2 = 0$  for a coset representatives; then  $G \cong \mathbb{Z}^2 \rtimes_{\sigma_z} \mathbb{Z}_2$ . Choosing  $r_z = 1$ , one has

$$(2n_{\bar{q},0} + r'_z)|0\rangle = |0\rangle$$

and  $\forall r'_z$  odd  $\exists n_{\bar{q},0}, n_{\bar{q},1} \in \mathbb{Z}$  such that such that the extension with  $c_{\bar{q}}'^2 = r'_z|0\rangle$  differs from that with  $c_{\bar{q}}^2 = 1$  for a coset representatives; then in this last case  $G$  is not a semidirect product.

■

We notice that  $G_4$  is the same group considered in Section ...

One can exploit the same methods provided in the two-dimensional case in order to construct all the extension of  $\mathbb{Z}^3$  by  $\mathbb{Z}_2$ . The subgroups of order 2 are five, isomorphic to  $\mathbb{Z}_2$ , and are respectively generated by:

$$-\mathbb{1}, \Sigma_{\pm} := \pm \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \Lambda_{\pm} := \pm \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

**Proposition 9.3.** *Let  $G$  be a non-Abelian  $\mathbb{Z}^3$ -by- $\mathbb{Z}_2$  group. Then  $G$  is isomorphic to one of the following groups:*

1.  $G_1 = \langle x_1, x_2, x_3, c \mid x_i x_j x_i^{-1} x_j^{-1}, c^2, c x_i c^{-1} x_i \rangle$ ,
2.  $G_2 = \langle x_1, x_2, x_3, c \mid x_i x_j x_i^{-1} x_j^{-1}, c^2, c x_1 c^{-1} x_1^{-1}, c x_{2,3} c^{-1} x_{2,3} \rangle$ ,
3.  $G_3 = \langle x_1, x_2, x_3, c \mid x_i x_j x_i^{-1} x_j^{-1}, c^2 x_1^{-1}, c x_{2,3} c^{-1} x_{2,3} \rangle$ ,

4.  $G_4 = \langle x_1, x_2, x_3, c \mid x_i x_j x_i^{-1} x_j^{-1}, c^2, c x_1 c^{-1} x_1, c x_{2,3} c^{-1} x_{2,3}^{-1} \rangle$ .
5.  $G_5 = \langle x_1, x_2, x_3, c \mid x_i x_j x_i^{-1} x_j^{-1}, c^2, c x_1 c^{-1} x_1, c x_{2,3} c^{-1} x_{3,2}^{-1} \rangle$ ,
6.  $G_6 = \langle x_1, x_2, x_3, c \mid x_i x_j x_i^{-1} x_j^{-1}, c^2, c x_1 c^{-1} x_1^{-1}, c x_{2,3} c^{-1} x_{3,2} \rangle$ ,
7.  $G_7 = \langle x_1, x_2, x_3, c \mid x_i x_j x_i^{-1} x_j^{-1}, c^2 x_1^{-1}, c x_{2,3} c^{-1} x_{3,2} \rangle$ .

*Proof.* One has to choose the only nontrivial 2-cocycle value  $f(\tilde{q}, \tilde{q}) = c_{\tilde{q}}^2$  among the invariant vectors of the particular automorphism chosen:

- For  $\varphi_{\tilde{q}} = -\mathbb{1}$ , the only invariant element of  $\mathbb{Z}^3$  is the zero vector. Then the only possibility is  $G \cong \mathbb{Z}^3 \rtimes_{-\text{id}} \mathbb{Z}_2$ .
- For  $\varphi_{\tilde{q}} = \Sigma_+$ , the invariant elements of  $\mathbb{Z}^3$  are the ones of the form  $r_0 |0\rangle$ , with  $r_0 \in \mathbb{Z}$ . Let us choose  $r_0 = 0$ : using Eq. (133), we have

$$(\mathbb{1} + \Sigma_1)(n_{\tilde{q},0} |0\rangle + n_{\tilde{q},1} |1\rangle + n_{\tilde{q},2} |2\rangle) + r'_0 |0\rangle = (2n_{\tilde{q},0} + r'_0) |0\rangle = 0,$$

namely  $\forall r'_0$  even  $\exists n_{\tilde{q},0}, n_{\tilde{q},1} \in \mathbb{Z}$  such that such that the extension with  $c_{\tilde{q}}^2 = r'_0 |0\rangle$  differs from that with  $c_{\tilde{q}}^2 = 0$  for a coset representatives. Then the only possibility is  $G \cong \mathbb{Z}^3 \rtimes_{\Sigma_+} \mathbb{Z}_2$ . Choosing  $r_0 = 1$ , one has

$$(2n_{\tilde{q},0} + r'_0) |0\rangle = |0\rangle$$

and  $\forall r'_0$  odd  $\exists n_{\tilde{q},0}, n_{\tilde{q},1} \in \mathbb{Z}$  such that such that the extension with  $c_{\tilde{q}}^2 = r'_0 |0\rangle$  differs from that with  $c_{\tilde{q}}^2 = 1$  for a coset representatives; then in this last case  $G$  is not a semidirect product.

- For  $\varphi_{\tilde{q}} = \Sigma_-$ , the invariant elements of  $\mathbb{Z}^3$  are the ones of the form  $r_1(|1\rangle + |2\rangle)$ , with  $r_1 \in \mathbb{Z}$ . Let us choose  $r_1 = 0$ : using Eq. (133) as above, we find that the only possibility is  $G \cong \mathbb{Z}^3 \rtimes_{\Sigma_-} \mathbb{Z}_2$ .
- For  $\varphi_{\tilde{q}} = \Lambda_+$ , the invariant elements of  $\mathbb{Z}^3$  are the ones of the form  $r_1(|1\rangle + |2\rangle)$ , with  $r_1 \in \mathbb{Z}$ . Let us choose  $r_1 = 0$ : using Eq. (133) as above, we find that the only possibility is  $G \cong \mathbb{Z}^3 \rtimes_{\Lambda_+} \mathbb{Z}_2$ .
- For  $\varphi_{\tilde{q}} = \Lambda_-$ , the invariant elements of  $\mathbb{Z}^3$  are the ones of the form  $r_0 |0\rangle + r_1(|1\rangle - |2\rangle)$ , with  $r_0, r_1 \in \mathbb{Z}$ . Let us choose  $r_1 = 0$ : using Eq. (133) as above, we find that the only possibility is  $G \cong \mathbb{Z}^3 \rtimes_{\Lambda_-} \mathbb{Z}_2$ . Choosing  $r_0 = 1$ , one has that  $G$  is not a semidirect product.







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 EUCLIDEAN QWS AND THE HYPERBOLIC CASE
 

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This final Chapter is devoted to the examination of some examples on qws on Cayley graphs derived making use of the methods and techniques developed throughout the present thesis work.

### 10.1 SOME SCALAR 2D EUCLIDEAN QWS

Let  $\mathcal{W}_1(\Gamma)$  be the family of the scalar qws on a given Cayley graph  $\Gamma(G, S_+)$  of a group  $G$ , and  $\mathcal{W}_p(\Gamma_p)$  the family of qws on the Cayley graph  $\Gamma_i(H, \tilde{S}_+)$  of a subgroup  $H \leq G$  of index  $i$ , given by a fixed regular tiling of  $\Gamma$  with respect to  $H$ . The qws on  $\Gamma_p$  have coin system of dimension  $p$ . Let us now identify the qws up to local unitary transformations (i.e. on the coin system) and changes of representation (coarse-grainings). These operations are all unitary, namely represents just changes of basis and the identification is well-posed. Since for all  $W \in \mathcal{W}_1(\Gamma)$  there exists a unique  $W' \in \mathcal{W}_p(\Gamma_p)$  such that  $W'$  is a coarse-graining of  $W$  up to a local change of basis, then clearly  $\mathcal{W}_1(\Gamma) \subseteq \mathcal{W}_p(\Gamma_p)$  holds. Moreover, if for all  $W \in \mathcal{W}_p(\Gamma_p)$  there exists a unique “refinement” mapping  $W$  to an element  $W' \in \mathcal{W}_1(\Gamma)$ , then also  $\mathcal{W}_p(\Gamma_p) \subseteq \mathcal{W}_1(\Gamma)$  holds. Thus, provided that one checks that up to a local change of basis the transition matrices for every walk in  $\mathcal{W}_p(\Gamma_p)$  can be written in the form of those of the coarse-graining of a walk in  $\mathcal{W}_1(\Gamma)$ , then also  $\mathcal{W}_1(\Gamma) = \mathcal{W}_p(\Gamma_p)$  holds.

In Appendix B we derive the most general family of qws on the 2D square lattice and on the 3D BCC lattice. One can see from Eqs. (174) and (192) that the transition matrices of the walks found are rank-one.

**Lemma 10.1.** *Let  $\{N_m\}_{m=1}^n$  be a finite set of finite-dimensional  $s \times s$  matrices over  $\mathbb{C}$  with all vanishing entries except for at least some entries in one column (possibly depending on the matrix). Then there always exists a basis in which all the matrices are represented with all entries being nonvanishing.*

*Proof.* Let us denote

$$N_m = \left( \sum_{i=1}^s v_{mi} |i\rangle \right) \langle j_m|.$$

Let  $U$  be a unitary matrix, then one has

$$UN_mU^\dagger = \sum_{i,l,r=1}^s v_{mi} U_{il} |l\rangle \langle r| U_{j_m r}^* = \sum_{l,r=1}^s \left( \sum_{i=1}^s v_{mi} U_{il} U_{j_m r}^* \right) |l\rangle \langle r| =: \sum_{l,r=1}^s n_{mlr} |l\rangle \langle r|.$$

Now, we have to pose the condition

$$n_{mlr} \neq 0 \quad \forall m, l, r. \quad (137)$$

We can always choose  $U_{pq} \neq 0$  for all  $p, q$ : thus condition (137) amounts to

$$\mathbf{v}_m \cdot \mathbf{u}_l := \sum_{i=1}^s v_{mi} U_{il} \neq 0 \quad \forall m, l. \quad (138)$$

The latter condition defines  $n \times s$  sets of linear equations in the components of the  $\mathbf{u}_l$ , namely the columns of  $U$ .  $U$  is unitary if and only if has orthonormal columns, then  $\mathbf{u}_l \cdot \mathbf{u}_{l'} = \delta_{ll'}$  holds. Take the set of solutions  $\mathcal{S}_{ml}$  of each  $\mathbf{v}_m \cdot \mathbf{u}_l = 0$  for  $m = 1, \dots, n$  and  $l = 1, \dots, s$ : these are  $(s-1)$ -dimensional hyperplanes, passing through the origin, in  $\mathbb{C}^s$  for every  $m, l$ . Now define

$$\mathcal{S} := \bigcup_{m=1}^n \bigcup_{l=1}^s \mathcal{S}_{ml}.$$

Then the problem (138) reduces to find a set  $\{\mathbf{u}_l^*\}_{l=1}^s$  of orthonormal vectors, not coinciding with a given reference system, in  $\mathbb{C}^s \setminus \mathcal{S}$ . Since  $\mathcal{S}$  is a finite union of  $(s-1)$ -dimensional hyperplanes passing through the origin, it is always possible to rotate a

given orthonormal reference system into the complement  $\mathbb{C}^S \setminus \mathcal{S}$ , and finally choose it as a solution  $\{\mathbf{u}_l^*\}_{l=1}^S$ . ■

We will now use Lemma 10.1 to find all the scalar QWS on Cayley graphs of the extensions of  $\mathbb{Z}^2$  (found in Section 9.2) and admitting a coarse-graining on the square lattice. First, we have to determine the admissible Cayley graphs of the groups found in Lemma 9.1. By Proposition 9.2, we have to consider just the split extensions, namely

1.  $G_1 \cong \mathbb{Z}^2 \rtimes_{-\text{id}} \mathbb{Z}_2$ ,
2.  $G_2 \cong \mathbb{Z}^2 \rtimes_{\sigma_x} \mathbb{Z}_2$ ,
3.  $G_3 \cong \mathbb{Z}^2 \rtimes_{\sigma_z} \mathbb{Z}_2$ .

Moreover, by same result, if  $S_+$  is a generating set for  $G_i$  and  $a, b$  generate the coarse-grained square lattice, then

$$S \supseteq \{a, ac, a^{-1}c, b^r c\} \vee S \supseteq \{b, bc, b^{-1}c, a^r c\}$$

for  $r = +1$  or  $r = -1$ . We remark that in Appendix B we also derived that it can't be  $e \in \tilde{S}$ . In each of the above cases, imposing (making use of condition (58))  $\tilde{S}_+ = \{a, b\}$  for the coarse-grained generating set of a possible Cayley graph of  $G_i$  and imposing the quadrangularity condition (71), it is easy to show that the only admissible Cayley graphs are  $\Gamma(G_i, S)$ , with  $S_+ = \{a, b, ac, bc\}$ .

We here write the coarse-grained transition matrices, derived using (60), for the three cases:

1. for from the coarse-graining of  $\Gamma(G_1, S)$

$$A_{+x} = \begin{pmatrix} z_x & z_{xc} \\ z_{x^{-1}c} & z_{x^{-1}} \end{pmatrix}, \quad A_{-x} = \begin{pmatrix} z_{x^{-1}} & z_{x^{-1}c} \\ z_{xc} & z_x \end{pmatrix} \quad x \in \{a, b\}; \quad (139)$$

2. for from the coarse-graining of  $\Gamma(G_2, S)$

$$A_{+x} = \begin{pmatrix} z_x & z_{xc} \\ z_{yc} & z_y \end{pmatrix}, \quad A_{-x} = \begin{pmatrix} z_{x^{-1}} & z_{x^{-1}c} \\ z_{y^{-1}c} & z_{y^{-1}} \end{pmatrix} \quad x, y \in \{a, b\} : x \neq y; \quad (140)$$

3. for from the coarse-graining of  $\Gamma(G_3, S)$

$$A_{\pm a} = \begin{pmatrix} z_{a^{\pm 1}} & z_{a^{\pm 1}c} \\ z_{a^{\pm 1}c} & z_{a^{\pm 1}} \end{pmatrix}, \quad A_{\pm b} = \begin{pmatrix} z_{b^{\pm 1}} & z_{b^{\pm 1}c} \\ z_{b^{\mp 1}c} & z_{b^{\mp 1}} \end{pmatrix}. \quad (141)$$

We first notice that, in all three cases, no isotropic scalar qw is admitted, since otherwise at least two matrices would be equal, but this is forbidden by the the form (174). Now one can see from (174) that the transition matrices of the walks found are column-matrices, then we just have to represent them with all non-vanishing entries and impose the symmetries of the coarse-grained scalar walks; if this is possible, then the resulting walks are the scalar walks on the extension of  $\mathbb{Z}^d$ .

We conclude this section looking for solutions in the tree cases. By Lemma 10.1, one can always represent the transition matrices (174) with all nonvanishing entries. Accordingly, we shall now just check that the symmetries of the above coarse-grained matrices can be implemented in those of (174).

1. There exists a unitary matrix  $U$  such that  $U^2 = I_2$  and  $UA_{+x}U^\dagger = A_{-x}$  for  $x = a, b$ . Imposing these two conditions to the transition matrices (174), combined with (48), one finds  $U = \sigma_x$  and that these transition matrices are, up to a relabelling  $b \rightleftharpoons b^{-1}$ , unitarily equivalent to those found in Proposition 7.1 for the case  $d = 2$  with  $V$  commuting with  $\sigma_y$ .
2. The set of transition matrices is invariant under conjugation by a unitary  $U$  such that  $U^2 = I_2$  and  $UA_{\pm a}U^\dagger = A_{\pm b}$ . Imposing these two conditions to the transition matrices (174), combined with (48), one finds  $U = \sigma_z$  and that the transition matrices are, up to a relabelling  $b \rightleftharpoons b^{-1}$ , unitarily equivalent to those found in Proposition 7.1 for the case  $d = 2$ . Accordingly, these class of qws coincides with the isotropic two-dimensional Euclidean qws.
3. The set of transition matrices is invariant under conjugation by a unitary  $U$  such that  $U^2 = I_2$ ,  $UA_{\pm a}U^\dagger = A_{\pm a}$  and  $UA_{+b}U^\dagger = A_{-b}$ . By direct inspection of (174), it is straightforward to see that such a  $U$  does not exist.

These results are relevant, since they show how the isotropy groups can be inherited through the coarse-graining, even without assuming it on the original qw. Further investigations are in order to study if scalar qws on  $\mathbb{Z}^d$ -by-finite groups are somehow equivalent to the isotropic qws on  $\mathbb{Z}^d$ .

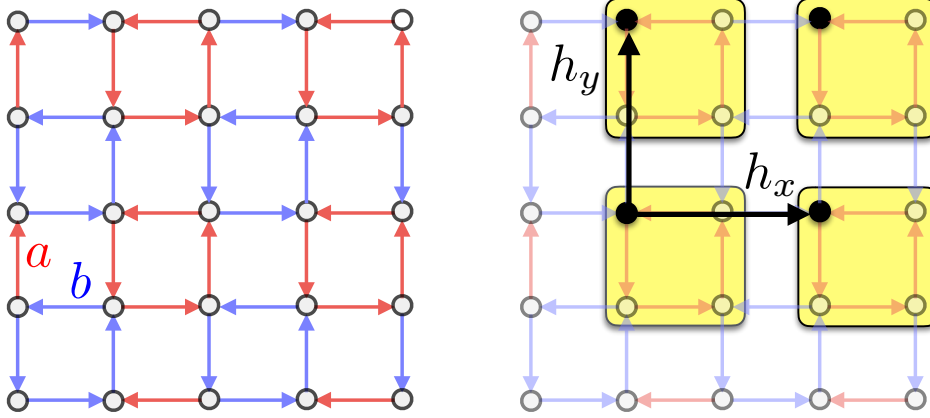


Figure 9: (Left) the Cayley graph of  $G$  corresponding to the presentation  $G = \langle a, b \mid a^4, b^4, (ab)^2 \rangle$ . (Right) A possible regular tiling of the Cayley graph of  $G$ , given by the subgroup isomorphic to  $\mathbb{Z}^2$  and generated by  $h_x = a^{-1}b$  and  $h_y = ba^{-1}$ . The subgroup has index four and we choose  $\{e, a, a^2, a^3\}$  as coset representatives.

## 10.2 EXAMPLE OF A MASSIVE VIRTUALLY ABELIAN QW

We now present the example of a qw, on the Cayley graph of a non-Abelian group  $G$ , whose evolution is analytically solved via the method developed in Chapter 5. The group is virtually Abelian, containing a subgroup  $H \cong \mathbb{Z}^2$  of index 4. The presentation

$$G = \langle a, b \mid a^4, b^4, (ab)^2 \rangle, \quad S_+ = \{a, b\},$$

corresponds to the Cayley graph shown in Fig. 9, being the simple square lattice, modulo the simple square lattice modulo a re-colouration and re-orientation of the edges.

The unitarity constraints for a qw

$$A = \sum_{g \in S} T_g \otimes A_g$$

leads to the following relations

$$A_{i-1}A_{j-1}^\dagger = A_{i-1}^\dagger A_{j-1} = A_i A_j^\dagger = A_i^\dagger A_j = 0 \quad i, j \in \{a, b\} : i \neq j, \quad (142)$$

$$A_i A_{j-1}^\dagger + A_{j-1} A_i^\dagger = A_{i-1}^\dagger A_j + A_j^\dagger A_{i-1} = 0 \quad i, j \in \{a, b\}. \quad (143)$$

From Eqs. (142) one can see that the case  $s = 2$  is not admissible, namely there exists no scalar qw on the Cayley graph  $\Gamma(G, S_+)$  (the quadrangularity condition is not satisfied). The simplest admissible case is for  $s = 2$ : in Appendix C.1 we derive the isotropic solutions, which are divided into the following two non-unitarily equivalent classes:

$$\begin{aligned} A_a^I &= \zeta^\pm Z \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, & A_b^I &= \zeta^\pm Z \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \\ A_{a^{-1}}^I &= \zeta^\mp Z \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, & A_{b^{-1}}^I &= \zeta^\mp Z \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \\ A_a^{II} &= A_{a'}^I, & A_b^{II} &= A_b^I, & A_{a^{-1}}^{II} &= A_{b^{-1}}^I, & A_{b^{-1}}^{II} &= A_{a^{-1}}^I, \end{aligned}$$

where  $\zeta^\pm := \frac{1 \pm i}{2}$  and  $Z := nI_2 + im\sigma_x$  with  $n^2 + m^2 = 1$ ,  $n, m \geq 0$ .

We now analytically solve this classes of qws applying the procedure of Section 5.2. The Abelian subgroup  $H \cong \mathbb{Z}^2$  of index 4 is the group generated by  $\mathbf{h}_x = a^{-1}b$  and  $\mathbf{h}_y = ba^{-1}$ . We now choose the regular tiling of the Cayley graph of  $G$  achieved by the coset partition

$$G = \bigcup_{j=0}^3 Hc_j, \quad c_j = a^j.$$

The plane waves on the cosets are given by

$$|\mathbf{k}\rangle_j := \frac{1}{2\pi} \sum_{\mathbf{x} \in H} e^{i\mathbf{k} \cdot \mathbf{x}} |\mathbf{x}a^j\rangle, \quad j \in \{0, 1, 2, 3\},$$

while computation of the action of the generators of  $G$  gives

$$\begin{aligned} T_a |\mathbf{k}\rangle_0 &= |\mathbf{k}\rangle_3, & T_a |\mathbf{k}\rangle_1 &= |\mathbf{k}\rangle_0, \\ T_a |\mathbf{k}\rangle_2 &= |\mathbf{k}\rangle_1, & T_a |\mathbf{k}\rangle_3 &= |\mathbf{k}\rangle_2, \\ T_b |\mathbf{k}\rangle_0 &= e^{ik_x} |\mathbf{k}\rangle_3, & T_b |\mathbf{k}\rangle_1 &= e^{iky} |\mathbf{k}\rangle_0, \\ T_b |\mathbf{k}\rangle_2 &= e^{-ik_x} |\mathbf{k}\rangle_1, & T_b |\mathbf{k}\rangle_3 &= e^{-iky} |\mathbf{k}\rangle_2, \\ T_{a^{-1}} |\mathbf{k}\rangle_0 &= |\mathbf{k}\rangle_1, & T_{a^{-1}} |\mathbf{k}\rangle_1 &= |\mathbf{k}\rangle_2, \\ T_{a^{-1}} |\mathbf{k}\rangle_2 &= |\mathbf{k}\rangle_3, & T_{a^{-1}} |\mathbf{k}\rangle_3 &= |\mathbf{k}\rangle_0, \\ T_{b^{-1}} |\mathbf{k}\rangle_0 &= e^{-iky} |\mathbf{k}\rangle_1, & T_{b^{-1}} |\mathbf{k}\rangle_1 &= e^{ik_x} |\mathbf{k}\rangle_2, \end{aligned}$$



$$T_{b^{-1}} |\mathbf{k}\rangle_2 = e^{ik_y} |\mathbf{k}\rangle_3, \quad T_{b^{-1}} |\mathbf{k}\rangle_3 = e^{-ik_x} |\mathbf{k}\rangle_0,$$

where  $k_x = \mathbf{k} \cdot \mathbf{h}_x$ ,  $k_y = \mathbf{k} \cdot \mathbf{h}_y$ . Accordingly, the coarse-grained qw takes the form

$$\mathcal{C}[A] = \int_B d\mathbf{k} |\mathbf{k}\rangle \langle \mathbf{k}|_H \otimes \mathcal{C}[A]_{\mathbf{k}},$$

where

$$\mathcal{C}[A]_{\mathbf{k}} = \begin{pmatrix} A_{k_y} & A'_{k_x} \\ A'_{-k_x} & A_{-k_y} \end{pmatrix},$$

$$A_k := \begin{pmatrix} 0 & A_a + e^{ik} A_b \\ A_{a^{-1}} + e^{-ik} A_{b^{-1}} & 0 \end{pmatrix}, \quad A'_k := \begin{pmatrix} 0 & A_{a^{-1}} + e^{-ik} A_{b^{-1}} \\ A_a + e^{ik} A_b & 0 \end{pmatrix}.$$

Diagonalizing the  $8 \times 8$  matrix  $\mathcal{C}[A]_{\mathbf{k}}$ , one can finally find the eigenvalues  $e^{i\omega_r^\pm(k_x, k_y)}$  ( $r = 1, 2$ ) of the walk—each with multiplicity 2. The dispersion relation is given by:

$$\omega_1^\pm = \pm \arccos \alpha(v, k_1, k_2) - \pi/4, \quad \omega_2 = \omega_1^\pm - \pi,$$

$$\alpha(v, k_1, k_2) := v \sqrt{\frac{1}{2} \left( \cos^2 \frac{k_x}{2} + \cos^2 \frac{k_y}{2} \right)},$$

where  $v = n$  (respectively  $v = m$ ) for the first (respectively second) class of solutions. The functions  $\omega_r$  provides kinematic information on the particle states (the eigenvectors of the qw's evolution operator). Close to the minimum of the  $\omega_r$ , namely for small  $k_x$  and  $k_y$ , the Dirac dispersion relation is recovered, with mass given by  $\mu = \sqrt{1 - v^2} \leq 1$ . For  $\mu = 1$ , the dispersion relation becomes flat: this behaviour is due to unitarity, as has already been observed in Refs. [39, 86, 136]. The non-Abelianity of the group  $G$ , in particular the cycles of order 4, induce a massive dynamics for the coarse-grained qw on the Abelian subgroup  $H$ , giving rise to the self-interacting term associated to the identical transition  $\tilde{T}_{\bar{e}}$ , having transition matrix

$$A_{\bar{e}} = \begin{pmatrix} B & B' \\ B' & B \end{pmatrix}, \quad (144)$$

$$B := \begin{pmatrix} 0 & A_a \\ A_{a^{-1}} & 0 \end{pmatrix}, \quad B' := \begin{pmatrix} 0 & A_{a^{-1}} \\ A_a & 0 \end{pmatrix}. \quad (145)$$

From (144) it is clear that the self-interaction term wraps the cycles formed by the generator  $a$ , mirroring the choice of the regular tiling. Indeed, as discussed in Section 5.3, its very existence depends on this choice.

We conclude noticing that, interestingly, a similar effect is found in Ref. [144], where a quantum walk on a cylinder is studied. Also in that case, the cyclic dimension induce the mass value of a set of Dirac-like equations.

### 10.3 QWS ON THE POINCARÉ DISK

Throughout the present work we mostly treated the case of groups quasi-isometric to Euclidean spaces  $\mathbb{R}^d$ . We now touch upon the case of hyperbolic spaces  $\mathbb{H}^d$ , namely metric spaces with a constant negative sectional curvature [145, 146]. In general, a model for hyperbolic spaces  $\mathbb{H}^d$  can be given by the space  $\{\mathbf{v} \in \mathbb{R}^d \mid \|\mathbf{v}\| < 1\}$  of open balls endowed with the metric defined as

$$d(\mathbf{v}_1, \mathbf{v}_2) := 2 \ln \frac{\|\mathbf{v}_1 - \mathbf{v}_2\| + \sqrt{\|\mathbf{v}_1\| \|\mathbf{v}_2\| - 2\mathbf{v}_1 \cdot \mathbf{v}_2 + 1}}{\sqrt{1 - \|\mathbf{v}_1\|} \sqrt{1 - \|\mathbf{v}_2\|}}.$$

In general,  $d$ -dimensional hyperbolic spaces lack rigidity results, contrarily to the Euclidean case (see Chapter 2). The simplest case is that of  $\mathbb{H}^2$ , modelled as the so-called *Poincaré disk model*. Although this is a well-studied model, even in this case rigidity results are lacking. A notable example of groups quasi-isometric to  $\mathbb{H}^2$  is constituted by the non-Euclidean crystallographic groups [147]: these are finitely generated groups of isometries of the hyperbolic plane  $\mathbb{H}^2$ . Clearly, any extension of finite index of these group is again quasi-isometric to  $\mathbb{H}^2$  (this happens also in the Euclidean case). An example of the Cayley graph of such a group is given in Figure 10. An important quantity to characterize finitely generated groups

**Definition 10.1** (Growth rate of finitely generated groups). *Let  $G$  be a finitely generated group and  $S$  a set of generators for  $G$ . Let us define the closed balls of radius  $n$  in the word metric  $d_G$  with respect to  $S$  as*

$$B_n(G, S) := \{g \in G \mid d_G(e, g) \leq n\}.$$

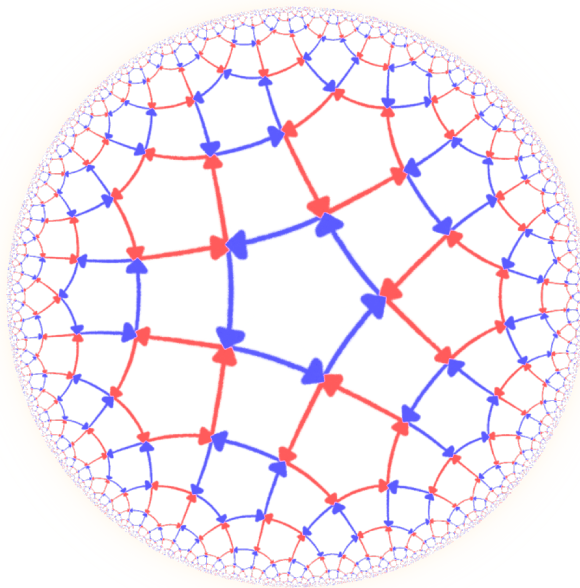


Figure 10: Cayley graph of a group which is quasi-isometric to the Poincaré disk, and corresponding to the presentation  $\langle a, b \mid a^5, b^5, (ab)^2 \rangle$ .

The growth rate of  $G$  with respect to the set of generators  $S$  is defined as the function

$$\#(n) := |B_n(G, S)|,$$

that is to say the number of elements of the closed ball of given radius  $n$ .

Virtually Abelian groups have polynomial growth, namely

$$\exists a, k < \infty : \#(n) \leq a(n^k + 1).$$

As a consequence of Gromov's Theorem [148], virtually Abelian groups can be thus suitably embedded in Euclidean spaces, as we know from Chapter 2. On the contrary, if a group is quasi-isometric to  $\mathbb{H}^d$ , then it has an exponential growth, namely

$$\exists b > 1 : \#(n) \geq b^n.$$

Every finitely generated group has at most exponential growth.

We conclude studying and solving the unitarity conditions of a qw on the Cayley graph shown in Figure 11. The unitarity conditions read:

$$A_i A_j^\dagger = A_i^\dagger A_j = A_i A_{j-1}^\dagger = A_i^\dagger A_{j-1} = 0 \quad i, j \in \{a, b\} : i \neq j, \quad (146)$$

$$A_i A_{i-1}^\dagger + A_{i-1} A_i^\dagger = A_i^\dagger A_{i-1} + A_{i-1}^\dagger A_i = 0 \quad i \in \{a, b\}. \quad (147)$$

From Eqs. (146) it is clear that the simplest admissible case is the one with a two-dimensional coin system. Therefore in Appendix C.2 we solve the constraints (146) and (147) for dimension  $s = 2$ . We report here the solution, which is given by the following family of transition matrices:

$$\begin{aligned} A_a &= \alpha X |0\rangle\langle 0|, & A_b &= \alpha X |1\rangle\langle 1|, \\ A_{a^{-1}} &= si\sqrt{1-\alpha^2} X |0\rangle\langle 0|, & A_{b^{-1}} &= si\sqrt{1-\alpha^2} X |1\rangle\langle 1|, \end{aligned}$$

where  $s$  is an arbitrary sign and  $X$  is a generic matrix commuting with  $\sigma_x$  with unit determinant, i.e. it has the form  $X = nI_2 + im\sigma_x$ , with  $n, m$  positive such that  $n^2 + m^2 = 1$ .

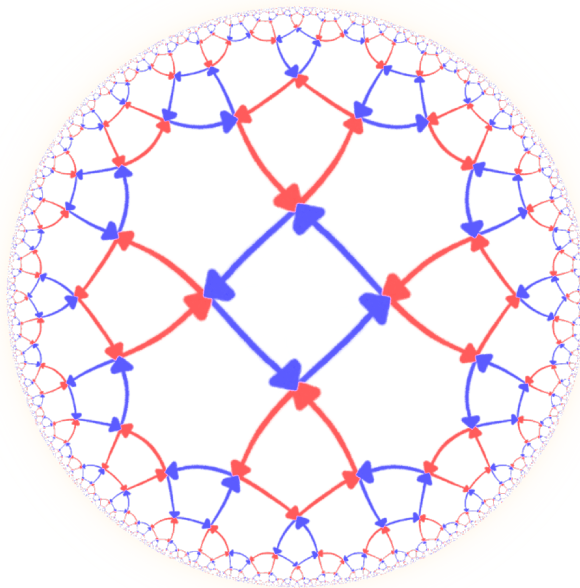


Figure 11: Cayley graph corresponding to the presentation  $\langle a, b \mid a^4, b^4, (ab)^3 \rangle$ . The graph is quasi-isometric to the Poincaré disk.

In the general non-Abelian case one cannot exploit the method previously developed in Chapters 3 and 5, and study the qw in the Fourier representations. In general, the unitary irreps are more than one-dimensional, and this does not allow to perform the mathematical description developed for virtually Abelian groups. Non-euclidean cases are very interesting cases from a geometric point of view, yet pathological when it comes to provide suitable representations for them.

Example of groups quasi-isometric to the Poincarè disk are Fuchsian groups and infinite discrete subgroups of the projective special linear group  $\mathrm{PSL}(2, \mathbb{R})$ . Unfortunately, it is not even known whether their right-regular representation admit a decomposition into finite-dimensional unitary irreps<sup>1</sup>. Indeed, it is already a hard problem to use the representations of general groups to study the kinematics and dynamics of the qws on them. Unfortunately, in the hyperbolic case very little is known about the irreducible representations and this is one of the reason why, to the best of our knowledge, a general method to extract differential equations on these kind of graphs is lacking.

**Remark 10.1.** *As we had the chance to realise throughout our investigation, paths of length 2 are the only relevant to the purpose of studying and solving the unitarity conditions for Qws on Cayley graphs (actually, this is true for arbitrary Qws on graphs, as can be seen from the general unitarity constraints (14) and (15)). As a consequence, the growth rate is not important to classify Qws and their unitarity conditions: Cayley graphs looking locally the same will also admit the same solutions to the unitarity conditions, namely the same Qws—if any—on them. For example, the group presented as  $\langle a, b \mid a^4, b^4, (ab)^n \rangle$  has the same paths of length 2 for every  $n \geq 3$ . Then the case  $n = 3$ , studied above, solves the unitarity conditions for a denumerable set of cases. For any  $n \geq 3$ , the Cayley graphs have the same global form, modulo the different length of the the cycles  $(ab)^n$ . Another example is given by the Cayley graph of the dihedral group constructed in Section 6.3: the Qws on the Cayley graph corresponding to the presentation  $D_\infty = \langle a, b, c, d \mid b^2, c^2, bda^{-1}, cda, baba, caca, bca^{-2} \rangle$  exhibit the same unitarity constraints given by all the dihedral groups presented as  $D_n = \langle a, b, c, d \mid b^2, c^2, bda^{-1}, cda, baba, caca, bca^{-2}, a^n \rangle$  for every  $n \geq 5$ . In this latter case, the relator  $a^n = e$  just sets a boundary condition for the graph, wrapping it into a strip.*

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<sup>1</sup> Private communication with Cornelia Druțu.

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## CONCLUSIONS AND OUTLOOKS

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In the *incipit* of this thesis work we have discussed the importance of operationalism and axiomatics in Physics. We supported the idea that QFTs can lie on a discrete framework, legitimised by the information-theoretical paradigm. QFT is still plagued by both mathematical and interpretative issues. On the other hand, QT has hitherto reached a solid foundation on operational and informational grounds. To some extent, an answer has already been given to Wheeler's question: *how come the quantum?*<sup>2</sup>

General Relativity (GR), the other most important theory of XX century besides QT, also suffers from interpretative problems. Are space and time *relational*, namely meaningful only in relation to each other and the other physical objects? What is the theoretical and operational statute of events? Does time possess a physical statute, or is it just there for mathematical convenience? How to interpret singularities? Is GR ultimately an effective theory?

From Ref. [149]: "Emergence from events has an operational motivation in requiring that every physical quantity—including space-time—be defined through precise measurement procedure". Many authors [150] agree in indicating that a (partial, at least) solution to these issues shall be found in order to face the next big open problem of contemporary Physics: formulating a theory which reconciles QT and GR, namely a Quantum Theory of Gravity (QG). As we argued, a discrete scenario would be natural in order to deal with the problem. Strikingly enough, Einstein exhibited the same conclusions in a letter to a former student of him:

But you have correctly grasped the drawback that the continuum brings. If the molecular view of matter is the correct (appropriate) one, i.e., if a part of the universe is to be represented by a finite number of moving points,

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<sup>2</sup> Besides, he emphatically indicated as the "supreme goal" to "*deduce the quantum from an understanding of existence*" [33].

then the continuum of the present theory contains too great a manifold of possibilities. I also believe that this too great is responsible for the fact that our present means of description miscarry with the quantum theory. [...] But we still lack the mathematical structure unfortunately. How much have I already plagued myself in this way!

Yet I see difficulties of principle here too. The electrons (as points) would be the ultimate entities in such a system (building blocks). *Are there* indeed such building blocks? Why are they all of equal magnitude? [...] With the continuum viewpoint one is better off in this respect, because one doesn't have to prescribe elementary building blocks from the beginning. Further, the old question of the vacuum! *But these considerations must pale beside the overwhelming fact: The continuum is more ample than the things to be described.*<sup>3</sup>

During the last decades, many authors developed some of the lacking mathematical structures which Einstein was looking for. Discrete mathematics is now a rich and deep discipline allowing to consider the continuum as an approximation of the discrete, and not rather, viceversa, the discreteness as an idealization of the continuum<sup>4</sup>. In Physics, among the efforts to formulate QG in discrete scenarios, we can cite: causal set theory [152], loop quantum gravity [153], and a recent operational approach of Lucien Hardy to GR [154].

The discrete (free) QFT we examined throughout this work, which we can call the *QCA theory of quantum fields (QCAFT)*, is formulated without making use of quantization rules, nor resorting to mechanical primitives [155]. QCAFT grounds on well-posed principles which are ubiquitous in physical models, and is endowed with an operational basis. Most importantly, it turned out to be suitable for the description of the well-known theory of Dirac and Maxwell free fields [87]. Moreover, the present thesis has relevance *per se* in the scope of QWs. We resorted to work methodologies pertaining statistical mechanics, solid state physics, and lattice gauge theories. Moreover, we used and developed techniques of mathematical physics aiding the investigation of QWs, and showed the relevance of these methods for the scopes of theoretical high energy physics. In the following we summarise our results and their significance.

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<sup>3</sup> The last emphasis is ours. These considerations date back to 1916 [151], right after Einstein's first formulation of GR!

<sup>4</sup> As an example, we mention that the most important axiomatic construction of the real numbers resort to properties of the rational numbers as primitives.



*Part i*

We sketched out a comparison between (discrete-time) classical rws and qws. The latter have been defined in a general context, and then analysed specialising to the case of qws on Cayley graphs. Indeed, the dynamical model of qws on Cayley graphs descends directly (in the noninteracting case) from the principles of QCAFT, which we outlined to a large degree of detail. Then, we needed the mathematical machinery of Group Theory to provide a precise account of the model. In particular, we mention the concept of quasi-isometry between generic metric spaces: via this equivalence relation we have been able to connect qws on Cayley graphs to smooth manifolds.

We paid particular attention to the Abelian case, having a Euclidean embedding. We systematised the free theory and presented a group-theoretical way to rigorously recover the continuum limit and write differential equations for the evolution. Finally, we introduced the relevant physical examples of the Weyl and Dirac qws in three space-dimensions.

*Part ii*

We proceeded developing a rigorous coarse-graining technique for qws on Cayley graphs. Its relevance is double. On the one hand, this method allows to prove structure results in principle for arbitrary classes of qws Cayley graphs. On the other hand, it served as a powerful tool to construct Cayley graphs admitting the implementation of qws. We thus could provide the first example of the explicit solution of the dynamics of qws with minimal algorithmic complexity, that is to say scalar qws.

More specifically, we showed that non-Abelian qws admitting a quasi-isometry to Euclidean spaces reduce to Abelian qws. Our technique allows to study a class of non-Abelian qws using the Fourier analysis, providing the first method to take the continuum limit also in non-Abelian case. In addition, we proved a classification theorem for general Abelian scalar qws, whose dynamics is trivial. Finally, a close examination of the isotropy principle in QCAFT has been performed, leading to a structure theorem for the isotropic spinorial qws (with a two-dimensional coin system) on  $\mathbb{Z}^d$  up to dimension  $d = 3$ . This also represents a full derivation from information-theoretical principles of the Weyl equation. Remarkably, this result—along with the other examples of qws derived from principles throughout this work—suggests a kind of universality of the Weyl and Dirac dynamics in this context.

*Part iii*

We dealt with the extension problem, namely the problem of constructing new groups starting from two fixed ones. We collected and expanded the sporadic results available in the mathematical literature on the explicit construction of group extensions. We then set our coarse-graining technique in the context of induced representations of groups: this is of computational benefit, allowing one to convert the problem of solving the unitarity constraints for scalar qws (hard) into a matricial problem (more feasible).

We thus tackled the problem of constructing Euclidean scalar walks through the construction of the most simple examples of infinite virtually Abelian groups. This allows one to derive scalar qws on them and study such qws as Abelian ones. We gave a first example of a qw on the Cayley graph of a group which is quasi-isometric to the Poincaré disk (having negative curvature). We thus showed that, via the dependence of the unitarity conditions solely on paths of length 2, the computational complexity of the problem does not increase with the graph growth rate.

## WHAT NEXT?

Most of the techniques and notions presented in the present work, as formulated, apply or can be easily generalized to QCAS. In a computational scenario, one possible line of investigation may be given by the connection between groups and e.g. Turing machines, along with its consequences for QCAFT (see Refs. [156, 157]). On the other hand, the constructions here exposed shall be of benefit in the context of QCAS on Cayley graphs, on the route towards a full, interacting QCAFT. The methods of resolution (shown in the Appendices) and the derived solutions themselves may possibly be useful to a simplification of the (linear terms of the) unitarity conditions of nonlinear QCAS, as investigated in Ref. [158]. In particular, one aim in order is to implement known symmetries in Quantum Electrodynamics and Quantum Chromodynamics with QCAS. To this purpose, the notion of isotropy, which proved to be a powerful symmetry to single out known QFT's dynamics, can come to aid. An open problem, for example, is to assess to what extent isotropy is inherited by QCAS under the coarse-graining procedure, and what such a property would imply.

Throughout this work, we mainly dealt with qws embedded in  $\mathbb{R}^d$ . We gave some structure results for low coin-dimension, finding ubiquitous Weyl-like and Dirac-like behaviours. The full emergent spacetime, then, is to be considered Minkowskian. Indeed, as discussed in the Introduction, also full Lorentz covariance is recovered in the

continuum limit. To this extent, we worked in a fixed flat-metric scenario. It is already known that in a discrete GR-like scenario with constant nonvanishing curvature is possible to implement QWS, simulating e.g. the Dirac equation [77, 78]. Yet, authors are nearly unanimous in saying that an acceptable theory of QG has to be background-independent [150]. We thus remark that, despite the fact that we considered a particular restriction of the model (i.e. the zero-curvature sector), QCAFT is in principle a background-independent theory. In order to implement a general relativistic scenario two main ways are viable: one can either find some effect of the evolution in the quantum network which mimics GR, or append an extra structure (as an additional field) to control the evolution of the emergent geometry. This would cope with the fact that the principles of the theory bound the graph to be fixed to the evolution law. Alternatively, one can consider an evolving network structure: a promising approach in this direction has been devised in Refs. [159–161]. If a dynamically evolving state is associated to the graph of interaction, then one may hope to recover right that geometry undergoing dynamical changes which is described by GR. This would mean to relax the principle of homogeneity: the graph would not (at least not entirely) encode the physical law any more. The problem of studying the emergent geometry would be still in order. The coarse-graining technique proved to be a solid tool to establish equivalence classes between different QWS and to study them via a unified tool. Remarkably, in the virtually (non-)Abelian case, it allowed to find differential equation for the evolution. Accordingly, this method or a suitable modification of it could be employed to systematically study the case of non-constant geometry, since general methods to approach the continuum limit even for non-zero fixed curvature are still lacking. A possible route is to investigate the study of “local abelianizations” of Cayley graphs, or even to entirely depart from a Cayley graph structure.

All of this bodes well for future enquiries.

*The answer to these questions can only be got by starting from the conception of phenomena which has hitherto been justified by experience, and which Newton assumed as a foundation, and by making in this conception the successive changes required by facts which it cannot explain. Researches starting from general notions, like the investigation we have just made, can only be useful in preventing this work from being hampered by too narrow views, and progress in knowledge of the interdependence of things from being checked by traditional prejudices.*

*This leads us into the domain of another science, of physics, into which the object of this work does not allow us to go today.*

[115]

# A

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## EXCLUSION OF CAYLEY GRAPHS OF $\mathbb{Z}^d$

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In Secs. A.1–A.4 we will exclude the infinite family of graphs arising from the following finite isotropy groups  $L < \mathcal{O}(3)$ :

1.  $A_4, S_4$  and their direct product with  $\mathbb{Z}_2$  (except for the cases in item 2);
2. the special instances of item 1 where the orbits contain the vertices of a truncated tetrahedron;
3.  $\mathbb{Z}_n, D_n$  for  $n = 3, 4, 6$  and their direct product with  $\mathbb{Z}_2$ ;
4. one special instance arising from  $D_2, D_2 \times \mathbb{Z}_2$ .

### A.1 EXCLUDING $A_4$ - AND $S_4$ -SYMMETRIC CAYLEY GRAPHS

In this subsection we use the convention that unwritten matrix elements are zero. We will consider the orbit of an arbitrary three-dimensional vector  $\mathbf{v} = (\alpha, \beta, \gamma)^T$  under the action of the finite groups  $L \cong A_4, S_4$  in  $\mathcal{O}(3)$ . To this purpose, as discussed in Section 7.1, we will use the real, orthogonal and three-dimensional faithful representations of  $L$ , identifying its representation with the group itself. In the present case of  $L \cong A_4, S_4$ , such representations coincide with the irreducible ones, since the reducible ones cannot be faithful (otherwise they would have orthogonal blocks of dimension at most 2, but  $A_4, S_4$  are not subgroups of  $\mathcal{O}(2)$ ).

We denote with  $\mathcal{O}_L(\mathbf{v})$  the family of orbits of  $\mathbf{v}$  under the action of  $L$ , parametrized by  $\alpha, \beta, \gamma$ . Each orbit satisfies a necessary condition to give rise to an isotropic presentation for  $\mathbb{Z}^d$  for  $d = 1, 2, 3$ .

We will make use of Prop. 7.2 to exclude an infinite family of presentations arising from  $L \cong A_4, S_4$ . Since by Eq. (104) we are interested in sums or differences of generators, the cases  $L \cong A_4 \times \mathbb{Z}_2, S_4 \times \mathbb{Z}_2$  are already accounted: their irreducible representations just add the inversion to the irreducible ones of  $A_4, S_4$ .

The groups  $L$  contain four isomorphic copies of  $\mathbb{Z}_3$ . Let us denote with  $D$  the generator of one of this cyclic subgroups. The content of Eqs. (104) for a fixed choice of  $i, j$  translates to the following. Suppose that for all  $A, B \in L_0 := \{0 \in M_3(\mathbb{R})\} \cup L$  one has:

$$(I - D)\mathbf{v} = s(A + tB)\mathbf{v} \Leftrightarrow (sA\mathbf{v} = \mathbf{v}) \vee (stB\mathbf{v} = \mathbf{v}), \quad (148)$$

( $s, t$  signs). Our strategy is now to solve the necessary conditions for the violation of (148), consisting in systems of the form

$$\forall A, B \in L_0, (I - D - s(A + tB))\mathbf{v} = 0. \quad (149)$$

These will produce some solutions  $\mathbf{v}_0$ . Then we can choose another vector in  $\mathcal{O}_L(\mathbf{v}_0)$ , impose again Eq. (149), and iterate until we end up either with the trivial solution, or with a system of linear equations for  $\alpha, \beta, \gamma$ . By Prop. 7.2, the only  $A_4$ - or  $S_4$ -symmetric Cayley graphs of  $\mathbb{Z}^3$  for which the unitarity conditions may be satisfied must then be found among the non-trivial solutions of the above systems. Since the condition (149) is only necessary, we need to check whether the solutions actually violate condition (148). The remaining differences  $(D - D^2)\mathbf{v}$  and  $(D^2 - I)\mathbf{v}$  are the orbit of  $(I - D)\mathbf{v}$  under  $D$ , then we can just solve (149) and check (148).

In the following we will show that (148) has only trivial solutions for  $A, B \in L$ , except for the special case where  $\mathbf{v} = \alpha(3, 1, 1)^T$ , that will be treated separately in Subsec. A.2. At the end of Subsec. A.1 we will then prove the same result in the case of  $B = 0$ .

It is useful to notice the following:

**Remark A.1.**  $\mathbf{v}_1 \in \mathbb{R}^3$  solves

$$(I - D - s(A + tB))\mathbf{v}_1 = 0$$

iff  $\mathbf{v}_2 := F_2^{-1}\mathbf{v}_1$  solves

$$F_1(I - D - s(A + tB))F_2\mathbf{v}_2 = 0,$$

for some arbitrary  $F_1, F_2 \in \text{GL}(3, \mathbb{R})$ . In particular, this is relevant in the case  $F_2 \in L$ , because it means that the orbits generated by the two solutions  $\mathbf{v}_1, \mathbf{v}_2$  coincide.

This remark will allow us to considerably reduce the number of systems we have to solve. In the following we will refer to a particular solution for (149) indifferently with: 1) the solution vector  $\mathbf{v}_0$ , or 2) the lattice which  $\mathbf{v}_0$  gives rise to, or 3) the polyhedron whose vertices are the elements of  $\mathcal{O}_L(\mathbf{v}_0)$ , or 4) any other vector in  $\mathcal{O}_L(\mathbf{v}_0)$ , or finally 5) the orbit  $\mathcal{O}_L(\mathbf{v}_0)$ . The cases we will end up with are the following:

1. The simple cubic lattice, generated orbiting  $\mathbf{v}_s = \alpha(1, 0, 0)^T$  under  $A_4$ : its vertices are all the signed permutations of the coordinates of  $\mathbf{v}_s$ .
2. The BCC lattice, generated orbiting  $\mathbf{v}_b = \alpha(1, -1, -1)^T$  under  $S_4$ : its vertices are all the signed permutations of the coordinates of  $\mathbf{v}_b$ .
3. The cuboctahedron, whose vertices are all the signed permutations of the coordinates of  $\mathbf{v}_c = \alpha(1, -1, 0)^T$  and are generated by orbiting  $\mathbf{v}_c$  under  $A_4$ .
4. The truncated tetrahedron, whose vertices are all the permutations with an even number of minus signs of the coordinates of  $\mathbf{v}_{tt} = \alpha(3, 1, 1)^T$  and are generated by orbiting  $\mathbf{v}_{tt}$  under  $A_4$ ; in addition, one can also find the solution including the inverses, which is given by  $\mathcal{O}_{S_4}(\mathbf{v}_{tt})$ .
5. The truncated octahedron, whose vertices are all the signed permutations of the coordinates of  $\mathbf{v}_{to} = \alpha(1, -2, 0)^T$  and are generated by orbiting  $\mathbf{v}_{to}$  under  $S_4$ .

One can easily check that  $\mathcal{O}_L(\mathbf{v}_0)$  for the five cases above actually are generating sets for some presentation of  $\mathbb{Z}^3$ .

In the following, we will choose  $D = R$  with  $R(x, y, z)^T = (z, x, y)^T$  ( $R$  is contained in the representation of both  $A_4$  and  $S_4$ ). As a consequence, we can consider  $A \neq B$ , since otherwise there are two possible cases:

1.  $(I - R)\mathbf{v} = \pm 2A\mathbf{v}$ , implying  $(A^{-1} - A^{-1}R)\mathbf{v} = \pm 2\mathbf{v}$ . Since  $A, R \in \mathcal{O}(3)$ , by the triangle inequality it must be

$$A^{-1}\mathbf{v} = \pm\mathbf{v}, \quad A^{-1}R\mathbf{v} = \mp\mathbf{v},$$

and in particular  $\mathbf{v} = -R\mathbf{v}$  holds. This implies  $\mathbf{v} = (0, 0, 0)^T$ .

2.  $(I - R)\mathbf{v} = 0$ , implying  $\mathbf{v} = \alpha(1, 1, 1)^T$ .

Finally, the reader can check that for  $\mathbf{v}_0 \in \{\mathbf{v}_s, \mathbf{v}_b, \mathbf{v}_c, \mathbf{v}_{to}\}$  condition (148) is not violated, thus excluding the cases of  $S_+ = \mathcal{O}_L(\mathbf{v}_0)$  by virtue of Prop. 7.2.

*Excluding  $A_4$ -symmetric Cayley graphs*

$A_4$  has a unique three-dimensional real irreducible representation, generated by the matrices:

$$X_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, R = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \tag{150}$$

We define

$$X_0 = I, X_2 = RX_1R^{-1}, X_3 = R^2X_1R^{-2}.$$

The group contains four isomorphic copies of  $\mathbb{Z}_3$ , generated respectively by the elements of the set  $\{R, X_1R, X_2R, X_3R\}$  (these are cyclic signed permutations of the coordinates).

We now choose the subgroup generated by  $R$  and consider the difference  $(I - R)\mathbf{v}$ , setting the condition (149) for any  $A, B \in A_4$ . Each of these define linear systems of three equations for  $\mathbf{v}$ . If  $A$  equals  $I$  or  $R$ , then it is easy to see that  $\exists G \in A_4$  such that  $G\mathbf{v} = s\mathbf{v}$  ( $s$  a sign): this implies that either  $\mathbf{v} = (0, \beta, \gamma)^T$  up to signed permutations, or  $\mathcal{O}_{A_4}(\mathbf{v}) = \mathcal{O}_{A_4}(\mathbf{v}_b)$ . The latter case has been already excluded. The remaining cases are then i)  $A, B \notin \{I, R\}$  or ii)  $\mathbf{v} = (0, \beta, \gamma)^T$  and signed permutations. Case (ii), however, will appear as a special instance of (i). In case (i), we have six cases for  $s(A + tB)$ :

$$1. s(X_i + tX_j) = \begin{pmatrix} 2s \\ \pm\zeta \\ 0 \end{pmatrix}, \text{ modulo permutations of the diagonal elements,}$$

with arbitrary sign  $s$  and for  $\zeta := 0, 2$ .

$$2. s(X_i + tX_jR) = \begin{pmatrix} s_1 & 0 & t_1 \\ t_2 & s_2 & 0 \\ 0 & t_3 & s_3 \end{pmatrix}, \text{ with } s_1s_2 + s_1s_3 + s_2s_3 = t_1t_2 + t_1t_3 + t_2t_3 = -1.$$



$$3. s(X_i + tX_j)R^2 = \begin{pmatrix} s_1 & t_1 & 0 \\ 0 & s_2 & t_2 \\ t_3 & 0 & s_3 \end{pmatrix}, \text{ with arbitrary signs } t_k, \text{ and } s_1s_2 + s_1s_3 + s_2s_3 = -1.$$

$$4. s(X_i + tX_j)R = \begin{pmatrix} & 2s \\ \pm\zeta & \\ & 0 \end{pmatrix} \text{ and permutations of the written elements, with arbitrary sign } s \text{ and } \zeta = 0, 2.$$

$$5. s(X_i + tX_j)R = \begin{pmatrix} 0 & t_1 & s_1 \\ s_2 & 0 & t_2 \\ t_3 & s_3 & 0 \end{pmatrix}, \text{ with arbitrary signs } t_k, \text{ and } s_1s_2 + s_1s_3 + s_2s_3 = -1.$$

$$6. s(X_i + tX_j)R^2 = \begin{pmatrix} & 2s \\ & \pm\zeta \\ 0 & \end{pmatrix} \text{ and permutations of the written elements, with arbitrary sign } s \text{ and } \zeta = 0, 2.$$

All the above mentioned permutations of elements and those between the  $s_i$  and  $t_i$  are performed by conjugation with  $R^{\pm 1}$ . Since

$$(I - R - sR(A + tB)R^{-1}) = R(I - R - s(A + tB))R^{-1},$$

by Remark A.1 we can just choose one permutation in each of the six cases to find the orbits of the solutions.

Accordingly, explicitly computing the expression

$$I - R - s(A + tB) = \begin{pmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix} - s(A + tB),$$

we end up with the following cases:

1.  $\begin{pmatrix} 1+2s & 0 & -1 \\ -1 & 1 \pm \zeta & 0 \\ 0 & -1 & 1 \end{pmatrix}$ , for  $s$  arbitrary sign.
2.  $\begin{pmatrix} 2 & -2 \\ -\zeta' & \zeta \\ 0 & 0 \end{pmatrix}$ ,  $\begin{pmatrix} 2 & 0 \\ -2 & \zeta \\ -\zeta' & 0 \end{pmatrix}$ ,  $\begin{pmatrix} 0 & -2 \\ -\zeta' & 2 \\ 0 & \zeta \end{pmatrix}$ ,  
with  $\zeta, \zeta' = 0, 2$ .
3.  $\begin{pmatrix} 2 & s_1 & -1 \\ -1 & \zeta & s_2 \\ s_3 & -1 & 0 \end{pmatrix}$ , with  $s_i$  arbitrary.
4.  $\begin{pmatrix} 1 & 0 & 2s-1 \\ -1 & 1 & 0 \\ 0 & \pm\zeta-1 & 1 \end{pmatrix}$ , with  $s$  arbitrary.
5.  $\begin{pmatrix} 1 & s_1 & 0 \\ -2 & 1 & s_2 \\ s_3 & -\zeta & 1 \end{pmatrix}$ , with  $s$  arbitrary.
6.  $\begin{pmatrix} 1 & 2s & -1 \\ -1 & 1 & 0 \\ \pm\zeta & -1 & 1 \end{pmatrix}$ , with  $s$  arbitrary.

The only solution to cases 1 and 4 is  $\mathcal{O}_{A_4}(\mathbf{v}_b)$ . Cases 3, 5 and 6 can be treated together since they exhibit a common structure: their solutions are  $\mathcal{O}_{A_4}(\mathbf{v}_b)$  (which has been already excluded by Prop. 7.2) and  $\mathcal{O}_{A_4}(\mathbf{v}_{tt})$  (which is excluded in Sec. A.2). The only relevant case is 2, since all the other cases have been already excluded.

In case 2, the most general orbits of solutions are  $\mathcal{O}_{A_4}(\mathbf{v}_i)$  for  $i = 1, 2, 3$ , where

$$\mathbf{v}_1 = \begin{pmatrix} \alpha \\ \beta \\ \alpha \end{pmatrix}, \mathbf{v}_2 = \begin{pmatrix} 0 \\ \beta \\ \gamma \end{pmatrix}, \mathbf{v}_3 = R^2 \mathbf{v}_2. \quad (151)$$

Nevertheless, for  $\mathbf{v} \in \{\mathbf{v}_2, \mathbf{v}_3\}$  the condition (148) is not violated. Indeed,  $\mathbf{v}_2$  was found as a solution of

$$(I - R + X_1 - RX_1)\mathbf{v}_2 = 0, \quad (152)$$

however  $X_1\mathbf{v}_2 = -\mathbf{v}_2$ , and thus Eq. (148) is satisfied. A similar argument holds for  $\mathbf{v}_3$ . By virtue of Prop. 7.2 the corresponding orbits  $\mathcal{O}_{A_4}(\mathbf{v}_2)$  and  $\mathcal{O}_{A_4}(\mathbf{v}_3)$  are excluded.

From the above analysis we already know that the only relevant solution is  $\mathbf{v}_1$  for case 2, modulo cyclic permutations. We now impose that  $X_1\mathbf{v}_1$ , which is in  $\mathcal{O}_{A_4}(\mathbf{v}_1)$ , is itself a solution of Eq. (149). Thus we impose

$$X_1\mathbf{v}_1 = \mathbf{w} \in \left\{ \begin{pmatrix} \alpha' \\ \beta' \\ \alpha' \end{pmatrix}, \begin{pmatrix} \alpha' \\ \alpha' \\ \beta' \end{pmatrix}, \begin{pmatrix} \beta' \\ \alpha' \\ \alpha' \end{pmatrix} \right\}.$$

The solutions are  $\mathcal{O}_{A_4}(\mathbf{v}_s)$  and  $\mathcal{O}_{A_4}(\mathbf{v}_b)$ : we can exclude also this last case.

#### *Excluding $S_4$ -symmetric Cayley graphs*

The group  $S_4$  contains  $A_4$  as a subgroup of index 2. The element connecting the two cosets is an involution, which we will denote with  $C$ .  $S_4$  has two three-dimensional irreducible representations: their elements are signed permutations matrices of three elements and the two representations coincide up to a minus sign on the elements in the coset  $CA_4$ . Nevertheless, in our case the sign is irrelevant, since we are considering combinations  $s(A + tB)$  of  $A, B \in S_4$  with  $s, t$  arbitrary signs. Accordingly, we consider the representation resulting from orbiting the elements generated by (150) under the left action of  $\{I, C\}$  with

$$C = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

whose effect is just an exchange of the first and third row.

Let us now define  $X'_i := CX_i$ . In order to perform the computation of  $s(A + tB)$ , we proceed as follows. We have to compute

$$\begin{aligned} & s(X_i + tX_j), s(X'_i + tX'_j), \\ & s(X_i + tX_jR), s(X'_i + tX'_jR), \\ & s(X'_i + tX_j), s(X'_i + tX_jR), s(X'_i + tX_jR^2) \end{aligned} \tag{153}$$

and then recover all the remaining combinations by right multiplication of these by  $R^{\pm 1}$ . For (153), we obtain the following cases:

$$\begin{aligned} 1. & \begin{pmatrix} \pm 2 & & \\ & \zeta & \\ & & 0 \end{pmatrix}, \begin{pmatrix} & & \pm 2 \\ & \zeta & \\ 0 & & \end{pmatrix}, \text{ considering all the permutations of elements and} \\ & \zeta = 0, \pm 2. \\ 2. & \begin{pmatrix} s_1 & & t_1 \\ t_2 & s_2 & \\ & t_3 & s_3 \end{pmatrix}, \begin{pmatrix} & t_1 & s_1 \\ t_2 & s_2 & \\ s_3 & & t_3 \end{pmatrix}, \begin{pmatrix} s_1 & & s_2 \\ & \zeta & \\ s_3 & & s_4 \end{pmatrix}, \\ & \begin{pmatrix} & & \zeta \\ t_2 & s_2 & \\ s_3 & t_3 & \end{pmatrix}, \begin{pmatrix} & t_1 & s_1 \\ & s_2 & t_2 \\ \zeta & & \end{pmatrix}, \text{ for } \zeta = 0, \pm 2. \end{aligned}$$

As mentioned above, one has to add to these cases the matrices resulting from a right multiplication of the previous ones by  $R^{\pm 1}$ , whose action is a cyclic permutation of the columns. Let us now consider

$$I - R = \begin{pmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix},$$

and derive the following matrices

$$I - R + s(A + tB)R^i, \quad i = 0, \pm 1 \tag{154}$$

for all the mentioned cases.

1. It's easy to verify that, in this case, either the matrices in Eq. (154) have trivial solution or their solutions are  $\mathcal{O}_{S_4}(\mathbf{v}_b)$  (already excluded) and  $\mathcal{O}_{S_4}(\mathbf{v}_{tt})$  (which will be treated in Section A.2).

$$\begin{aligned}
2. & \begin{pmatrix} 1+s_1 & & t_1-1 \\ t_2-1 & 1+s_2 & \\ & t_3-1 & 1+s_3 \end{pmatrix}, \begin{pmatrix} 1 & & \zeta-1 \\ t_2-1 & 1+s_2 & \\ s_3 & t_3-1 & 1 \end{pmatrix}, \\
& \begin{pmatrix} 1 & t_1 & s_1-1 \\ s_2-1 & 1 & t_2 \\ t_3 & s_3-1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & \zeta & -1 \\ s_2-1 & 1 & t_2 \\ t_3 & -1 & 1+s_3 \end{pmatrix}, \\
& \begin{pmatrix} 1+t_1 & s_1 & -1 \\ -1 & 1+t_2 & s_2 \\ s_3 & -1 & 1+t_3 \end{pmatrix}, \begin{pmatrix} 1+\zeta & & -1 \\ -1 & 1+t_2 & s_2 \\ & s_3-1 & 1+t_3 \end{pmatrix}, \\
& \begin{pmatrix} 1 & t_1 & s_1-1 \\ t_2-1 & 1+s_2 & \\ s_3 & -1 & 1+t_3 \end{pmatrix}, \begin{pmatrix} 1+t_1 & s_1 & -1 \\ s_2-1 & 1+t_2 & \\ & -1 & \zeta+1 \end{pmatrix}, \\
& \begin{pmatrix} 1+t_1 & s_1 & -1 \\ s_2-1 & 1 & t_2 \\ & t_3-1 & 1+s_3 \end{pmatrix}, \begin{pmatrix} 1+s_1 & & t_1-1 \\ t_2-1 & 1 & s_2 \\ & \zeta-1 & 1 \end{pmatrix}, \\
& \begin{pmatrix} 1+s_1 & & t_1-1 \\ -1 & 1+t_2 & s_2 \\ t_3 & s_3-1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & t_1 & s_1-1 \\ -1 & 1+s_2 & t_2 \\ \zeta & -1 & 1 \end{pmatrix}, \\
& \begin{pmatrix} 1+s_1 & & s_2-1 \\ -1 & 1+\zeta & \\ s_3 & -1 & 1+s_4 \end{pmatrix}, \begin{pmatrix} 1 & s_2 & s_1-1 \\ \zeta-1 & 1 & \\ & s_4-1 & 1+s_3 \end{pmatrix}, \\
& \begin{pmatrix} 1+s_2 & s_1 & -1 \\ -1 & 1 & \zeta \\ s_4 & s_3-1 & 1 \end{pmatrix}.
\end{aligned}$$

The above set can be partitioned into equivalence classes according to the relation:

$$N \sim M \Leftrightarrow \exists F \in S_4, F' \in \mathbf{GL}(3, \mathbb{R}) : N = F'MF. \quad (155)$$

By Remark A.1 the above equivalence relation preserves the orbits of solutions of the linear systems. It is easy to check that there are five equivalence classes represented by the following matrices:

$$M_1 = \begin{pmatrix} 1 + s_1 & & s_2 - 1 \\ -1 & 1 + \zeta & \\ s_3 & -1 & 1 + s_4 \end{pmatrix},$$

$$M_2 = \begin{pmatrix} 1 + s_1 & & t_1 - 1 \\ t_2 - 1 & 1 + s_2 & \\ & t_3 - 1 & 1 + s_3 \end{pmatrix},$$

$$M_3 = \begin{pmatrix} 1 & t_1 & s_1 - 1 \\ t_2 - 1 & 1 + s_2 & \\ s_3 & -1 & 1 + t_3 \end{pmatrix},$$

$$M_4 = \begin{pmatrix} 1 & t_1 & s_1 - 1 \\ s_2 - 1 & 1 & t_2 \\ t_3 & s_3 - 1 & 1 \end{pmatrix},$$

$$M_5 = \begin{pmatrix} 1 & \zeta & -1 \\ s_2 - 1 & 1 & t_2 \\ t_3 & -1 & 1 + s_3 \end{pmatrix}.$$

The solutions for  $M_4, M_5$  are  $\mathcal{O}_{S_4}(\mathbf{v}_s), \mathcal{O}_{S_4}(\mathbf{v}_b)$  (that have been already excluded) and  $\mathcal{O}_{S_4}(\mathbf{v}_{tt})$ , that will be treated in Section A.2.

The three remaining cases are given in the following:

- For  $M_1$  one has  $\mathcal{O}_{S_4}(\mathbf{v}_s), \mathcal{O}_{S_4}(\mathbf{v}_b), \mathcal{O}_{S_4}(\mathbf{v}_c), \mathcal{O}_{S_4}(\mathbf{v}_{tt})$ , and  $\mathcal{O}_{S_4}(\mathbf{v}_1), \mathcal{O}_{S_4}(\mathbf{v}_2)$ , with

$$\mathbf{v}_1 = \begin{pmatrix} \alpha \\ \alpha \\ \beta \end{pmatrix}, \quad \mathbf{v}_2 = \alpha \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix};$$

The systems in the same equivalence class are connected by the permutations  $F \in \{R^{\pm 1}, C, CR^{\pm 1}\}$ .

- For  $M_2$  one has  $\mathcal{O}_{S_4}(\mathbf{v}_1)$  and  $\mathcal{O}_{S_4}(\mathbf{v}_3)$ , with

$$\mathbf{v}_3 = \begin{pmatrix} 0 \\ \alpha \\ \beta \end{pmatrix};$$

- For  $M_3$  one has  $\mathcal{O}_{S_4}(\mathbf{v}_s), \mathcal{O}_{S_4}(\mathbf{v}_b), \mathcal{O}_{S_4}(\mathbf{v}_c), \mathcal{O}_{S_4}(\mathbf{v}_{to}), \mathcal{O}_{S_4}(\mathbf{v}_1)$  and  $\mathcal{O}_{S_4}(\mathbf{v}_4)$ , with

$$\mathbf{v}_4 = \begin{pmatrix} \alpha \\ \beta \\ \frac{\alpha+\beta}{2} \end{pmatrix}.$$

The systems in the same equivalence class are connected by the permutations  $F \in \{R^2, C\}$ .

We notice that  $\mathbf{v}_2$  is a particular case of  $\mathbf{v}_4$ , then we can just treat the latter. On the other hand, the vectors in  $\mathcal{O}_{S_4}(\mathbf{v}_3)$  cannot be solutions for  $M_i$  with  $i \neq 2$ , otherwise the orbit is reduced to  $\mathcal{O}_{S_4}(\mathbf{v}_s)$ , or  $\mathcal{O}_{S_4}(\mathbf{v}_c)$ , or  $\mathcal{O}_{S_4}(\mathbf{v}_{to})$ , which are ruled out. The remaining case of  $\mathcal{O}_{S_4}(\mathbf{v}_3)$  can be then excluded via the same analysis of case 2 in the previous section.

We end up with  $\mathcal{O}_{S_4}(\mathbf{v}_1), \mathcal{O}_{S_4}(\mathbf{v}_4)$ . We observe that imposing that  $X_2\mathbf{v}_1$  is a solutions for  $M_1, M_2, M_3$  gives rise to  $\mathcal{O}_{S_4}(\mathbf{v}_s), \mathcal{O}_{S_4}(\mathbf{v}_b), \mathcal{O}_{S_4}(\mathbf{v}_c)$ . As for  $\mathcal{O}_{S_4}(\mathbf{v}_4)$ , imposing that  $X_2\mathbf{v}_4$  is a solution leads to  $\mathcal{O}_{S_4}(\mathbf{v}_{tt}), \mathcal{O}_{S_4}(\mathbf{v}_{to})$ , and  $\mathcal{O}_{S_4}(\mathbf{v}_5)$  with  $\mathbf{v}_5 = \alpha(5, 3, 1)^T$ . However, it's easy to verify that  $(I - X_2R)\mathbf{v}_5$  is uniquely determined as sum of elements of  $\{\mathbf{0}, \mathcal{O}_{S_4}(\pm\mathbf{v}_5)\}$ , leading us to exclude this last case by virtue of Prop. 7.2.

Finally, as anticipated at the beginning of the present section, we can exclude  $(I - R)\mathbf{v} = \pm A\mathbf{v}$  for  $A \in L$  and  $L \cong A_4, S_4$ : by direct inspection of the representation matrices of  $S_4$ , it turns out that this condition leads to  $\mathcal{O}_{S_4}(\mathbf{v}_c)$ .

## A.2 EXCLUSION OF THE TRUNCATED TETRAHEDRON

In this section we make use of the three-dimensional irreducible representation of  $A_4$  provided in Section A.1 in order to exclude, by means of the unitarity conditions, the graph whose primitive cell is the set of vertices of the truncated tetrahedron. This also excludes the case where the inverses are contained in  $S_+$ . For notation convenience,

we will use the Pauli matrices notation  $\sigma_x := X_1$ ,  $\sigma_y := X_2$ , and  $\sigma_z := X_3$ , and use the vector  $\mathbf{w}_{tt} = \alpha(1, 1, 3)^T$  instead of  $\mathbf{v}_{tt}$  as a representative of the orbit  $\mathcal{O}_{A_4}(\mathbf{v}_{tt})$ . In the following we will also denote the elements  $G\mathbf{w}_{tt}$  (for  $G \in A_4$ ) with the shorthand  $G$ .

Let  $U$  be a faithful unitary and (generally projective) representation of  $A_4$  in  $\text{SU}(2)$ . We will denote the transition matrices as

$$A_{\pm G} := U_G A_{\pm I} U_G^\dagger, \quad (156)$$

with  $G \in A_4$ . From the unitarity conditions, choosing  $\mathbf{h}'' = 2\mathbf{w}_{tt}$ , one derives the form

$$A_{\pm I} := \alpha_{\pm} V |\pm\rangle \langle \pm|, \quad (157)$$

with  $\{|+\rangle, |-\rangle\}$  orthonormal basis,  $\alpha_{\pm} > 0$  and  $V$  unitary. Consider the following unitarity conditions:

$$A_I A_W^\dagger + A_{-W} A_{-I}^\dagger = 0, \quad W = X, Y.$$

By multiplication on the right by  $A_I$  we obtain

$$A_I A_W^\dagger A_I = 0,$$

implying that  $U_W$  must be antidiagonal in the  $\{|+\rangle, |-\rangle\}$  basis or in  $\{V|+\rangle, V|-\rangle\}$ . On the other hand, from

$$A_I A_{-R}^\dagger + A_R A_{-I}^\dagger = 0,$$

one gets

$$A_{-I} A_R^\dagger A_{-I} = 0, \quad (158)$$

meaning that  $U_R$  must be diagonal in  $\{|+\rangle, |-\rangle\}$  or  $\{V|+\rangle, V|-\rangle\}$ .

Let us now suppose that  $U_X$  is antidiagonal in  $\{|+\rangle, |-\rangle\}$  and  $U_Y$  antidiagonal in  $\{V|+\rangle, V|-\rangle\}$  (or viceversa): then, since

$$U_R U_X U_R^\dagger = s_1 U_Y, \quad U_R U_Y U_R^\dagger = s_2 U_Z, \quad (159)$$



( $s_1, s_2$  arbitrary signs) all of the  $U_G$  for  $G = X, Y, Z$  would be antidiagonal in one of the two bases, but this violates the algebra of  $D_2 \equiv \{I, X, Y, Z\}$  in  $A_4$ . Accordingly, choosing the  $\{|+\rangle, |-\rangle\}$  basis and imposing

$$U_X U_Y = t_1 U_Y U_X = t_2 U_Z, \quad U_G^2 = t_3 I \quad (160)$$

(for  $G = X, Y, Z$  and  $t_1, t_2, t_3$  arbitrary signs), it is easy to see that up to a change of basis we can always take:

$$U_G = i\sigma_G, \quad G = X, Y, Z$$

with  $|+\rangle, |-\rangle$  eigenvectors of  $\sigma_Z$ . This implies that, in order to satisfy (159),  $U_R$  cannot have vanishing elements in  $\{|+\rangle, |-\rangle\}$  and then by Eq. (158) it must be diagonal in  $\{V|+\rangle, V|-\rangle\}$ . Consequently we must have:

$$U_R := V D V^\dagger, \quad (161)$$

where  $D = \text{diag}(e^{i\epsilon}, e^{-i\epsilon})$  in  $\{|+\rangle, |-\rangle\}$  and  $e^{3i\epsilon}$  is a sign. As a consequence, using conditions (160) one sees that the  $U_X, U_Y, U_Z$  cannot have vanishing elements in  $\{V|+\rangle, V|-\rangle\}$ . This in turn implies, by Eq. (159), that  $V$  cannot have vanishing elements in  $\{|+\rangle, |-\rangle\}$ .

Let us now pose

$$V = \begin{pmatrix} \rho e^{i\theta} & \tau e^{i\varphi} \\ -\tau e^{-i\varphi} & \rho e^{-i\theta} \end{pmatrix} : \rho, \tau > 0, \rho^2 + \tau^2 = 1.$$

Multiplying on the left by  $A_{-I}^\dagger$  the following unitarity condition

$$A_I A_{RX}^\dagger + A_{-RX} A_{-I}^\dagger + A_R A_Y^\dagger + A_{-Y} A_{-R}^\dagger = 0,$$

and reminding that  $A_{-I}^\dagger A_R A_Y^\dagger = 0$  by Eq. (161), one has

$$A_{-I}^\dagger A_{-RX} A_{-I}^\dagger + A_{-I}^\dagger A_{-Y} A_{-R}^\dagger = 0.$$

Now, substituting Eq. (157), and using definition (156), the nonvanishing matrix element of the previous identity in the basis  $\{|+\rangle, |-\rangle\}$  is

$$\begin{aligned} \langle -|V^\dagger U_{RX} V|-\rangle \langle -|U_{RX}^\dagger|-\rangle &= \\ &= -e^{i\epsilon} \langle -|V^\dagger U_Y V|-\rangle \langle -|U_Y^\dagger U_R|-\rangle. \end{aligned}$$

Recalling the form of  $V$  given above and using the fact that  $U_{RX} = t' U_R U_X$  ( $t'$  a sign) and that  $U_R$  cannot have vanishing elements in the basis  $\{|+\rangle, |-\rangle\}$ , for the previous equation we finally obtain

$$\cos(\theta_1 + \varphi_1) = -i \sin(\theta_1 + \varphi_1) e^{2i\epsilon},$$

which has no solution.

### A.3 EXCLUSION OF $\mathbb{Z}_n, D_n, \mathbb{Z}_n \times \mathbb{Z}_2$ AND $D_n \times \mathbb{Z}_2$ , WITH $n = 3, 4, 6$

The aim of the present section is: 1) to construct the real, orthogonal and three-dimensional faithful representations of the groups  $L \in \{\mathbb{Z}_n, D_n, \mathbb{Z}_n \times \mathbb{Z}_2, D_n \times \mathbb{Z}_2 \mid n = 3, 4, 6\}$ , and 2) to exclude all the graphs arising from  $L$  by means of the unitarity conditions.

By the classification theorem for real matrices of finite order given in Ref. [162], any matrix in  $O(3)$  of order  $n$  is similar to one of the form

$$R_{\theta,s} := \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & s \end{pmatrix},$$

with  $\theta = \frac{2z\pi}{n}$ ,  $z$  integer and  $s$  a sign. The matrices  $R_{\theta,s}$  represent the generators for the subgroups of order  $n = 3, 4, 6$  in  $L$ . We can generate the orbits of  $L$  starting from the generic vector (up to a rotation around the  $z$ -axis) given by  $\mathbf{v}_1 = (1, 0, h)^T$ . It is easy to show that the only matrices in  $O(3)$  of order 2 commuting with  $R_{\theta,s}$  for all  $\theta$

and  $s$  are  $R_{0,t}$  and  $R_{\pi,t}$ : they represent the generators of  $L/\mathbb{Z}_n$  for  $L \cong \mathbb{Z}_n \times \mathbb{Z}_2$  or  $L/D_n$  for  $L \cong D_n \times \mathbb{Z}_2$ . On the other hand, the involutions

$$S_{\varphi,r} := \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ \sin \varphi & -\cos \varphi & 0 \\ 0 & 0 & r \end{pmatrix}$$

are the only ones such that  $S_{\varphi,r}R_{\theta,s}S_{\varphi,r}^{-1} = S_{\varphi,r}R_{\theta,s}S_{\varphi,r} = R_{\theta,s}^{-1}$ . This implies that the  $S_{\varphi,r}$  represent the generators for the subgroups of reflections when  $L$  is a dihedral group. Therefore, in general, the elements of  $\mathcal{O}_L(\mathbf{v}_1)$  lie on the two circumferences which are parallel to the  $xy$ -plane at heights  $z = \pm h$ .

In order to solve the unitarity conditions, it is necessary to determine the paths with length 2 constructed by elements in  $\{\mathbf{0}\} \cup \mathcal{O}_L(\mathbf{v}_1)$ : by the above analysis, the problem is reduced to a two-dimensional problem, since the form of the vectors in  $\mathcal{O}_L(\mathbf{v}_1)$  is  $\mathbf{v}_i = (x_i, y_i, \pm h)^T := (\cos \chi_i, \sin \chi_i, \pm h)^T$ . Accordingly, it is easy to see that

$$\mathbf{v}_i \pm \mathbf{v}_j = s\mathbf{v}_l + t\mathbf{v}_p, \quad \mathbf{v}_i, \mathbf{v}_j, \mathbf{v}_l, \mathbf{v}_p \neq \mathbf{0}, \quad (s, t \text{ signs})$$

implies  $(x_i, y_i) = s(x_l, y_l)$  or  $(x_i, y_i) = t(x_p, y_p)$ .

**Case  $n = 4$ .** There are at least two inequivalent orthogonal representations of  $L \in \{\mathbb{Z}_4, D_4, \mathbb{Z}_4 \times \mathbb{Z}_2, D_4 \times \mathbb{Z}_2\}$ , since the element of order 4 can be either represented by  $R_{\frac{\pi}{2},-}$  or  $R_{\frac{\pi}{2},+}$ . We shall now analyse the two different cases.

$R_{\frac{\pi}{2},-}$  generates the four vectors

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 0 \\ h \end{pmatrix}, \mathbf{v}_2 = \begin{pmatrix} 0 \\ 1 \\ -h \end{pmatrix}, \mathbf{v}_3 = \begin{pmatrix} -1 \\ 0 \\ h \end{pmatrix}, \mathbf{v}_4 = \begin{pmatrix} 0 \\ -1 \\ -h \end{pmatrix}.$$

The differences  $\mathbf{v}_i - \mathbf{v}_j \neq \mathbf{0} \forall i, j \in \{1, 2, 3, 4\}$  are uniquely determined as sums of elements of  $\{\mathbf{0}, \mathcal{O}_L(\pm \mathbf{v}_1)\}$ . Accordingly, there is a cyclic subgroup of order 4 (i.e.  $\mathbb{Z}_4$ ) whose orbit satisfies Eq. (104) and thus, invoking Proposition 7.1 (we remind that the representation  $U$  must be faithful), we exclude the representation containing  $R_{\frac{\pi}{2},-}$ .

Taking now  $R_{\frac{\pi}{2},+}$ , the orbit is

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 0 \\ h \end{pmatrix}, \mathbf{v}_2 = \begin{pmatrix} 0 \\ 1 \\ h \end{pmatrix}, \mathbf{v}_3 = \begin{pmatrix} -1 \\ 0 \\ h \end{pmatrix}, \mathbf{v}_4 = \begin{pmatrix} 0 \\ -1 \\ h \end{pmatrix}.$$

We have that the vectors

$$\mathbf{v}_1 + \mathbf{v}_2, \quad \mathbf{v}_1 - \mathbf{v}_3 \tag{162}$$

are uniquely determined as sum of elements of  $\{\mathbf{0}, \mathcal{O}_L(\pm\mathbf{v}_1)\}$ . Let us denote with  $R$  the matrix representing  $R_{\frac{\pi}{2},+}$  in  $\text{SU}(2)$  and proceed as in Section A.2. From now on in the present section we use the notation of Eq. (156) and perform calculations in the  $\{|+\rangle, |-\rangle\}$  basis. Multiplying on the right by  $A_{\mathbf{v}_1}$  the unitarity conditions associated to the vectors in (162), we obtain

$$A_{\mathbf{v}_1} R A_{-\mathbf{v}_1}^\dagger R^\dagger A_{\mathbf{v}_1} = 0, \quad A_{\mathbf{v}_1} R^2 A_{\mathbf{v}_1}^\dagger R^{2\dagger} A_{\mathbf{v}_1} = 0. \tag{163}$$

By the first of conditions (163), up to a change of basis we can impose

$$R = \begin{pmatrix} \mu & 0 \\ 0 & \mu^* \end{pmatrix}, \quad R^4 = sI$$

( $s$  arbitrary sign); using the second condition, it follows that

$$R^2 = \begin{pmatrix} \mu^2 & 0 \\ 0 & \mu^{*2} \end{pmatrix} = V \begin{pmatrix} 0 & \nu \\ -\nu^* & 0 \end{pmatrix} V^\dagger, \tag{164}$$

and thus necessarily  $\mu^2 \neq \mu^{*2}$ . Consider now the unitarity condition

$$A_{\mathbf{v}_1} A_{\mathbf{v}_2}^\dagger + A_{-\mathbf{v}_2} A_{-\mathbf{v}_1}^\dagger + A_{\mathbf{v}_4} A_{\mathbf{v}_3}^\dagger + A_{-\mathbf{v}_3} A_{-\mathbf{v}_4}^\dagger = 0.$$

Multiplying the last equation by  $A_{\mathbf{v}_1}$  on the right and taking the adjoint we get <sup>1</sup>

<sup>1</sup> One has  $A_{-\mathbf{v}_2} A_{-\mathbf{v}_1}^\dagger A_{\mathbf{v}_1} = 0$  since  $A_{-\mathbf{v}_1}^\dagger A_{\mathbf{v}_1} = 0$ , and  $A_{\mathbf{v}_4} A_{\mathbf{v}_3}^\dagger A_{\mathbf{v}_1} = 0$ , since  $A_{\mathbf{v}_3}^\dagger A_{\mathbf{v}_1} = R^2 A_{\mathbf{v}_1}^\dagger R^{2\dagger} A_{\mathbf{v}_1}$  and  $A_{\mathbf{v}_1}^\dagger R^2 A_{\mathbf{v}_1} = \alpha_+^2 |+\rangle \langle +| V^\dagger R^2 V |+\rangle \langle +|$ , and by Eq. (164)  $\langle +| V^\dagger R^2 V |+\rangle = 0$ .

$$A_{\mathbf{v}_1}^\dagger A_{\mathbf{v}_2} A_{\mathbf{v}_1}^\dagger + A_{\mathbf{v}_1}^\dagger A_{-\mathbf{v}_4} A_{-\mathbf{v}_3}^\dagger = 0,$$

which amounts to

$$\begin{aligned} & \frac{\alpha_+^2}{\alpha_-^2} \langle + | R^\dagger | + \rangle \langle + | V^\dagger R V | + \rangle = \\ & = -\nu^* \langle - | R^\dagger | - \rangle \langle + | V^\dagger R^3 V | - \rangle. \end{aligned} \quad (165)$$

Posing now

$$V^\dagger R V = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix},$$

with  $a, b \neq 0$  since otherwise  $V^\dagger R^2 V$  cannot be anti-diagonal (see Eq. (164)), we have that

$$V^\dagger R^3 V = (V^\dagger R V)(V^\dagger R^2 V) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \begin{pmatrix} 0 & \nu \\ -\nu^* & 0 \end{pmatrix}.$$

Accordingly, Eq. (165) leads to

$$\frac{\alpha_+^2}{\alpha_-^2} = -\mu^2,$$

which is impossible, since  $\mu^2 \neq \mu^{*2}$ .

**Cases  $n = 3, 6$ .** The representations of  $L \in \{\mathbb{Z}_n, D_n, \mathbb{Z}_n \times \mathbb{Z}_2, D_n \times \mathbb{Z}_2 \mid n = 3, 6\}$  must contain  $R_{\frac{2\pi}{3}, +}$ , which generates a subgroup  $K$  isomorphic to  $\mathbb{Z}_3$ :  $\mathcal{O}_K(\mathbf{v}_1)$  is given by the following vectors:

$$\mathbf{v}_l = \begin{pmatrix} \cos \frac{2\pi}{3}(l-1) \\ \sin \frac{2\pi}{3}(l-1) \\ h \end{pmatrix}, \quad l \in \{1, 2, 3\}.$$

We denote the representation matrix of  $R_{\frac{2\pi}{3}, +}$  in  $\text{SU}(2)$  with  $U_{\frac{2\pi}{3}}$ .

If  $\mathbf{v}_1 - \mathbf{v}_2$  is uniquely determined as sum of elements of  $\{\mathbf{0}, \mathcal{O}_L(\pm \mathbf{v}_1)\}$  (a particular case is given by the condition  $h = 0$ ), we can exclude this case by Proposition 7.2.

Let us then suppose that  $\mathbf{v}_1 - \mathbf{v}_2$  is not uniquely determined as sum of elements of  $\{\mathbf{0}, \mathcal{O}_L(\pm \mathbf{v}_1)\}$  (in particular  $h \neq 0$ ). Then, by the above analysis,  $\mathcal{O}_L(\mathbf{v}_1)$  must contain

$$\mathbf{v}_l = \begin{pmatrix} -\cos \frac{2\pi}{3}(l-1) \\ -\sin \frac{2\pi}{3}(l-1) \\ h \end{pmatrix}, \quad l \in \{4, 5, 6\}$$

(such that  $\mathbf{v}_1 - \mathbf{v}_2 = \mathbf{v}_5 - \mathbf{v}_4$ ). Again, via the above arguments on the representations of  $L$ , is easy to see that  $\mathbf{v}_1 + \mathbf{v}_2$  is uniquely determined as sum of elements of  $\{\mathbf{0}, \mathcal{O}_L(\pm \mathbf{v}_1)\}$ . Then, from condition

$$A_{\mathbf{v}_1} A_{-\mathbf{v}_2}^\dagger + A_{\mathbf{v}_2} A_{-\mathbf{v}_1}^\dagger = 0,$$

by multiplying on the right by  $A_{\mathbf{v}_1}$ , we get

$$A_{\mathbf{v}_1} A_{-\mathbf{v}_2}^\dagger A_{\mathbf{v}_1} = 0.$$

Up to a change of basis  $U_{\frac{2\pi}{3}} = \text{diag}(e^{i\epsilon}, e^{-i\epsilon})$  holds with  $e^{3i\epsilon} = \pm 1$ , and  $\epsilon \notin \{0, \pi\}$ . Let  $U_\pi$  represent the element of  $L$  mapping  $\mathbf{v}_1$  to  $\mathbf{v}_4$ . This element is an involution and there are only two cases (by inspection of the groups  $L$  here considered)

$$U_\pi U_{\frac{2\pi}{3}} U_\pi^\dagger = \begin{cases} s U_{\frac{2\pi}{3}} \\ s' U_{\frac{2\pi}{3}}^\dagger \end{cases} \quad (166)$$

( $s, s'$  signs). Recalling that the representation  $U \subset \text{SU}(2)$  is faithful and  $U_{\frac{2\pi}{3}}^3 = tI$  ( $t$  a sign), it is easy to verify that the previous two conditions on  $U_{\frac{2\pi}{3}}, U_\pi$  are satisfied respectively only if

1.  $U_\pi$  is diagonal;
2.  $U_\pi$  is anti-diagonal.

Multiplying by  $A_{\mathbf{v}_1}$  on the right the unitarity condition associated to the difference  $\mathbf{v}_1 - \mathbf{v}_4$

$$A_{\mathbf{v}_1} A_{\mathbf{v}_4}^\dagger + A_{-\mathbf{v}_4} A_{-\mathbf{v}_1}^\dagger = 0,$$

one also gets

$$A_{\mathbf{v}_1} A_{\mathbf{v}_4}^\dagger A_{\mathbf{v}_1} = 0,$$

namely either  $A_{\mathbf{v}_4}^\dagger A_{\mathbf{v}_1} = 0$  or  $A_{\mathbf{v}_1} A_{\mathbf{v}_4}^\dagger = 0$ . This implies that a)  $V^\dagger U_\pi V$  is anti-diagonal or b)  $U_\pi$  is anti-diagonal. In case a), multiplying by  $A_{\mathbf{v}_1}$  on the right the unitarity condition

$$A_{\mathbf{v}_1} A_{\mathbf{v}_2}^\dagger + A_{-\mathbf{v}_2} A_{-\mathbf{v}_1}^\dagger + A_{\mathbf{v}_5} A_{\mathbf{v}_4}^\dagger + A_{-\mathbf{v}_4} A_{-\mathbf{v}_5}^\dagger = 0,$$

it follows that

$$A_{\mathbf{v}_1} A_{\mathbf{v}_2}^\dagger A_{\mathbf{v}_1} + A_{-\mathbf{v}_4} A_{-\mathbf{v}_5}^\dagger A_{\mathbf{v}_1} = 0; \quad (167)$$

in case b) multiplying by  $A_{\mathbf{v}_1}^\dagger$  on the right the unitarity condition

$$A_{\mathbf{v}_1}^\dagger A_{\mathbf{v}_2} + A_{-\mathbf{v}_2}^\dagger A_{-\mathbf{v}_1} + A_{\mathbf{v}_5}^\dagger A_{\mathbf{v}_4} + A_{-\mathbf{v}_4}^\dagger A_{-\mathbf{v}_5} = 0, \quad (168)$$

and taking the adjoint, it follows that

$$A_{\mathbf{v}_1} A_{\mathbf{v}_2}^\dagger A_{\mathbf{v}_1} + A_{\mathbf{v}_1} A_{-\mathbf{v}_5}^\dagger A_{-\mathbf{v}_4} = 0. \quad (169)$$

Let us now pose

$$V^\dagger U_{\frac{2\pi}{3}} V = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix},$$

where  $a \neq 0$  since  $U_{\frac{2\pi}{3}}^3 = tI$ . In case a), from (167) one then has

$$\frac{\alpha_+^2}{\alpha_-^2} e^{i\epsilon} = - \langle - | U_\pi^\dagger U_{\frac{2\pi}{3}} U_\pi | - \rangle,$$

which cannot be satisfied neither in case 1 nor in case 2. On the other hand in case b), from (169) one has

$$\frac{\alpha_+^2}{\alpha_-^2} a^* e^{i\epsilon} = -e^{-i\epsilon} \langle - | V^\dagger U_\pi^\dagger U_{\frac{2\pi}{3}}^\dagger U_\pi V | - \rangle,$$

and being  $U_\pi$  anti-diagonal, one has

$$\frac{\alpha_+^2}{\alpha_-^2} a^* e^{2i\epsilon} = - \langle - | V^\dagger U_{\frac{2\pi}{3}} V | - \rangle = -a^*,$$

which is impossible, since  $e^{3i\epsilon} = \pm 1$ , for  $\epsilon \notin \{0, \pi\}$ .

#### A.4 REMAINING PRESENTATIONS ARISING FROM $\mathbb{Z}_2$ , $D_2$ AND $D_2 \times \mathbb{Z}_2$

By the argument of Section A.3, any matrix of order 2 in  $\mathcal{O}(3)$  is similar to

$$M_{s,t} := \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & t \end{pmatrix},$$

with  $s, t$  signs. Accordingly, up to conjugation, any three-dimensional orthogonal representation of a group  $L \in \{\mathbb{Z}_2, D_2, D_2 \times \mathbb{Z}_2\}$  contains  $M_{s,t}$ . If  $s \neq t$ , any matrix  $N$  of order 2 in  $\mathcal{O}(3)$  commuting with  $M_{s,t}$  is either  $M_{s',t'}$ , or of the form:

$$N = \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ \sin \varphi & -\cos \varphi & 0 \\ 0 & 0 & r \end{pmatrix},$$

with  $r$  a sign. Being the two dimensional block a reflection matrix, there exists a similarity transformation which maps it to  $\pm \sigma_z$  (and leaving  $M_{s,t}$  invariant). Thus the real, orthogonal and three-dimensional faithful representations of the groups here considered contain just  $M_{s,t}$  and

$$N_{r_1, r_2} := \begin{pmatrix} r_1 & 0 & 0 \\ 0 & -r_1 & 0 \\ 0 & 0 & r_2 \end{pmatrix}.$$

The problem reduces to combine signs in  $M_{s,t}, N_{r_1, r_2}$  to give rise to faithful representations of  $L$ . It is easy to check that they give rise to the integer lattice, the square lattice



or the BCC lattice (one can include the inverses or not). Nevertheless, there are two ways of providing a minimal generating set (namely such that  $S_+ \neq S_-$ ) for  $\mathbb{Z}^3$  and whose Cayley graph is associated with the BCC lattice. Such presentations are both generated by  $D_2$ : one is made with the vertices of a tetrahedron, as shown in Fig. 2; the second one corresponds to the vertices of the upper face of the cell given by the following vectors

$$\mathbf{v}_0 = \begin{pmatrix} 1 \\ 1 \\ h \end{pmatrix}, \mathbf{v}_1 = \begin{pmatrix} -1 \\ -1 \\ h \end{pmatrix}, \mathbf{v}_2 = \begin{pmatrix} -1 \\ 1 \\ h \end{pmatrix}, \mathbf{v}_3 = \begin{pmatrix} 1 \\ -1 \\ h \end{pmatrix}.$$

We notice that excluding this solution allows us to exclude the case including the inverses, namely  $S_+ = S_-$ .

From the unitarity conditions one has:

$$A_{\mathbf{v}_0} A_{\mathbf{v}_1}^\dagger A_{\mathbf{v}_0} = 0, \quad (170)$$

$$A_{\mathbf{v}_0} A_{-\mathbf{v}_i}^\dagger A_{\mathbf{v}_0} = 0, \quad i = 2, 3, \quad (171)$$

$$A_{\mathbf{v}_0} A_{-\mathbf{v}_1}^\dagger + A_{\mathbf{v}_1} A_{-\mathbf{v}_0}^\dagger + A_{\mathbf{v}_2} A_{-\mathbf{v}_3}^\dagger + A_{\mathbf{v}_3} A_{-\mathbf{v}_2}^\dagger = 0. \quad (172)$$

From (170) and the form of Eqs. (156),(157) for the transition matrices, we get  $U_1 = i\sigma_1$  (we use the equivalent notation for Pauli matrices:  $\sigma_0 := I, \sigma_1 := \sigma_X, \sigma_2 := \sigma_Y, \sigma_3 := \sigma_Z$ ), up to a change of basis; from (176) we end up with the two cases:

$$1. \quad A_{-\mathbf{v}_2}^\dagger A_{\mathbf{v}_0} = A_{-\mathbf{v}_3}^\dagger A_{\mathbf{v}_0} = 0,$$

$$2. \quad A_{-\mathbf{v}_2}^\dagger A_{\mathbf{v}_0} = A_{\mathbf{v}_0} A_{-\mathbf{v}_3}^\dagger = 0,$$

since  $A_{\mathbf{v}_0} A_{-\mathbf{v}_2}^\dagger = A_{\mathbf{v}_0} A_{-\mathbf{v}_3}^\dagger = 0$  is forbidden in order to respect the  $D_2$  algebra, while the case  $A_{-\mathbf{v}_3}^\dagger A_{\mathbf{v}_0} = A_{\mathbf{v}_0} A_{-\mathbf{v}_2}^\dagger = 0$  is accounted by the symmetry of the unitarity conditions under the exchange  $2 \leftrightarrow 3$ . In case 1, the condition is incompatible with a faithful representation of  $D_2$  in  $\text{SU}(2)$ . In case 2, we have  $U_G = i\sigma_G$  and  $U_2 = VDV^\dagger$  with  $D$  diagonal, implying  $U_2 = sV(i\sigma_3)V^\dagger$  ( $s$  a sign). Then, up to a global sign, one has

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} i & s \\ -s & -i \end{pmatrix},$$

and from (172) we obtain

$$A_{\mathbf{v}_0} A_{-\mathbf{v}_1}^\dagger A_{\mathbf{v}_0} + A_{\mathbf{v}_2} A_{-\mathbf{v}_3}^\dagger A_{\mathbf{v}_0} = 0,$$

which, using the form of Eqs. (156) and (157) for the transition matrices along with the previous results, leads to  $-2\alpha_+^2 \alpha_- = 0$ , contradicting the assumption  $\alpha_\pm \neq 0$ .

# B

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## DERIVATION OF THE SCALAR QWS

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### B.1 TWO SPACE-DIMENSIONS

We here derive the most general qws with  $s = 2$  on

$$G = \langle h_1, h_2 | h_1 h_2 h_1^{-1} h_2^{-1} \rangle.$$

Let us introduce the *polar decomposition* for the transition matrices:  $\forall A \in \text{GL}_n(\mathbb{C})$  there exists  $V$  unitary and  $P$  positive semidefinite such that  $A = VP$ .

$$\begin{aligned} A_{+i} A_{-i}^\dagger &= A_{-i}^\dagger A_{+i} = 0, \\ A_{+i} A_{\mp j}^\dagger + A_{\pm j} A_{-i}^\dagger &= 0, \\ A_{-i}^\dagger A_{\pm j} + A_{\mp j}^\dagger A_{+i} &= 0, \end{aligned} \tag{173}$$

for  $i, j \in \{h_1, h_2\}$  and  $i \neq j$ . The first one implies

$$A_{\pm i} = \alpha_{\pm i} V_i |\pm i\rangle \langle \pm i|,$$

where  $\{|-i\rangle, |+i\rangle\}$  are orthonormal basis and  $\alpha_{\pm i} > 0 \forall i$  and we posed  $V_{+i} = V_{-i} =: V_i$ , since it's easy to show that this is possible in view of the non-uniqueness of the polar decomposition in case of matrices which are not full-rank.

The second and third of Eqs. (173) imply

$$\begin{aligned} A_{+i}A_{\pm j}^{\dagger}A_{+i} &= A_{-i}A_{\pm j}^{\dagger}A_{-i} = 0 \\ \Rightarrow \langle +i | \mp j \rangle \langle \mp j | V_j^{\dagger} V_i | +i \rangle &= \langle -i | \pm j \rangle \langle \pm j | V_j^{\dagger} V_i | -i \rangle = 0. \end{aligned}$$

It's easy to see that at least one among  $\langle \mp j | V_j^{\dagger} V_i | +i \rangle$  and  $\langle \pm j | V_j^{\dagger} V_i | -i \rangle$  must be vanishing. The cases are just two:

1.  $\langle \pm j | V_j^{\dagger} V_i | \pm i \rangle = 0 \Rightarrow |\pm i\rangle = |\pm j\rangle := |0\rangle, |1\rangle;$
2.  $\langle \mp j | V_j^{\dagger} V_i | \pm i \rangle = 0 \Rightarrow |\pm i\rangle = |\mp j\rangle := |0\rangle, |1\rangle;$

(up to a phase factor which is not relevant in defining the transition matrices). Then  $V_j^{\dagger} V_i$  is anti-diagonal in the basis  $\{|0\rangle, |1\rangle\}$ , say  $V_1 =: W = V \begin{pmatrix} 0 & \mu \\ \nu & 0 \end{pmatrix}$ , where  $V := V_2$ . Using the second and third of Eqs. (173) and Eq. [normalization], one gets in both cases  $\mu = -\nu^*$ ,  $\alpha_{+1} = \alpha_{-1} =: \alpha$  and  $\alpha_{+2} = \alpha_{-2} = \sqrt{1 - \alpha^2}$ . Substituting and changing basis to set  $\nu = 1$ , one gets

$$\begin{aligned} A_{+1} &= \alpha V |1\rangle \langle 0|, \quad A_{-1} = -\alpha V |0\rangle \langle 1|, \\ A_{+2} &= \sqrt{1 - \alpha^2} V |0\rangle \langle 0|, \quad A_{-2} = \sqrt{1 - \alpha^2} V |1\rangle \langle 1|, \end{aligned} \tag{174}$$

for the case 1, while case 2 is recovered just swapping  $+2 \leftrightarrow -2$ . A posteriori, it is simple to see that including the identical transition  $e$  in the set of generators would not satisfy unitarity.

## B.2 THREE SPACE-DIMENSIONS

We here derive the most general qws with  $s = 2$  on

$$G = \langle h_1, h_2, h_3, h_4 | h_i h_j h_i^{-1} h_j^{-1}, h_1 h_2 h_3 h_4 \rangle$$

There are three kinds of different paths of length 2 giving rise to unitarity conditions:

- (a)  $\pm 2h_i$ , (b)  $\pm h_i \mp h_j$ , (c)  $\pm(h_i + h_j)$ ,

for  $h_i, h_j \in S_+$ . Similarly to the two-dimensional case, from condition (a) we obtain a general expression for the transition matrices:

$$A_{\pm i} = \alpha_{\pm i} V_i |\pm i\rangle \langle \pm i|, \quad (175)$$

with  $\{|-i\rangle, |+i\rangle\}$  orthonormal basis and  $\alpha_{\pm i} > 0 \forall i$ . On the other hand, condition (b) amounts to

$$\begin{aligned} A_{+i} A_{+j}^\dagger + A_{-j} A_{-i}^\dagger &= 0, \\ A_{+i}^\dagger A_{+j} + A_{-j}^\dagger A_{-i} &= 0. \end{aligned} \quad (176)$$

Exploiting the form of (175) and using (176) we get

$$A_{+i} A_{+j}^\dagger A_{+i} = 0 \quad \Rightarrow \quad A_{+i} A_{+j}^\dagger = 0 \quad \vee \quad A_{+j}^\dagger A_{+i} = 0, \quad (177)$$

therefore one of the two cases

$$\begin{aligned} 1. \quad A_{\pm i} &= \alpha_{\pm i} V_i |\pm i\rangle \langle \pm i|, & 2. \quad A_{\pm i}^\dagger &= \alpha_{\pm i} V_i^\dagger V_i |\pm i\rangle \langle \pm i| V_i^\dagger, \\ A_{\pm j} &= \alpha_{\pm j} V_j |\mp i\rangle \langle \mp i|. & A_{\pm j}^\dagger &= \alpha_{\pm j} V_j^\dagger V_i |\mp i\rangle \langle \mp i| V_i^\dagger. \end{aligned}$$

hold. In case 1  $A_{+j} A_{+i}^\dagger = A_{+i} A_{+j}^\dagger = 0$  implies  $A_{+j} A_{+i}^\dagger \neq 0$ , while in case 2  $A_{+i}^\dagger A_{+j} = A_{+j}^\dagger A_{+i} = 0$  implies  $A_{+j}^\dagger A_{+i} \neq 0$ : since there are four elements in  $S_+$ , it is easy to see that, for a fixed  $+i$ , conditions in (177) can be satisfied at most for two different values of  $+j$ . Being six the possible couples, either the first or the second condition must be satisfied for at least two couples with a fixed  $+i$ . Thus one has (modulo relabeling the  $h_m$ ) three set of conditions:

$$\begin{aligned} A_{+1} A_{+2}^\dagger &= A_{+1} A_{+3}^\dagger = A_{+2} A_{+4}^\dagger = 0, \\ A_{+2}^\dagger A_{+3} &= A_{+1}^\dagger A_{+4} = A_{+3}^\dagger A_{+4} = 0, \end{aligned} \quad (178)$$

or

$$\begin{aligned} A_{+1} A_{+2}^\dagger &= A_{+1} A_{+3}^\dagger = A_{+2} A_{+4}^\dagger = A_{+3} A_{+4}^\dagger = 0, \\ A_{+2}^\dagger A_{+3} &= A_{+1}^\dagger A_{+4} = 0, \end{aligned} \quad (179)$$

or the previous one modulo the exchange of  $A_{+i}$  and  $A_{+i}^\dagger$ , i.e. equivalently modulo PT symmetry  $A_{\mathbf{k}} \mapsto A_{\mathbf{k}}^\dagger$  (it is then sufficient to solve the first two sets of equations).

Imposing the common conditions in Eqs. (178) and (179) we obtain:

$$\begin{aligned} A_{+1} &= \alpha_{+1}V_1M, & A_{-1} &= \alpha_{-1}V_1(1-M), \\ A_{+2} &= \alpha_{+2}V_2(1-M), & A_{-2} &= \alpha_{-2}V_2M, \\ A_{+3} &= \alpha_{+3}V_3(1-M), & A_{-3} &= \alpha_{-3}V_3M, \\ A_{+4} &= \alpha_{+4}V_4M, & A_{-4} &= \alpha_{-4}V_4(1-M), \end{aligned}$$

(where  $M := |0\rangle\langle 0|$ ,  $1-M := |1\rangle\langle 1|$  are arbitrary one-dimensional projectors)  $V_1^\dagger V_4$ ,  $V_2^\dagger V_3$  having vanishing diagonal elements. This form of the solutions is equivalent to (179).

Imposing (176) we find

$$\begin{aligned} \alpha_{+1}\alpha_{+4}V_1MV_4^\dagger + \alpha_{-1}\alpha_{-4}V_4(1-M)V_1^\dagger &= 0, \\ \alpha_{+2}\alpha_{+3}V_2(1-M)V_3^\dagger + \alpha_{-2}\alpha_{-3}V_3MV_2^\dagger &= 0, \end{aligned}$$

implying that

$$\begin{aligned} \alpha_{+1}\alpha_{+4} &= \alpha_{-1}\alpha_{-4}, \\ \alpha_{+2}\alpha_{+3} &= \alpha_{-2}\alpha_{-3}, \\ V_1^\dagger V_4, V_2^\dagger V_3 &\in \text{SU}(2). \end{aligned} \tag{180}$$

Also, we have

$$\begin{aligned} \alpha_{+1}\alpha_{+2}MV_1^\dagger V_2(1-M) + \alpha_{-1}\alpha_{-2}MV_2^\dagger V_1(1-M) &= 0, \\ \alpha_{+1}\alpha_{+3}MV_1^\dagger V_3(1-M) + \alpha_{-1}\alpha_{-3}MV_3^\dagger V_1(1-M) &= 0, \\ \alpha_{+2}\alpha_{+4}(1-M)V_2^\dagger V_4M + \alpha_{-2}\alpha_{-4}(1-M)V_4^\dagger V_2M &= 0, \\ \alpha_{+3}\alpha_{+4}(1-M)V_3^\dagger V_4M + \alpha_{-3}\alpha_{-4}(1-M)V_4^\dagger V_3M &= 0, \end{aligned} \tag{181}$$

implying  $(V_i^\dagger V_j)_{01} = -(V_i^\dagger V_j)_{10}^*$  for the couples  $(i, j) = (1, 2), (1, 3), (2, 4), (3, 4)$ . Then we can pose

$$V_i^\dagger V_j := \begin{pmatrix} \rho_{ij}e^{i\theta_{ij}} & \sqrt{1-\rho_{ij}^2}e^{i\varphi_{ij}} \\ -\sqrt{1-\rho_{ij}^2}e^{-i\varphi_{ij}} & \rho_{ij}e^{-i\theta'_{ij}} \end{pmatrix}, \quad \rho_{14} = \rho_{23} = 0. \tag{182}$$

Notice that, from (181),

$$\rho_{ij} \neq 1 \quad \Rightarrow \quad \theta_{ij} = \theta'_{ij}, \quad \alpha_{+i}\alpha_{+j} = \alpha_{-i}\alpha_{-j}, \quad \forall (h_i, h_j) \in S_+ \times S_+ \quad (183)$$

also holds. Using the equality  $V_i^\dagger V_l = V_i^\dagger V_j V_j^\dagger V_l$ , it is easy to show that

$$\rho_{12} = \sqrt{1 - \rho_{13}^2} = \sqrt{1 - \rho_{24}^2} = \rho_{34} \quad (184)$$

holds and, recalling Eqs. (180) and (183) and taking determinants, one also realizes that

$$V_i^\dagger V_j \in \mathbf{SU}(2) \quad \forall (i, j) \in S_+ \times S_+; \quad (185)$$

in particular, this holds  $\forall \rho_{ij} \in [0, 1]$  and one has  $\theta_{ij} = \theta'_{ij}$  in Eq. (185).

Accordingly, the only three possible cases are

$$(i) \quad \rho_{12} \neq 0, 1; \quad (ii) \quad \rho_{12} = 1; \quad (iii) \quad \rho_{12} = 0.$$

From paths of the form (c) these conditions follow:

$$\begin{aligned} \alpha_{+1}\alpha_{-2}V_1MV_2^\dagger + \alpha_{-1}\alpha_{+2}V_2(1-M)V_1^\dagger + \\ + \alpha_{-3}\alpha_{+4}V_3MV_4^\dagger + \alpha_{+3}\alpha_{-4}V_4(1-M)V_3^\dagger = 0, \end{aligned} \quad (186)$$

$$\begin{aligned} \alpha_{+1}\alpha_{-2}MV_1^\dagger V_2M + \alpha_{-1}\alpha_{+2}(1-M)V_2^\dagger V_1(1-M) + \\ + \alpha_{-3}\alpha_{+4}MV_3^\dagger V_4M + \alpha_{+3}\alpha_{-4}(1-M)V_4^\dagger V_3(1-M) = 0, \end{aligned} \quad (187)$$

$$\begin{aligned} \alpha_{-1}\alpha_{+3}V_3(1-M)V_1^\dagger + \alpha_{+1}\alpha_{-3}V_1MV_3^\dagger + \\ + \alpha_{+2}\alpha_{-4}V_4(1-M)V_2^\dagger + \alpha_{-2}\alpha_{+4}V_2MV_4^\dagger = 0, \end{aligned} \quad (188)$$

$$\begin{aligned} \alpha_{-1}\alpha_{+3}(1-M)V_3^\dagger V_1(1-M) + \alpha_{+1}\alpha_{-3}MV_1^\dagger V_3M + \\ + \alpha_{+2}\alpha_{-4}(1-M)V_4^\dagger V_2(1-M) + \alpha_{-2}\alpha_{+4}MV_2^\dagger V_4M = 0, \end{aligned} \quad (189)$$

$$\begin{aligned} & \alpha_{-1}\alpha_{+4}MV_4^\dagger V_1(1-M) + \alpha_{+1}\alpha_{-4}MV_1^\dagger V_4(1-M) + \\ & + \alpha_{+2}\alpha_{-3}MV_3^\dagger V_2(1-M) + \alpha_{-2}\alpha_{+3}MV_2^\dagger V_3(1-M) = 0. \end{aligned} \quad (190)$$

We shall use these equations in order to show that cases (ii) and (iii) lead to nontrivial solutions connected via a swap  $2 \leftrightarrow 3$ , while case (i) cannot satisfy unitarity.

**Case (i).** Recalling that in this case  $\rho_{ij} \neq 1 \forall (i, j)$ , then from Eqs. (180), (183) it's easy to derive that  $\alpha_{+i} = \alpha_{-i} =: \alpha_i \forall h_i \in S_+$ . We can use this condition in Eq. (187), along with  $\rho_{12} = \rho_{34}$ , obtaining  $\alpha_1\alpha_2 = \alpha_3\alpha_4$ . Similarly, since  $\rho_{13} = \rho_{24}$ , from Eq. (189) also  $\alpha_1\alpha_3 = \alpha_2\alpha_4$  follows. One thus straightforwardly has:  $\alpha_1 = \alpha_4$  and  $\alpha_2 = \alpha_3$ . Then again from Eqs. (187) and (189) it follows that  $e^{i\theta_{12}} = -e^{i\theta_{34}}$ ,  $e^{i\theta_{13}} = -e^{i\theta_{24}}$ . Finally, multiplying Eq. (186) by  $V_1^\dagger$  to the left and by  $V_2$  to the right and using the two identities just found, the first matrix element reads

$$1 - (1 - \rho_{12}^2) - \rho_{13}^2 + e^{i(\theta_{14} - \theta_{23})} = 0 \quad \Rightarrow \quad 2\rho_{12}^2 - 1 = -e^{i(\theta_{14} - \theta_{23})},$$

meaning that either  $\rho_{12} = 1$  or  $\rho_{12} = 0$ , which is absurd.

**Case (ii).** Recalling Eq. (184), from Eq. (187) one obtains  $\alpha_{\pm 1}\alpha_{\mp 2} = \alpha_{\mp 3}\alpha_{\pm 4}$  and  $V_1^\dagger V_2 = -V_3^\dagger V_4$ , while from (186) one gets  $\alpha_{\pm 1}\alpha_{\mp 2} = \alpha_{\pm 3}\alpha_{\mp 4}$  and

$$V_1^\dagger V_4 = -V_2^\dagger V_3; \quad (191)$$

plugging the latter in Eq. (190) one gets  $\alpha_{+1}\alpha_{-4} + \alpha_{+2}\alpha_{-3} = \alpha_{-1}\alpha_{+4} + \alpha_{-2}\alpha_{+3}$ , which, using the conditions on the  $\alpha_i$  just found, reads

$$\frac{\alpha_{+1}\alpha_{-4}}{\alpha_{+1}\alpha_{-2}} + \frac{\alpha_{+2}\alpha_{-3}}{\alpha_{+4}\alpha_{-3}} = \frac{\alpha_{-1}\alpha_{+4}}{\alpha_{-1}\alpha_{+2}} + \frac{\alpha_{-2}\alpha_{+3}}{\alpha_{-4}\alpha_{+3}}$$

and finally

$$\frac{\alpha_{+4}\alpha_{-4} + \alpha_{+2}\alpha_{-2}}{\alpha_{-2}\alpha_{+4}} = \frac{\alpha_{+4}\alpha_{-4} + \alpha_{+2}\alpha_{-2}}{\alpha_{+2}\alpha_{-4}},$$

implying  $\alpha_{-2}\alpha_{+4} = \alpha_{+2}\alpha_{-4}$ . Combining this condition with those already found, we just end up with the two conditions:  $\alpha_{+i} = \alpha_{-i} =: \alpha_i$  and  $\alpha_1\alpha_2 = \alpha_3\alpha_4$ .



Posing now  $\theta := \theta_{21}, \varphi := \varphi_{31}, V := V_1$  and noticing that  $V^\dagger V_4 = -V_2^\dagger V_3 = -V_2^\dagger V V^\dagger V_3$  (where we used Eq. (191)), we finally find the transition matrices:

$$\begin{aligned}
 A_{+1} &= \alpha_1 V |0\rangle \langle 0|, & A_{-1} &= \alpha_1 V |1\rangle \langle 1|, \\
 A_{+2} &= \alpha_2 e^{i\theta} V |1\rangle \langle 1|, & A_{-2} &= \alpha_2 e^{-i\theta} V |0\rangle \langle 0|, \\
 A_{+3} &= -\alpha_3 e^{i\varphi} V |0\rangle \langle 1|, & A_{-3} &= \alpha_3 e^{-i\varphi} V |1\rangle \langle 0|, \\
 A_{+4} &= -\alpha_4 e^{-i(\theta+\varphi)} V |1\rangle \langle 0|, & A_{-4} &= \alpha_4 e^{i(\theta+\varphi)} V |0\rangle \langle 1|,
 \end{aligned} \tag{192}$$

along with the condition  $\alpha_1 \alpha_2 = \alpha_3 \alpha_4$  and being  $V$  an arbitrary unitary. With a change of basis, we can set the phase factor  $e^{i\varphi} = 1$ .

**Case (iii).** Similarly to the previous derivation, from Eq. (189) we get  $V_1^\dagger V_3 = -V_2^\dagger V_4$ , while from Eq. (186) we have  $V_1^\dagger V_4 = V_2^\dagger V_3$ . Then, from the form of  $V_1^\dagger V_3, V_1^\dagger V_4$  the identity  $V_1^\dagger V_2 = V_1^\dagger V_3 V_3^\dagger V_2 = V_1^\dagger V_3 V_4^\dagger V_1 = V_4^\dagger V_1 V_3^\dagger V_1$  holds. Moreover, using Eqs. (188), (189) and (190), one likewise can derive the conditions  $\alpha_{+i} = \alpha_{-i} =: \alpha_i$  and  $\alpha_1 \alpha_3 = \alpha_2 \alpha_4$ . At this point one easily realizes that this solution is connected to the previous one via a swap  $2 \leftrightarrow 3$ . Again, a posteriori, it is simple to see that including the identical transition  $e$  in the set of generators would not satisfy unitarity.



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## DERIVATION OF THE SPINORIAL QWS

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### C.1 DERIVATION OF THE MASSIVE VIRTUALLY ABELIAN QW

Here we derive the walk in Section 10.2 on the Cayley graph  $G = \langle a, b \mid a^4, b^4, (ab)^2 \rangle$ . Assuming the isotropy of the walk, we show how to solve the unitarity constraints Eqs. (142) and (143) obtained from the above Cayley graph. We take the polar decomposition<sup>1</sup> of the QW transition matrices  $A_g = V_g P_g$  ( $g \in S = \{a, b, a^{-1}, b^{-1}\}$ ) and considering that  $P_q = P_q^\dagger$ , the conditions in Eq. (142) become

$$V_{i\pm 1} P_{i\pm 1} P_{j\pm 1} V_{j\pm 1}^\dagger = 0, \quad (193)$$

$$P_{i\pm 1} V_{i\pm 1}^\dagger V_{j\pm 1} P_{j\pm 1} = 0. \quad (194)$$

Being the  $V$  matrices unitary, we need to have  $P_{i\pm 1} P_{j\pm 1} = 0$ , and being both  $P_i$  and  $P_j$  nonnull (all transition matrices are nonnull by definition) they must be both rank one. Moreover, from (193) one has

$$P_{i\pm 1} = \alpha_{i\pm 1} |+_i\rangle \langle +_i|, \quad P_{j\pm 1} = \alpha_{j\pm 1} |-_i\rangle \langle -_i|,$$

with  $\alpha_g > 0$  and  $\{|+_g\rangle, |-_g\rangle\}$  orthonormal bases for  $\mathbb{C}^2$ . From equation (194) we get  $\langle +_{i\pm 1} | V_{i\pm 1}^\dagger V_{j\pm 1} | -_{i\pm 1} \rangle = 0$  and, since  $V_{i\pm 1}^\dagger V_{j\pm 1}$  is unitary, it must be diagonal on the

<sup>1</sup> Every complex square matrix admits a so called *polar decomposition*, namely  $\forall M \in \mathcal{M}(2 \times 2, \mathbb{C}) \exists V \in \mathcal{M}(2 \times 2, \mathbb{C})$  unitary,  $P \in \mathcal{M}(2 \times 2, \mathbb{C})$  semi-positive definite :  $M = VP$ .

basis  $\{|+_{i\pm 1}\rangle, |-_{i\pm 1}\rangle\}$  (with entries corresponding to phases). The  $V_g$  are not uniquely determined by the polar decomposition, since the  $A_g$  are not full rank. In fact, if  $A_{i\pm 1} = V_{i\pm 1} P_{i\pm 1}$  holds for a  $V_{i\pm 1}$ , there exists an infinite class of unitary matrices  $V'_{i\pm 1}$  such that  $A_{i\pm 1} = V'_{i\pm 1} P_{i\pm 1}$ : all the unitary matrices

$$V'_{i\pm 1} = V_{i\pm 1} \left( |+_{i\pm 1}\rangle \langle +_{i\pm 1}| + e^{i\theta_{i\pm 1}} |-_{i\pm 1}\rangle \langle -_{i\pm 1}| \right) \quad (195)$$

give the same polar decomposition for  $A_{i\pm 1}$ . The same freedom holds for  $A_{j\pm 1}$ ,  $j \neq i$  and one can always fix it computing

$$\begin{aligned} V'_{i\pm 1}{}^\dagger V'_{j\pm 1} &= e^{i\theta_{j\pm 1}} \langle +_{i\pm 1}| V_{i\pm 1}{}^\dagger V_{j\pm 1} |+_{i\pm 1}\rangle |+_{i\pm 1}\rangle \langle +_{i\pm 1}| \\ &\quad + e^{-i\theta_{i\pm 1}} \langle -_{i\pm 1}| V_{i\pm 1}{}^\dagger V_{j\pm 1} |-_{i\pm 1}\rangle |-_{i\pm 1}\rangle \langle -_{i\pm 1}| \end{aligned}$$

and posing  $e^{i\theta_{j\pm 1}} \langle +_{i\pm 1}| V_{i\pm 1}{}^\dagger V_{j\pm 1} |+_{i\pm 1}\rangle = 1$  and  $e^{-i\theta_{i\pm 1}} \langle -_{i\pm 1}| V_{i\pm 1}{}^\dagger V_{j\pm 1} |-_{i\pm 1}\rangle = 1$ . Accordingly one has

$$V'_{i\pm 1}{}^\dagger V'_{j\pm 1} = I \implies V'_{j\pm 1} = V'_{i\pm 1} \quad (196)$$

that leads to the following structure for the transition matrices

$$A_a = \alpha_a V |+_a\rangle \langle +_a|, A_b = \alpha_b V |-_a\rangle \langle -_a|, \quad (197)$$

$$A_{a^{-1}} = \alpha_{a^{-1}} W |+_{a^{-1}}\rangle \langle +_{a^{-1}}|, \quad (198)$$

$$A_{b^{-1}} = \alpha_{b^{-1}} W |-_{a^{-1}}\rangle \langle -_{a^{-1}}|, \quad (199)$$

with  $\alpha_g > 0$  and  $\{|+_q\rangle, |-_q\rangle\}$  orthonormal bases for  $\mathbb{C}^2$ .

Combining (142) and (143) one obtains

$$A_{i^{-1}} A_i{}^\dagger A_{j^{-1}} = 0, \quad A_i A_{i^{-1}}{}^\dagger A_j = 0,$$

$$A_j A_{i^{-1}}{}^\dagger A_i = 0, \quad A_{j^{-1}} A_i{}^\dagger A_{i^{-1}} = 0.$$

and using the expression (197) for the  $A_g$  we get

$$\begin{aligned}
\langle +_a | +_{a-1} \rangle \langle -_{a-1} | W^\dagger V | +_a \rangle &= 0, \\
\langle -_a | -_{a-1} \rangle \langle +_{a-1} | W^\dagger V | -_a \rangle &= 0, \\
\langle +_a | -_{a-1} \rangle \langle +_{a-1} | W^\dagger V | +_a \rangle &= 0, \\
\langle -_a | +_{a-1} \rangle \langle -_{a-1} | W^\dagger V | -_a \rangle &= 0.
\end{aligned} \tag{200}$$

Considering that  $\langle +_a | -_{a-1} \rangle = 0 \Leftrightarrow | +_a \rangle = | +_{a-1} \rangle \Leftrightarrow \langle -_a | +_{a-1} \rangle = 0$  (up to phase factors that would not appear in the  $A_g$ ), condition (200) can be satisfied only in two cases

1.  $\langle +_{a-1} | W^\dagger V | -_a \rangle = \langle -_{a-1} | W^\dagger V | +_a \rangle = 0,$
2.  $\langle -_{a-1} | W^\dagger V | -_a \rangle = \langle +_{a-1} | W^\dagger V | +_a \rangle = 0.$

Let's note that just two of the matrix elements which appear in (??) can be zero: indeed, suppose by contradiction that this is not be the case, let's define  $U$  any of the possible matrices which connect the two orthonormal bases found; thus  $U^\dagger W^\dagger V$  would have at least three vanishing matrix elements, but this is absurd for it is unitary. Accordingly, the two cases are:

1. 
$$\begin{aligned}
A_a^I &= \alpha_a \mu W | + \rangle \langle + | & A_b^I &= \alpha_b \nu W | - \rangle \langle - | \\
A_{a-1}^I &= \alpha_{a-1} W | + \rangle \langle + | & A_{b-1}^I &= \alpha_{b-1} W | - \rangle \langle - |,
\end{aligned}$$
2. 
$$\begin{aligned}
A_a^{II} &= \alpha_a \mu W | + \rangle \langle + | & A_b^{II} &= \alpha_b \nu W | - \rangle \langle - | \\
A_{a-1}^{II} &= \alpha_{a-1} W | - \rangle \langle - | & A_{b-1}^{II} &= \alpha_{b-1} W | + \rangle \langle + |,
\end{aligned}$$

with  $\mu, \nu$  phase factors and each of them can be equal either to  $i$  or to  $-i$ . From the condition (48),  $W$  is found simply substituting the  $A_g$  and inverting the resulting relation, while from the normalization condition one can find the  $\alpha_g$ . The transition matrices for the case 1 are

$$\begin{aligned}
A_a^I &= \zeta^\pm \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, & A_b &= \zeta^\pm \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \\
A_{a-1}^I &= \zeta^\mp \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, & A_{b-1}^I &= \zeta^\mp \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.
\end{aligned}$$

where  $A_{a^{-1}}^I = (A_a^I)^\dagger$ ,  $A_{b^{-1}}^I = (A_b^I)^\dagger$ ,  $\zeta^\pm := \frac{1 \pm i}{2}$ , while the solutions 2 are the same up to the swap  $a^{-1} \leftrightarrow b^{-1}$ .

For  $G := \langle a, b \mid a^4, b^4, (ab)^2 \rangle$  the only transitive graph automorphism of  $S_+ = \{a, b\}$  is the swap  $a \leftrightarrow b$  of the generators. It is easy to verify that this automorphism is represented by the unitary matrix  $\sigma_x$ . Accordingly we see that by left multiplication of the transition matrices by a unitary matrix commuting with  $\sigma_x$ —whose general form is

$$Z_\pm = nI \pm im\sigma_x,$$

for  $n, m \geq 0$  and  $n^2 + m^2 = 1$ —both the unitarity conditions and the isotropy group of the qw are unchanged. This shows that whole class of isotropic qws on  $G$  is obtained by left multiplication of the above solutions by the matrix  $Z_\pm = nI \pm im\sigma_x$ .

### C.2 DERIVATION OF THE QW ON THE POINCARÉ DISK

We here derive the hyperbolic qws presented in Section 10.3. From Eqs. (146) choosing  $(i, j) = (a, b), (a^{-1}, b^{-1})$ , and recalling the results of the preceding Section, the transition matrices has the form

$$\begin{aligned} A_a &= \alpha V |0\rangle\langle 0|, & A_b &= \alpha V |1\rangle\langle 1|, \\ A_{a^{-1}} &= \beta W |0\rangle\langle 0|, & A_{b^{-1}} &= \beta W |1\rangle\langle 1|, \end{aligned}$$

where  $V$  and  $W$  are unitary matrices. By the normalization condition (30), one also has  $\beta = \sqrt{1 - \alpha^2}$ . Choosing then in Eqs. (146) the pair  $(i, j) = (b, a^{-1})$ , one obtains

$$[V^\dagger W, \sigma_z] = 0,$$

and then we can set

$$W = e^{i\theta} \begin{pmatrix} \mu & 0 \\ 0 & \mu^* \end{pmatrix}, \quad |\mu|^2 = 1.$$

Then, substituting into Eq. 147 one gets the conditions

$$e^{i\theta}\mu = s_1i, \quad e^{i\theta}\mu^* = s_2i \quad s_1 \text{ and } s_2 \text{ signs,}$$

which imply that  $\mu = s_3i$  with  $s_3$  a sign. Accordingly, relabelling the signs, the transition matrices read

$$\begin{aligned} A_a &= \alpha V |0\rangle\langle 0|, & A_b &= \alpha V |1\rangle\langle 1|, \\ A_{a^{-1}} &= s_1i\sqrt{1-\alpha^2}V |0\rangle\langle 0|, & A_{b^{-1}} &= s_2i\sqrt{1-\alpha^2}V |1\rangle\langle 1|. \end{aligned}$$

Imposing isotropy, namely imposing that there exists a unitary  $U \in \text{SU}(2)$  such that  $UA_{a^{\pm 1}}U^\dagger = A_{b^{\pm 1}}$ , one finds  $s := s_1 = s_2$ . Imposing condition (48) (recalling that we can always choose the global phase factor) amounts to set  $V = I_2$ . Now we can left-multiply the transition matrices by an arbitrary unitary  $X$  commuting with  $U$ . Since it must be  $U^2 = -I_2$ , that is to say

$$U = \begin{pmatrix} 0 & v \\ -v^* & 0 \end{pmatrix}, \quad |v|^2 = 1,$$

up to a change of basis we can always choose  $U = \sigma_x$ . Thus up to a change of basis one has  $X = nI_2 + im\sigma_x$ , with  $n, m$  positive such that  $n^2 + m^2 = 1$ . Finally, the transition matrices are given by

$$\begin{aligned} A_a &= \alpha X |0\rangle\langle 0|, & A_b &= \alpha X |1\rangle\langle 1|, \\ A_{a^{-1}} &= si\sqrt{1-\alpha^2}X |0\rangle\langle 0|, & A_{b^{-1}} &= si\sqrt{1-\alpha^2}X |1\rangle\langle 1|. \end{aligned}$$





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