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## Algebraic Walk Theory

P.-L Giscard

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UNIVERSITÉ DU LITTORAL  
CÔTE D'OPALE



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Présentée par

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# Algebraic Walk Theory

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# Foreword

## Acknowledgements

I am heavily indebted to my family, in particular to my wife, for the profound support I received from her throughout the years that we shared.

I am grateful to the people of the Laboratoire de Mathématiques Pures et Appliquées Joseph Liouville: firstly, they gave me food and shelter in the form of a permanent research position, ending years of wandering and anxiety. Secondly, they have proven to be marvellous colleagues, great Magic players and mathematical luminaries, making the LMPA into a remarkably enjoyable work environment on top of a place of constant mathematical learning.

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María Ronco deserves a special mention for her patience, humility and brilliance: *patience* because I first contacted her in 2016 about a research project which we still have not finished since every step along the way I need to learn something anew; *humility* because I was a postdoctoral researcher and she is a researcher of international stature who not only answered my unclear questions and even came to visit but she also consistently took the time and effort to come down to my level so the project would progress; *brilliance* because she regularly discovers fundamental objects and laws of algebra yet seems oblivious to the size of her achievements. María is uniquely fluent in mathematics and languages alike and a constant traveler: I hope to be part of her voyage in the years to come.

## On real authorship

Almost all of the results presented in this *Habilitation à Diriger des Recherches* are the fruits of extended collaborations. These results should by no means be attributed to myself alone and the present thesis should certainly not be taken to be a claim of this. The researchers who, by their work, contributed to 'walk theory' and are therefore effectively authors of this thesis are (in alphabetical order):

Franka Bause, Tolga Birkandan, Christian Bonhomme, Zheng Choo, Loïc Foissy, Mohammadali Foroozandeh, Jean Fromentin, Dieter Jaksch, Théo Karaboghossian, Nils Kriege, Kevin Lui, Cécile Mammez, Stefano Pozza, Paul Rochet, María Ronco, Manon Ryckebusch, Aditya Tamar, Simon James Thwaite, Richard C. Wilson.

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## Mode of presentation

Mathematicians probably prefer proofs to theorems. Proofs are often—though not always—either trivial or lengthy and technical. For this reason and given my goal of presenting an overarching view of a theory of walks, I have decided in all but a few cases to either briefly sketch or completely omit proofs while concentrating on results. The proofs are all available and published (hence accessible to the inquisitive reader) but the tentative vision of a coherent theory of walks offered by a mass of results concentrated in a single report can only be found here.



# Contents

## Introduction

<b>1</b>	<b>The two branches of walk theory</b>	<b>9</b>
1.1	NAP-co-preLie bialgebra on walks . . . . .	9
1.2	Hike monoids . . . . .	10

## Part 1: The fundamental bialgebraic structure on walks

<b>2</b>	<b>NAP-co-preLie bialgebra on graph walks</b>	<b>12</b>
2.1	Co-preLie co-algebra of walks . . . . .	13
2.2	Non-associative permutative algebra of walks . . . . .	15
2.3	NAP-co-preLie bialgebra . . . . .	16
2.4	Path-Sum theorem . . . . .	17
<b>3</b>	<b>Implications and applications to differential calculus</b>	<b>19</b>
3.1	The $\star$ -product . . . . .	20
3.2	Path-sum representation of the solution of systems of non-autonomous ODEs . . . . .	26
3.3	Tridiagonalization of differential systems: $\star$ -Lanczos algorithm . . . . .	29
<b>4</b>	<b>Further applications of the path-sum theorem</b>	<b>32</b>
4.1	Statistical inference . . . . .	32
4.2	Quantum dynamics . . . . .	33
4.3	Representation of Heun functions . . . . .	38

## Part 2: Extending number theory to walks on graphs

<b>5</b>	<b>Walk theory: combinatorics on hike monoids</b>	<b>42</b>
5.1	On the necessity of a theory of walks . . . . .	42
5.2	Hike monoids and number theory . . . . .	44
5.3	Algebraic relations between hikes series . . . . .	48
<b>6</b>	<b>Number-theoretic sieves on hikes</b>	<b>52</b>
6.1	Asymptotic enumeration of walks by their last erased loop . . . . .	52
6.2	Proof of the infinite sieve theorem . . . . .	55
6.3	Relation with the self-avoiding polygons counting problem . . . . .	60
<b>7</b>	<b>Exact enumeration formulas for simple cycles and simple paths</b>	<b>62</b>
7.1	Counting from weakly connected subgraphs . . . . .	62
7.2	Algorithmic analysis of the counting formulae . . . . .	64
7.3	Counting via convolutions over induced subgraphs . . . . .	67
7.4	An Hopf algebra structure for the hikes . . . . .	69
<b>8</b>	<b>On the <i>tenuous</i> relation between walks and their graphs</b>	<b>72</b>
8.1	Realizable cycle structures in digraphs . . . . .	72
8.2	Simple graphs do not relate well with their simple cycles . . . . .	76
8.3	Invariants of hike monoids . . . . .	77

<b>9 Further applications of hike monoids</b>	<b>80</b>
9.1 Cycle counting in social analysis and computer science . . . . .	80
9.2 Sieves on hikes as a cycle centrality measure . . . . .	82

## Conclusion

<b>10 And from there...</b>	<b>86</b>
10.1 Exotic umbral calculi for path-sum solutions to non-linear ODEs and PDEs . . . . .	86
10.2 Sieves on hikes . . . . .	88

<b>List of Symbols</b>	<b>90</b>
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<b>Bibliography</b>	<b>92</b>
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# Publications

This is a list of published material I authored or co-authored since completion of my DPhil in August 2014.

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# Chapter 1

## The two branches of walk theory

All the results presented here realize a coherent albeit incomplete body of work on a *theory of walks*, its necessity, applications and *implications*. Though they may seem disparate at first sight, they fall into two distinct but closely related branches, which differ only in the role played by the initial vertex of closed walks.

### 1.1 NAP-co-preLie bialgebra on walks

The first branch concerns a bialgebraic structure on graph walks and its consequences throughout mathematics. The structure arises from a simple procedure, now known as *Lawler's loop erasing* [123], first conceived in the context of percolation theory to randomly generate simple paths-walks where all vertices are distinct—from a sample of random walks [115, 121, 119, 116]. The procedure consists of a chronological removal of cycles (called loops in Lawler's original work) as one walks along on the graph: consider for instance the complete graph  $K_4$  on 4 vertices and label these vertices with integers 1 through 4. Walking along the path  $1 \rightarrow 2 \rightarrow 1 \rightarrow 3 \rightarrow 4 \rightarrow 3 \rightarrow 1 \rightarrow 3$  on the graph and removing cycles whenever they appear, we are left with the simple path  $1 \rightarrow 3$  after having successively 'erased' the cycles  $1 \rightarrow 2 \rightarrow 1$ , then  $3 \rightarrow 4 \rightarrow 3$  and finally  $1 \rightarrow 3 \rightarrow 1$ . Note how  $1 \rightarrow 3 \rightarrow 1$  does not appear contiguously in the original walk. Once terminated, Lawler's loop-erasing has eliminated a set of cycles, all of whose internal vertices are distinct, leaving a possibly trivial walk-skeleton behind. If the initial walk was itself a cycle, this skeleton is the empty walk on the initial vertex (also called length-0 walk) and otherwise it is a self-avoiding path. Remark that because the loop-removal occurs in a chronological fashion, Lawler's process is strongly non-Markovian: complete knowledge of all the past steps of a walk is required to decide the current and future erased sections at any point of the walk.

In Chapter 2 we show that Lawler's procedure, which formally sends a walk to a family of closed walks and at most one open path, correspond to a pre-Lie co-product. This dual of this co-structure is a non-associative permutative algebra based on a product called nesting, which consists of inserting walks into another one according to specific rules. Nesting induces a remarkable property which led to its discovery even before its relation to Lawler's process was uncovered: any walk admits a unique factorisation into nesting products of simple cycles and simple paths. These, it turns out, are exactly the primitive elements of the co-preLie structure and precisely those loops and walk skeleton produced by Lawler's loop-erasing.

The unique factorisation property sustains extremely powerful combinatorial results, allowing in particular for a sophisticated resummation of all walks between any two vertices of a graph into a single branched continued fraction of finite depth and breadth over the simple cycles and simple paths of the graph, known as path-sum. Path-sums, which were first devised from purely combinatorial arguments during my PhD thesis, have since found an astounding number of applications, in quantum mechanics, black hole theory, chemistry and in various fields of mathematics including probability theory, linear algebra, differential calculus and numerical analysis. Some of these are presented in Chapter 4. Surprisingly, this line of ideas has proven particularly fertile in its *implications* even more than through its applications. Indeed, in the case of differential equations, the very fact that a path-sum formulation of the solution of a problem *ought to exist* implied the existence of novel mathematical results. As an example, we shall cite in particular the  $\star$ -product on distributions, the tridiagonalization of systems of non-autonomous Ordinary Differential Equations (ODEs) and more; subjects which, at first sight, might seem very far from walks indeed. This area of research, the results of which are in Chapter 3, is now especially active notably in the pursuit of novel formal solutions to systems of non-autonomous, fractional, non-linear ODEs as well as Partial Differential Equations (PDEs).

## 1.2 Hike monoids

The second branch of research results from quotienting out the initial vertex (i.e. the root) of the walks in the bialgebraic structure mentioned above. This is a rather dramatic step as in Lawler's process, which is inherently chronological, the initial vertex is the start of history and the point from which all erasing decisions are taken. Dually, for nesting, the initial vertex of a closed walk determines the few places where a walk may be inserted into another. To properly describe the objects obtained from walks and sets of walks on removing the information about the starting point necessitates a return to a lower level presentation: words on the formal alphabet directed edges  $w_{i \rightarrow j} \in E$  of the graph  $G = (V, E)$ . Changing the starting point, we see that the backtrack  $w_{1 \rightarrow 2} w_{2 \rightarrow 1}$  must represent the same object as  $w_{2 \rightarrow 1} w_{1 \rightarrow 2}$ . Since exchanging  $w_{1 \rightarrow 2}$  and  $w_{2 \rightarrow 1}$  passes from one presentation to the other, this implies in general that two edges with different starting points must be allowed to commute in the word representations of the same object. Meanwhile, walks  $1 \rightarrow 2 \rightarrow 1 \rightarrow 3 \rightarrow 1$  and  $1 \rightarrow 3 \rightarrow 1 \rightarrow 2 \rightarrow 1$  remain distinct. So the words  $w_{1 \rightarrow 2} w_{2 \rightarrow 3} w_{3 \rightarrow 1}$  and  $w_{1 \rightarrow 3} w_{3 \rightarrow 2} w_{2 \rightarrow 1}$  represent distinct objects. This implies that edges with identical starting points—here  $w_{1 \rightarrow 2}$  and  $w_{1 \rightarrow 3}$ —must not be allowed to commute.

These two rules define the Cartier-Foata monoids. We shall see that a purely cycle-based vision also exists for these monoids and closed walks are now really heaps of cycles on the graph, the combinatorial properties of which are described by semi-commutative monoids called *hike monoids*. Algebraically and combinatorially these monoids obey a semi-commutative extension of number theory presented in Chapter 5. This approach is particularly well suited to enumeration purposes, in Chapter 7 we present novel formulas for counting the simple cycles and simple paths as well as the best general purpose algorithm for this task. This is because all the theoretical tools developed for number theory continue to exist in walk theory, where they share the same relations with one-another. We may therefore exploit these well-understood tools in the novel context of walks. In this framework, the semi-commutative extension of the Prime Number Theorem is a famous open problem, namely that of counting asymptotically the number of self-avoiding polygons of length  $\ell$  as  $\ell \rightarrow \infty$  on infinite regular lattices. Pursuing this idea, in Chapter 6 we use number theoretic sieves to obtain closed form finite, explicit results for enumerating walks per their last erased loops on infinite lattices.

The need for a dedicated mathematical field of study devoted to walks independently from graph theory is exemplified by results from this branch. In Chapter 8 we show that the hike monoidal structure of walks is essentially independent from the topology of the graphs that sustains them. In particular, deciding whether an arbitrary Cartier-Foata monoid is a hike monoid, i.e. if some arrangement of cycles on a graph exists at all, turns out to be extremely difficult.

Applications of the results of this branch beyond pure mathematics are presented in Chapter 9. Here we use the number-theoretic sieves to rate the importance of cycles in real-world networks. As these cycles represent feedback processes in the exchanges between the entities forming the complex system modeled by the network, ranking their importance might lead to uncovering properties of the system itself. For example we show how the sieves are sensitive enough to predict which plant proteins will be targeted by pathogens and which proteins participate in biological complexes.

# **Part 1: The fundamental bialgebraic structure on walks**

## Chapter 2

# NAP-co-preLie bialgebra on graph walks

We begin by showing that a co-preLie structure on graph walks arises naturally from Lawler's loop erasing. In addition, slightly relaxing the chronological constraints by allowing simultaneous erasures under some compatibility conditions leads to Hopf algebra structures on the tensor and symmetric algebras of graph walks.

In §2.2 we show that Lawler's process is also naturally associated with a non-associative permutative product, known as nesting [76], which satisfies the Livernet compatibility condition [125] with the co-preLie co-product defined here. This provides the very first concrete example of the NAP - co-preLie operad in a 'living' context. This construction appears to be of paramount importance given the pervasive use of graph-walks in mathematics and mathematical-physics. In particular this leads to a useful bridge between formal sums over infinite families of walks and branched continued fractions, the path-sum theorem §2.4.

### Notations and definitions

We consider a non-empty digraph  $G$  as defined throughout this work. The set of all walks on a graph  $G$  is denoted  $\mathcal{W}(G)$ .

Consider a walk  $\omega = w_0 \dots w_\ell$ . A *subwalk* of a walk  $\omega = w_0 \dots w_\ell$  is any walk  $w_k \dots w_{k'}$  where  $0 \leq k \leq k' \leq \ell$ . If  $k \neq k'$  and  $w_k = w_{k'}$ , we designate by  $\omega^{k,k'} := w_k w_{k+1} \dots w_{k'}$  the *closed subwalk* of  $\omega$  with root  $w_k$ . In a complementary way, we define the *remainder* section  $\omega_{k,k'} := w_0 \dots w_k w_{k'+1} \dots w_\ell$  to be what remains of  $\omega$  after removal of the section  $\omega^{k,k'}$ . Note, for convenience we denote  $\omega_{k,k'}^{l,l'}$  for  $(\omega_{k,k'})^{l,l'}$ , the section  $w_l \dots w_{l'}$  erased from the remainder  $\omega_{k,k'} = w_0 \dots w_k w_{k'+1} \dots w_\ell$ . This means in particular that in  $\omega_{k,k'}^{l,l'}$ , integers  $k, k', l$  and  $l'$  all refer to indices from  $\omega$ .

A rooted walk in which all vertices are distinct is said to be a *simple path* or *self-avoiding walk*. The set of all such walks on a digraph  $G$  is denoted  $\text{SAW}(G)$ . The set of all simple cycles on  $G$  is  $\text{SAP}(G)$ . For  $G$  any (directed multi)graph, to ease the notation, we also denote by  $\mathcal{W}(G)$  the  $K$ -vector space spanned by all walks,  $K$  being a field of characteristic 0. For a walk  $\omega \in \mathcal{W}(G)$ , we designate by  $V(\omega)$  the support of  $\omega$ , that is the set of *distinct* vertices visited by  $\omega$ ; and by  $E(\omega)$  the *multiset* of directed edges visited by  $\omega$ .

As stated above, Lawler's loop-erasing procedure consists in erasing all cycles from a walk  $\omega$  in the *chronological* order in which they appear. Formally, it is a selection-quotient process which transforms a walk into its self-avoiding skeleton. To construct the algebraic structures associated with Lawler's procedure we must not only consider its end product but also what it produces during its intermediary stages and what it removes from the walk, in its original context:

**Definition 2.0.1** (Loop-erased sections). Let  $G$  be a digraph and consider  $\omega = w_0 \dots w_\ell \in \mathcal{W}(G)$ . The set  $\text{LES}(\omega)$  of loop-erased sections is the set of all *closed subwalks* of  $\omega$  *erased* by Lawler's procedure.

**Example 2.0.1.** On the complete graph  $K_5$  on 5 vertices (including self-loops), consider the walk  $\omega = 12324522$ . The simple cycles erased by Lawler's procedure are  $\omega^{1,3} = 232$ ,  $\omega^{3,6} = 2452$  and  $\omega^{6,7} = 22$  and the set of erased closed subwalks of  $\omega$  is therefore,

$$\text{LES}(12324522) = \{\omega^{1,3}, \omega^{3,6}, \omega^{1,6}, \omega^{6,7}, \omega^{3,7}, \omega^{1,7}\} = \{232, 2452, 232452, 22, 24522, 2324522\}.$$

**Definition 2.0.2** (Loop-erased walks). Let  $G$  be a digraph and  $\omega = w_0 \dots w_\ell \in \mathcal{W}(G)$  of length  $\ell$ . For  $0 \leq k \leq \ell$ , we designate  $\text{LEW}_k(\omega)$ , called loop-erased walk  $\omega$  at step  $k$ , to be what is left of  $\omega$  after its first  $k$  steps while performing Lawler's procedure.

By the definitions of  $\text{LES}(\omega)$  and  $\text{LEW}(\omega)$  we obtain what was remarked above, namely that loop-erased sections may not straddle over one-another, a consequence of their step-by-step erasure in chronological order:

**Lemma 2.0.1.** *Let  $G$  be a digraph and  $\omega = w_0 \dots w_\ell \in \mathcal{W}(G)$ . Then  $\omega^{k,k'} \in \text{LES}(\omega)$  if and only if there does not exist a pair of integers  $0 \leq l < k < l' < k' \leq \ell$  with  $w_k = w_{k'} \neq w_l = w_{l'}$  and  $\omega^{l,l'} \in \text{LES}(\omega)$*

We remark that the notion of loop-erased walks allows for an alternative but equivalent definition of that of loop-erased section:

**Remark** (A recursive procedure for constructing  $\text{LES}(\omega)$ ). Let  $G$  be a digraph and consider  $\omega = w_0 \dots w_\ell \in \mathcal{W}(G)$ . The set  $\text{LES}(\omega)$  of loop-erased sections of  $\omega = w_0 \dots w_\ell$  is constructed recursively as follows. Initialise with  $\text{LES}(\omega) = \emptyset$ . Then for  $k \in \{1, \dots, \ell - 1\}$ , if  $w_{k+1} \in V(\text{LEW}_k(\omega))$  denote  $k'$ , the greatest integer such that  $0 \leq k' \leq k$  and  $w_{k'} = w_{k+1}$ . If  $k'$  exists, then:

1. add the closed walk  $\omega^{k',k+1} = w_{k'} \dots w_{k+1}$  to  $\text{LES}(\omega)$ ;
2. if there exists  $\omega^{k'',k'} \in \text{LES}(\omega)$ , add the closed walk  $\omega^{k'',k+1} = w_{k''} \dots w_{k+1}$  to  $\text{LES}(\omega)$  as well.

While equivalent to Definition 2.0.1, the above formulation is more formal in flavor and recursive in nature, thus better suited to algorithm designs and easier to wield in proofs.

## 2.1 Co-preLie co-algebra of walks

From a walk  $\omega$ , Lawler's process, once terminated, produces a set of erased simple cycles and one self-avoiding skeleton (possibly trivial). It is therefore natural to seek a co-product which to the walk  $\omega$  would associate a sum over erased sections  $\omega^{k,k'}$  and associated remainders  $\omega_{k,k'}$ , so that  $\omega$  could be obtained back from these through grafting of the former onto the latter. The 'grafting' product appropriate to that end, known as *nesting* is presented in §2.2 is permutative non-associative reflecting Lawler's process' chronological constraints. It is difficult to maintain any form of compatibility with nesting via such an indiscriminate procedure as cutting out all loop-erased sections however, as not all pairs  $(\omega^{k,k'}, \omega_{k,k'})$  can be consistently grafted back to form the original walk; and when grafting is possible, it may be so in more than one way. These problems arise from certain ladders and all corollas, respectively.

Consider first an instance of the former,  $\omega = 1233231$ , which is a ladder in the sense that the self-loop 33 is attached 'on top of' cycle 232, itself attached to the 'base' triangle 1231. Here  $\omega^{2,3} = 33$  is a valid loop-erased section of  $\omega$ , yet can be grafted back onto  $\omega_{2,3}$  in two distinct ways: one producing  $\omega$  and the other yielding the walk  $\omega' = 1232331$ . Remark how in  $\omega'$ , the self-loop 33 occurs one level below its original location in  $\omega$  since it is now attached directly to the 'base' triangle 1231. Algebraically such instances correspond to cases where the nesting product fails to be associative. Second, for the issue with corollas, i.e. bouquets of closed walks with the same root, consider e.g.  $\omega = 12131$ . Here both  $121, 131 \in \text{LES}(\omega)$ ; yet cutting e.g.  $\omega^{0,2} = 121$  and grafting it back onto  $\omega_{0,2} = 131$  either gives back the walk  $\omega = 12131$  or the completely different one  $\omega' = 13121$ . Algebraically, these instances translate into cases where the nesting product fails to be commutative.

### Admissible cuts

To resolve the difficulties mentioned above, which become extensive when taken together in arbitrary long walks, we must refine the set of loop-erased sections that can be cut out of the original walk by the co-product. Here, as earlier, the major hurdle is due to the chronological constraints inherent to Lawler's process. Because of this, special attention must be paid to erased sections that appear within longer erased sections, the latter providing the temporal context of the former:

**Definition 2.1.1** (Temporal context of an erased section). Let  $G$  be a digraph,  $\omega \in \mathcal{W}(G)$  and  $\omega^{k,k'} \in \text{LES}(\omega)$ . We denote  $\text{LES}(\omega)_{k,k'}^< \subset \text{LES}(\omega)$  the subset of loop-erased sections  $\omega^{l,l'}$  which *strictly* include  $\omega^{k,k'}$  as left subwalk, i.e.  $l \leq k < k' < l'$ . Because we require  $k' < l'$  strictly,  $\text{LES}(\omega)_{k,k'}^<$  may be empty. Otherwise, we denote  $\omega_{k,k'}^{\min}$  the smallest element of  $\text{LES}(\omega)_{k,k'}^<$  for inclusion.

By construction, if  $\omega_{k,k'}^{\min}$  exists, it is the tightest erased section which comprises  $\omega^{k,k'}$  entirely. It provides the relevant temporal context for  $\omega^{k,k'}$  since anything outside of  $\omega_{k,k'}^{\min}$  creates no further chronological constraints on  $\omega^{k,k'}$  beyond those on  $\omega_{k,k'}^{\min}$ . We can now control the loop-erased sections that a co-product may extract by admitting only those cuts which are corollas within their relevant temporal context and only if those cuts are contiguous subwalks including the last petals of the corolla:

**Definition 2.1.2** (Admissible cuts). Let  $G$  be a digraph and  $\omega = w_1 \dots w_\ell \in \mathcal{W}(G)$ . A non-empty loop-erased section  $\omega^{k,k'} := w_k w_{k+1} \dots w_{k'} \in \text{LES}(\omega)$  is an *admissible cut* of  $\omega$  when  $\omega^{k,k'} \neq \omega$  and either  $\omega^{l,l'} := \omega_{k,k'}^{\min}$  does not exist or  $w_k$  does not appear in  $w_{k'+1} \dots w_{l'}$ . The set of admissible cuts of  $\omega$  is denoted  $\text{AdC}(\omega)$ .

The condition that for  $\omega^{k,k'} \in \text{LES}(\omega)$ ,  $\omega^{l,l'} := \omega_{k,k'}^{\min}$  either does not exist or  $w_k$  does not appear in  $w_{k'+1} \cdots w_{l'}$  implies that admissible cuts can only be made right to left in the walk, that is from the latest to the earliest, in *reverse chronological order*. The notion of admissible cut is well defined because the property of being admissible does not depend on the order in which admissible cuts are considered and removed from the original walk. In particular, if a loop-erased section is an admissible cut of an admissible cut of a walk or of its remainder, then it is an admissible of that walk and vice-versa. This is significant because it indicates that, in spite of the strong chronological constraints created by Lawler's process, cutting out admissible cuts does not alter the other cuts relevant temporal context and thence, their admissibility:

**Proposition 2.1.1.** *Let  $G$  be a digraph and  $\omega \in \mathcal{W}(G)$ .*

**Case 1.** *If  $k < k' < l < l'$  or  $l < l' < k < k'$  then,*

$$\omega^{k,k'} \in \text{AdC}(\omega) \text{ and } \omega^{l,l'} \in \text{AdC}(\omega_{k,k'}) \iff \omega^{l,l'} \in \text{AdC}(\omega) \text{ and } \omega^{k,k'} \in \text{AdC}(\omega_{l,l'}).$$

**Case 2.** *If  $k < l < l' \leq k'$  then,*

$$\omega^{k,k'} \in \text{AdC}(\omega) \text{ and } \omega^{l,l'} \in \text{AdC}(\omega^{k,k'}) \iff \omega^{l,l'} \in \text{AdC}(\omega) \text{ and } \omega_{l,l'}^{k,k'} \in \text{AdC}(\omega_{l,l'}).$$

This Proposition is the central result on which all other proofs pertaining to the co-structure are built. The rather long proof of the Proposition, given in [57], works entirely by contradiction, treating every possible configuration of loops in a walk on a case-by-case basis. It is close in spirit to the original proof of the path-sum theorem [76], which relies on a case-by-case analysis of the configuration of loops in walks in conjunction with combinatorial arguments.

## Co-product definition

With the notion of admissible cut, we may now formally define the co-product associated to Lawler's process, by mapping a walk to a sum over all its admissible cuts tensored with their remainders:

**Definition 2.1.3** (Co-product). Let  $G$  be a digraph. The co-product associated to Lawler's process is the linear map  $\Delta_{\text{CP}}$  defined by,

$$\Delta_{\text{CP}} : \begin{cases} \mathcal{W}(G) & \rightarrow \mathcal{W}(G) \otimes \mathcal{W}(G) \\ \omega & \mapsto \Delta_{\text{CP}}(\omega) = \sum_{\omega^c \in \text{AdC}(\omega)} \omega_c \otimes \omega^c. \end{cases}$$

An essential property of this co-product is that a walk is primitive for it if and only if it is a simple path or a simple cycle. This is the ultimate algebraic explanation for the role these objects play in the path-sum theorem.

**Proposition 2.1.2.** *Let  $G$  be a digraph and  $\omega \in \mathcal{W}(G)$ . Then,  $\Delta_{\text{CP}}(\omega) = 0 \iff \omega \in \text{SAW}(G) \cup \text{SAP}(G)$ .*

## Co-preLie property

Having established the definition of the co-product associated to the Lawler process and identified its primitive walks, we now turn to the co-algebraic structure it gives to the walk vector space  $\mathcal{W}(G)$ . Recall that:

**Definition 2.1.4.** A co-preLie co-algebra is a couple  $(\mathcal{V}, \Delta)$  where  $\mathcal{V}$  is a vector space and  $\Delta : \mathcal{V} \rightarrow \mathcal{V} \otimes \mathcal{V}$  is a linear map such that for any  $v \in \mathcal{V}$  the following relation is satisfied

$$(\Delta \otimes \text{Id} - \text{Id} \otimes \Delta) \circ \Delta(v) = (\text{Id} \otimes \tau) \circ (\Delta \otimes \text{Id} - \text{Id} \otimes \Delta) \circ \Delta(v)$$

where  $\text{Id}$  is the identity map and  $\tau$  is the twisting linear map,  $\tau : \mathcal{V} \otimes \mathcal{V} \rightarrow \mathcal{V} \otimes \mathcal{V}$ ,  $\tau(u \otimes v) = v \otimes u$ .

**Theorem 2.1.1.** *The vector space  $\mathcal{W}(G)$ , equipped with the coproduct  $\Delta_{\text{CP}}$ , is a co-preLie (but not co-unital) co-algebra.*

There exists two proofs of this result. The first is a direct verification of the co-preLie property based on the properties of admissible cuts. The second proof obtains the theorem as a corollary of the Hopf structure on the tensor algebra generated by  $\mathcal{W}(G)$  via a brace coalgebra construction. Note that the Hopf structure on the tensor algebra is a corollary of the properties of admissible cuts, in particular Proposition 2.1.1.

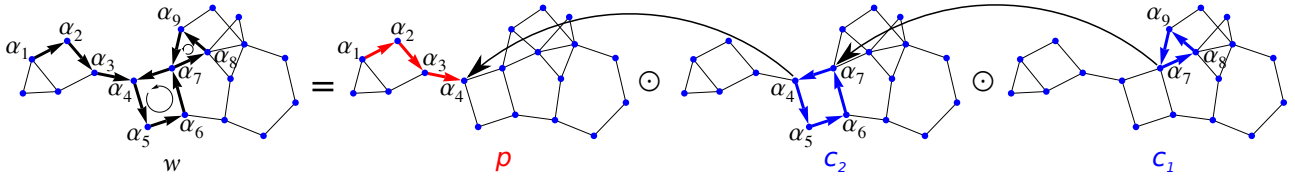


Figure 2.1: An example of nesting: the walk  $w = \alpha_1\alpha_2\alpha_3\alpha_4\alpha_5\alpha_6\alpha_7\alpha_8\alpha_9\alpha_7\alpha_4$  is obtained upon inserting the triangle  $c_1 = \alpha_7\alpha_8\alpha_9\alpha_7$  into the square  $c_2 = \alpha_4\alpha_5\alpha_6\alpha_7\alpha_4$  and then into the simple path  $p = \alpha_1\alpha_2\alpha_3\alpha_4$ , that is  $w = p \odot (c_2 \odot c_1)$ .

## Chronological structure of walks

Lemma 2.0.1 and Proposition 2.1.1 strongly suggest that any walk on any graph is chronologically equivalent to a tree where the root node is the self-avoiding skeleton of the walk and each non-root node stands for a simple cycle, see Theorem 2.1.2 below. In that tree, Lawler’s procedure erases nodes from the leaves down to the root and operates on the branches from left to right (or more precisely along the direction given to time). That is, time totally orders the walk’s tree structure.

**Definition 2.1.5** (Time-ordering of the admissible cuts). Let  $G$  be a digraph and  $\omega \in \mathcal{W}(G)$ . Assuming that  $\text{AdC}(\omega) \neq \emptyset$  we define the relation  $\leq_{\odot}$  on  $\text{AdC}(\omega)$  as follows:

$$\omega^{k,k'}, \omega^{l,l'} \in \text{AdC}(\omega) : \omega^{k,k'} \leq_{\odot} \omega^{l,l'} \iff l \leq k < k' \leq l' \text{ or } k < k' < l < l'.$$

That is,  $\omega^{k,k'} \leq_{\odot} \omega^{l,l'}$  if and only if either  $\omega^{k,k'}$  is erased prior to  $\omega^{l,l'}$  or, if both are erased simultaneously,  $\omega^{k,k'}$  began after  $\omega^{l,l'}$ .

With this definition, the set of admissible cuts of a walk is totally ordered chronologically. As a consequence, all walks are temporal trees in the following sense. For a walk  $\omega$  one can always construct an unique tree  $t(\omega)$  whose nodes and leaves represent simple cycles eliminated by Lawler’s process from  $\omega$ . Two nodes are linked in the tree if and only if the child node is a cycle that is found inside of the parent node in the walk. The theorem makes this intuitive presentation rigorous:

**Theorem 2.1.2.** *Let  $G$  be a digraph and  $\omega \in \mathcal{W}(G)$ . Then  $\omega$  has the temporal-structure of a tree  $t(\omega)$  whose nodes are totally ordered by  $\leq_{\odot}$  according to a reverse depth-first order.*

Although the tree  $t(\omega)$  to which a walk is mapped depends on the walk  $\omega$ , an universal tree can be constructed for all walks of a given digraph  $G$ . Considering only the trees  $t(\kappa)$  obtained from walks with no repeated sections produces a finite number of structurally distinct trees from all walks on  $G$ . These trees can be ordered partially by inclusion and the resulting poset always admits an unique maximum. This maximum tree is of paramount importance to  $G$ : it is one of the few invariants of its hike monoid (see Chapter 5 and §8.3) and dictates the shape of the branched continued fraction in the path-sum theorem §2.4.

## 2.2 Non-associative permutative algebra of walks

### Nesting product

Nesting was first introduced in [76] during my PhD thesis. The motivation for doing so was solely combinatorial: the definition aimed at ensuring the existence and uniqueness of the factorisation of walks into products of “cycle-irreducible” objects. The nesting product crafted in consequence *turns out* to be closely related to Lawler’s process in that the factors of a walk per nesting are exactly the admissible loop-erased sections of that walk. This is remarkable since nesting was devised independently from Lawler’s ideas, implying that existence and uniqueness of walk factorisations is necessarily tied with the chronological ordering of the edges of a walk. In this section we give an updated, streamlined definition of nesting. After detailing its relation with the co-preLie coproduct introduced earlier, we discuss results on the NAP-co-preLie bialgebraic structure on walks.

Let  $\omega = w_1w_2 \cdots w_n$  be a walk. By the loop-erasing procedure, we obtain that  $w$  can be seen as a self-avoiding skeleton on top of which are attached closed-walks (loops)  $\ell_1, \dots, \ell_n$ , i.e.

$$\omega = \omega_1\ell_1\omega_2\ell_2 \cdots \ell_n\omega_{n+1} \quad (2.2.1)$$

where  $\omega_j$  are (possibly trivial) self-avoiding vertex sequences. If  $\omega$  is open we denote  $\text{rad}(\omega) := \omega_1\omega_2 \cdots \omega_{n+1}$  its self-avoiding skeleton. If instead  $\omega$  is closed, we define  $\text{rad}(\omega) := \text{rad}(\omega')$  to be the self-avoiding skeleton of the open walk  $\omega' := w_1w_2 \cdots w_{n-1}$  obtained from  $\omega$  by removing its last vertex.



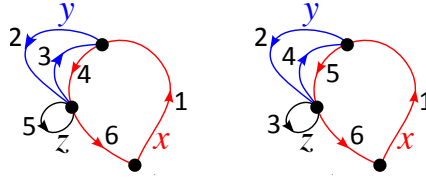


Figure 2.2: Illustration of the inherent non-associativity of walk construction from Lawler's erased loops reflected in nesting's lack of associativity. Left: walk  $\omega = (x \odot y) \odot z$ . Right: walk  $\omega = x \odot (y \odot z)$ .

The decomposition expounded in Eq. 2.2.1 holds recursively: we can decompose all  $\ell_i$  closed walks by seeing them as comprising closed walks on their radicals  $\text{rad}(\ell_i)$ . We can continue in this fashion until all closed walks invoked in the decomposition are simple cycles. The set of the simple cycles so obtained is unique, coincides with the loops erased in Lawler's procedure. Furthermore there is a unique way to build  $w$  back from these loops [76].

**Definition 2.2.1** (Nesting product). Consider  $(a, b) \in \mathcal{W}(G)^2$  with  $b$  a cycle with root  $\beta$ . Then the couple  $(a, b)$  is nestable if and only if  $\beta$  occurs in  $\text{rad}(a)$ , no closed walk is already attached to  $\beta$  in  $\text{rad}(a)$  and no vertex that is visited by  $\text{rad}(a)$  before  $\beta$  is also visited by  $b$ .

For a nestable couple  $(a, b)$ , the nesting product  $a \odot b$  is defined as the walk whose vertex sequence is formed by replacing the *last* appearance of  $\beta$  in  $a$  by the entire vertex sequence of  $b$ .

Nesting is neither commutative nor associative, however for  $x, y, z \in \mathcal{W}(G)$ , if  $(x, y)$  and  $(x, z)$  are both nestable couples then  $(a \odot b) \odot c = (a \odot c) \odot b$  since  $\text{rad}(a \odot b) = \text{rad}(a)$ . As a consequence:

**Proposition 2.2.1.** *The nesting product is a Non-Associative Permutative (NAP) product and  $(\mathcal{W}(G), \odot)$  is a NAP-algebra*

A compatibility relation between nesting and the co-preLie coproduct  $\Delta_{\text{CP}}$  exists as a corollary of the properties of admissible cuts. Indeed, take  $a, b \in \mathcal{W}(G)$ , if  $(a, b)$  is nestable then  $\{b\} \cup \text{AdC}(b) \subset \text{AdC}(a \odot b)$  and  $\text{AdC}(a \odot b) = \{a, b\} \cup \text{AdC}(a) \cup \text{AdC}(b)$  since by Proposition 2.1.1 no admissible cut of  $a \odot b$  may straddle over  $a$  and  $b$ . Thus:

**Corollary 2.2.1.** *Let  $G$  be a digraph,  $a, b \in \mathcal{W}(G)$ , then  $(\Delta_{\text{CP}}, \odot)$  share the Livernet compatibility condition,*

$$\Delta_{\text{CP}} \circ \odot = \text{Id}^{\otimes 2} + (\odot \otimes \text{Id}) \circ (\text{Id} \otimes \tau)(\Delta \otimes \text{Id}) + (\odot \otimes \text{Id}) \circ (\text{Id} \otimes \Delta)$$

that is, using Sweedler's notation,

$$\Delta_{\text{CP}}(a \odot b) = a \otimes b + a \odot b_{(1)} \otimes b_{(2)} + a_{(1)} \odot b \otimes a_{(2)}$$

and  $(\mathcal{W}(G), \odot, \Delta_{\text{CP}})$  forms a NAP-co-preLie bialgebra.

## 2.3 NAP-co-preLie bialgebra

Corollary 2.2.1 states that walks obey a NAP-co-preLie bialgebra structure. They are therefore merely an example of realization of this bialgebra, albeit a natural and eminently important one. A preLie-coNAP structure, dual of that of interest here was first studied by Livernet [125] yet much general algebraic and operadic results on the structure remain to be established. The example offered by walks is currently the main stimulus for such studies. Since the problem of identifying the simple cycles and simple paths on a graph is paramount to many applications, see e.g. Chapters 5–9 and given that these are the primitive elements of the co-algebra of walks, it is natural to seek the projection map onto these elements within the bialgebraic structure. The formula for this projection was discovered by Ronco, then proven independently by Ronco and Foissy.

Let  $(A, \bullet, \Delta)$  be a connected NAP-co-preLie bialgebra, that is  $(A, \mu)$  is a NAP algebra,  $(A, \Delta)$  a co-preLie co-algebra and  $\bullet, \Delta$  share the Livernet compatibility condition. For any  $n \in \mathbb{N}$  define the maps  $\Delta_n : A \rightarrow A^{\otimes(n+1)}$  recursively by setting  $\Delta_0 = \text{Id}_A$  and, for  $n \geq 1$ ,

$$\Delta_n := \sum_{i=1}^n \left( \text{Id}_A^{\otimes(i-1)} \otimes \Delta \otimes \text{Id}_A^{\otimes(n-i)} \right) \circ \Delta_{n-1}.$$

Dually define the maps  $\mu_n : A^{\otimes(n+1)} \rightarrow A$  by

$$\mu_n(a_0 \otimes a_1 \otimes \dots \otimes a_n) := (\dots((a_0 \bullet a_1) \bullet a_2) \dots) \bullet a_n.$$

**Definition 2.3.1.** Let  $E : A \rightarrow A$  be the linear map  $E := \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \mu_n \circ \Delta_n$ .

**Theorem 2.3.1** (Foissy, Ronco, unpublished). *Let  $(A, \bullet, \Delta)$  be connected NAP-co-preLie bialgebra. Let  $\text{Prim}(A)$  be the set of primitive elements of  $A$ . Then the linear map  $E$  is the Eulerian idempotent of  $A$ , in particular it satisfies that  $a \in \text{Prim}(A) \iff E(a) = a$  and for any  $a, b \in A$ ,  $E(a \bullet b) = 0$ .*

This theorem proven by direct combinatorial arguments notably implies the existence of explicit formulas for counting simple cycles on graph. Foissy offers an alternative form for  $E$  in terms of trees which, by Theorem 2.1.2, is also immediately interpretable in terms of walks. The Eulerian idempotent enters a formula for the identity map on  $A$ , which reconstructs all the elements of  $A$  out of its primitive elements. This formula can be partially resummed leading to the path-sum theorem. This line of proof for the path-sum theorem, purely algebraic, is the subject of ongoing work. Without it the only proof of the path-sum theorem is a combinatorial one based on the uniqueness of the factorisation of walks into nesting products of erased loops.

## 2.4 Path-Sum theorem

The main interest of the existence and uniqueness of the factorisation of walks into nestings of primitive elements of its co-algebraic structure is that it allows resummations of families of terms in series of walks. These turn the series into an expression that involves only the primitive elements of the bialgebraic structure, that is the simple cycles and simple paths of  $G$ . This is analogous to how the fundamental theorem of arithmetic leads to the existence of Euler products for the Riemann zeta function and other totally multiplicative functions on the integers. This observation is made rigorous in Part 2 of this work where the relation with number theory is fully elucidated.

Let  $\alpha$  and  $\omega$  be two vertices on  $G$ , let  $\mathcal{W}(G)_{\alpha\omega}$  be the set of all walks on  $G$  from  $\alpha$  to  $\omega$ ,  $\Pi(G)_{\alpha\omega}$  be the set of simple paths from  $\alpha$  to  $\omega$  and  $\Gamma(G)_\alpha$  the set of simple cycles from  $\alpha$  to itself. The formal series of all walks from  $\alpha$  to  $\omega$  on  $G$  is the formal sum over  $\mathcal{W}(G)_{\alpha\omega}$ ,

$$\Sigma_{G; \alpha\omega} := \sum_{w \in \mathcal{W}(G)_{\alpha\omega}} w.$$

In other words, the coefficient of  $w$  in  $\Sigma_{G; \alpha\omega}$ , denoted is 1 if  $w \in \mathcal{W}(G)_{\alpha\omega}$  and 0 otherwise.

By using the fact that every open walk can be factorised into a simple path and a collection of nested cycles, we rewrite  $\Sigma_{G; \alpha\omega}$  as a series over simple paths by modifying each path in the series to include all collections of cycles that can be nested off the vertices it visits. To preserve the vertex-edge notation of walks, we implement this modification by replacing each vertex  $\alpha$  in a simple path by a ‘dressed vertex’  $(\alpha)'_G$  defined to represent the characteristic series of all cycles that can be nested off  $\alpha$  on  $G$ :

$$(\alpha)'_G := \sum_{c \in \mathcal{W}(G)_{\alpha\alpha}} c = \Sigma_{G; \alpha\alpha}. \quad (2.4.1)$$

We rewrite this characteristic series as a series over simple cycles  $\gamma \in \Gamma(G)_\alpha$  by replacing each vertex  $\mu$  visited by a simple cycle  $\gamma$  by a dressed vertex representing the characteristic series of all the cycles that can be nested off  $\mu$  on the appropriate subgraph of  $G$ . Applying this procedure recursively yields a representation of the formal series  $\Sigma_{G; \alpha\omega}$  as a branched continued fraction of finite depth and breadth which only involves simple paths and simple cycles of  $G$ , the *path-sum*.

To present the path-sum theorem we need the vertex-edge notation for walks, where e.g. walk  $w = \alpha\beta\omega$  is written  $w = (\alpha)(\alpha\beta)(\beta)(\beta\omega)(\omega)$ . Then:

**Theorem 2.4.1** (Path-sum theorem). *The formal series over all walks from  $\alpha$  to  $\omega$  on  $G$  has the following expression,*

$$\Sigma_{G; \alpha\omega} = \sum_{\Pi(G)_{\alpha\omega}} (\alpha)'_G (\alpha\nu_1) (\nu_1)'_{G \setminus \{\alpha\}} \cdots (\nu_{\ell(p)-1}\omega) (\omega)'_{G \setminus \{\alpha, \nu_1, \dots, \nu_{\ell(p)-1}\}}, \quad (2.4.2a)$$

where  $p = (\alpha\nu_1 \cdots \nu_{\ell(p)-1}\omega)$  is a simple path of length  $\ell(p)$  from  $\alpha \equiv \nu_0$  to  $\omega \equiv \nu_{\ell(p)}$ , and  $(\alpha)'_G$  denotes the dressed vertex  $\alpha$  on  $G$ , defined as the formal series of all cycles off  $\alpha$  on  $G$  and given explicitly by

$$(\alpha)'_G = \left[ (\alpha) - \sum_{\gamma \in \Gamma(G)_\alpha} (\alpha)(\alpha\mu_1) (\mu_1)'_{G \setminus \{\alpha\}} (\mu_1\mu_2) \cdots (\mu_{\ell(\gamma)-1})'_{G \setminus \{\alpha, \mu_1, \dots, \mu_{\ell(\gamma)-1}\}} (\mu_{\ell(\gamma)-1}\alpha)(\alpha) \right]^{-1}, \quad (2.4.2b)$$

with  $\gamma = (\alpha\mu_1 \cdots \mu_{\ell(\gamma)-1}\alpha)$  a simple cycle of length  $\ell(\gamma)$  off  $\alpha$ .

The formal series  $\Sigma_{G; \alpha\omega}$  is expressed recursively in terms of formal series on subgraphs of  $G$ . We term these formal series the dressed vertices, and denote them by e.g.  $(\mu_j)'_{G \setminus \{\alpha, \mu_1, \dots, \mu_{j-1}\}}$ . These subseries are

in turn obtained through Eq. (2.4.2b), but on the subgraphs of  $G$  (e.g.  $G \setminus \{\alpha, \mu_1, \dots, \mu_{j-1}\}$  in the case of  $(\mu_j)'_{G \setminus \{\alpha, \mu_1, \dots, \mu_{j-1}\}}$ ). The recursion stops when vertex  $\mu_j$  has no neighbour on this subgraph. In this case the dressed vertex is given by

$$(\mu_j)'_{G \setminus \{\alpha, \mu_1, \dots, \mu_{j-1}\}} = \sum_{n \geq 0} (\mu_j \mu_j)^n = \begin{cases} [(\mu_j) - (\mu_j \mu_j)]^{-1} & \text{if the loop } (\mu_j \mu_j) \text{ exists,} \\ (\mu_j) & \text{otherwise,} \end{cases} \quad (2.4.3)$$

where  $(\mu_j)$  is the trivial walk off the vertex  $\mu_j$ . Note that this trivial walk is a local unit in the  $(\mathcal{W}(G), \odot)$  algebra. The recursive nature of Eq. (2.4.2b) implies that the result of the path-sum theorem for  $\Sigma_{G; \alpha\omega}$  yields a formal continued fraction involving only simple cycles and simple paths. On finite digraphs, the depth of this continued fraction is necessarily finite.

The path-sum theorem has proven to have an extremely wide range of applications, e.g. for expressing analytic matrix functions [181, 77, 63]. At first I thought this was owing to the ubiquity of graph walks throughout mathematics, physics, chemistry and, via network analysis, into computer science and biology. *The problem with this view is that it contrasts with the mathematically extremely limited scope of the theorem.* Indeed, recall that the fundamental result of algebraic graph theory is that powers of the ordinary adjacency matrix  $\mathbf{A}$  of a graph  $G$  counts the walks on that graph [19], for  $n \in \mathbb{N}$ ,  $(\mathbf{A}^n)_{i,j}$  is the number of walks of length  $n$  from vertex  $i$  to vertex  $j$  on  $G$ . This result generalises naturally to labelled adjacency matrix  $\mathbf{W}_{i,j} := w_{i,j} \mathbf{A}_{i,j}$  where  $w_{i,j}$  are formal labels (see also p. 44). Then it becomes readily apparent that, formally,

$$\Sigma_{G; \alpha\omega} = \text{Id} + \mathbf{W} + \mathbf{W}^2 + \dots = (\text{Id} - \mathbf{W})^{-1}.$$

In other terms, all the path-sum theorem does is express a resolvent. Alarmingly, resolvents are only to be found in linear problems since one verifies easily that if  $r = (1 - a)^{-1}$  then  $r$  solves the linear equation  $a.r = r - 1$ . Having paid attention to that, it becomes apparent that the theorem's sole reason for being useful is that resolvents appear far more often than could reasonably be expected. This in turn, I now see as a manifestation of the existence of exotic umbral calculi on finite and infinite dimensional vector spaces, see the discussion in §10.1.

## Chapter 3

# Implications and applications to differential calculus

The most promising field of applications of the path-sum theorem is that of differential equations. While re-investigating more closely the original [77] path-sum formulation of the ordinary matrix-exponential, it appeared that a path-sum expression for a more general object, the *time-ordered exponential* was possible. This object arises in coupled systems of linear ordinary differential equations with non-constant coefficients (also known as non-autonomous systems of ODEs),

$$\frac{d}{dt}\mathbf{U}(t) = \mathbf{A}(t)\mathbf{U}(t), \quad \mathbf{U}(0) = \text{Id},$$

where  $\mathbf{A}$  is a matrix of smooth functions of time and  $\mathbf{U}$ , known as the evolution operator, is the solution that is sought after. Under the assumption that  $\mathbf{A}$  commutes with itself at all times, i.e.  $\mathbf{A}(t')\mathbf{A}(t) - \mathbf{A}(t)\mathbf{A}(t') = \mathbf{0}$  for all  $t', t \in I$ , then  $\mathbf{U}$  is the ordinary matrix exponential of  $\mathbf{A}$ ,  $\mathbf{U}(t) = \exp\left(\int_0^t \mathbf{A}(\tau) d\tau\right)$ . In general, however, the evolution operator has no known explicit form in terms of  $\mathbf{A}$  and is rather expressed as

$$\mathbf{U}(t) = \mathfrak{T} \exp\left(\int_0^t \mathbf{A}(\tau) d\tau\right).$$

Here  $\mathfrak{T}$  represents the time-ordering (or path-ordering) operator defined as

$$\mathfrak{T}[\mathbf{A}(t')\mathbf{A}(t)] = \begin{cases} \mathbf{A}(t')\mathbf{A}(t), & \text{if } t' \geq t, \\ \mathbf{A}(t)\mathbf{A}(t'), & \text{otherwise.} \end{cases}$$

The action of this operator transforms the series representation of the ordinary matrix-exponential function into a matrix-valued Peano-Baker series (also known as Dyson series [47]) involving an infinite sum of nested integrals. This series is frankly unwieldy, hinders theoretical analyses of the solution, is computationally costly to evaluate and purely perturbative from a physical point of view.<sup>1</sup> Furthermore the time-ordered exponential cannot be evaluated via direct diagonalisation of  $\mathbf{A}$ . Only two analytical methods have been devised to evaluate the time-ordered exponential:<sup>2</sup>

- If the matrix  $\mathbf{A}$  is periodic, i.e. for all  $t \in I$  there exists  $T > 0$  with  $\mathbf{A}(t + T) = \mathbf{A}(t)$ , then 19th century Floquet theory dictates that the evolution operator takes on the form  $\mathbf{U}(t) = \mathbf{P}(t) \exp(\mathbf{F}t)$ . In this expression  $\mathbf{P}(t)$  a periodic time-dependent matrix and  $\mathbf{F}$  a constant matrix, both of which are determined in the Fourier domain from the solution to an *infinite-dimensional* but autonomous linear system of ODEs. This system can only be solved approximately by truncating it to a finite size either analytically [23], or otherwise via numerical procedures [86, 82]. Floquet formalism was first used by Shirley [185], who successfully applied it to study the quantum dynamics of a linearly polarised excitation in magnetic resonance. Shirley obtained low orders analytical approximations for the now celebrated Bloch-Siegert effect [24].

- The second analytical approach, discovered in 1954, is that of Magnus series [129]. It posits that the evolution operator can be expressed as an ordinary exponential  $\mathbf{U} = \exp \Omega(t)$  and gives an expression for  $\Omega(t)$  as

<sup>1</sup>That is, the terms of the series involve powers of a parameter that should be small to guarantee rapid enough convergence for an acceptable approximation to be reached by truncation of the series in applications.

<sup>2</sup>A plethora of numerical methods have been devised: (i) Fer and Magnus-Floquet hybrids [187, 133], (ii) Zassenhaus and Suzuki-Trotter propagator approximations [30, 45, 140]; (iii) Flow-equation approaches [197]; (iv) Average Hamiltonian Theory [199, 89]; and many more case-specific methods. The expansions presented above all suffer from various drawbacks including: the divergence of the representation at long times; the perturbative nature of the numerical or theoretical approach; the non-avoidable propagation of errors at long time; the failure to find exact solutions even in  $2 \times 2$  cases.

an increasingly intricate infinite series of nested commutators of  $\mathbf{A}$  with itself at different times. This series is so complicated to write explicitly that it is rarely calculated beyond its first two terms. Most importantly, Magnus expansion suffers from severe and incurable divergences as already mentioned by Magnus [129] and Fel'dman [53], now well studied [34, 136, 99, 176]. Ultimately, these result from the inherently faulty assumption that  $\Omega(t)$  even exists, see Example 3.2.1 page 27 for an explicit case where  $\mathbf{U}$  presents a negative real eigenvalue. While not restricted to periodic matrices it is well known that Magnus expansion suffers from a further two limitations for such matrices: the stroboscopic detection of events, and the impossibility to take into account more than one characteristic period. In spite of all this, Magnus series are very much in use nowadays in quantum physics [23], notably because they guarantee the unitarity of the approximated solutions even when the series diverges (!).

The observation, first made in 2015 [67] that the time-ordered exponential is amenable to a path-sum formulation is thus striking on two accounts:

- 1) It constitutes the only exact expression of the time-ordered exponential that involves a *finite* number of  $(\star)$ operations;
- 2) It both necessitates and implies the existence of a novel product, the  $\star$ -product, which induces a Fréchet-Lie group structure on distributions [175].

The existence of formal expressions for the solution of differential problems in  $\star$ -algebras opens the floodgates to classical linear algebra methods for solving problems in the differential context. This is exemplified by the  $\star$ -Lanczos algorithm reported here in §3.3 and consequent theorem regarding the tridiagonalization of systems of non-autonomous ODEs. *These results are among the unexpected implications of the path-sum theorem, yet by no mean corollaries of it.*

**Remark** (Fiber bundles and space-time graphs). Before we delve in the detailed treatment of non-autonomous ODEs, let us sketch the reason why there should even exist a path-sum formulation of time-ordered exponentials.

Consider a graph  $G$  whose edges are endowed with smooth time-dependent weight functions of  $\mathcal{C}^\infty[I]$ . This may be encoded by a time-dependent adjacency matrix  $\mathbf{A}(t)$ ,  $t \in I$ . At a given time  $t$ , some of these weights may be 0 so the graph  $G(t)$  so-obtained may be topologically different from another  $G(t')$  for  $t' \neq t$ . This view is rather inconvenient because one cannot decide whether a walk passing from a vertex  $i$  to a vertex  $j$  from time  $t$  to time  $t'$  exists at all, unless one knows the continuous family of graphs  $\{G(\tau)\}_{\tau \in [t, t']}$ . It is thus more convenient to encode this family into a single larger, semi-continuous graph-like object  $\mathfrak{G}$  so that time slicing  $\mathfrak{G}$  at time  $t$  recovers  $G(t)$  while space slicing  $\mathfrak{G}$  at edge  $w_{i \rightarrow j}$  yields the time-dependent weight function for this edge. Now we verify that if the edge set of  $\mathfrak{G}$  is just the trivial fiber-bundle  $E \times \mathcal{C}^\infty[I]^{|E|}$  then  $\mathbf{A}(t)$  commutes with itself at all times and the sum of all *space-time* walks on  $\mathfrak{G}$  is the ordinary matrix exponential of  $\mathbf{A}(t)$ .<sup>3</sup> If instead the edge set of  $\mathfrak{G}$  is a nontrivial fiber bundle, then  $\mathbf{A}$  fails to commute with itself at different times and the sum of all space-time walks on  $\mathfrak{G}$  is now a time-ordered exponential. As a sum of walks it must admit a path-sum representation as per the path-sum theorem. In this view the  $\star$ -product defined below appears naturally from the continuous extension of the matrix-product, continuously generating the walking process along the time dimension, just as the ordinary matrix product generates discrete walk steps along the space dimension.

### 3.1 The $\star$ -product

To present the path-sum formulation of the time-ordered exponential, we must first introduce the algebraic structure in which this formulation makes sense and the product on which it is based. While we introduced the  $\star$ -product in [67, 69], we here follow the more recent presentation by Ryckebusch2023 [175].

#### Definition

Let  $I$  be a compact subspace of  $\mathbb{R}$ . We write  $\mathcal{C}^\infty(I^2)$  for the set of smooth functions on an open neighborhood of  $I^2$  and  $\mathcal{C}^\infty(I)$  for the set of smooth functions on an open neighborhood of  $I$ . Let  $\mathcal{D}$  be the set of distributions  $d$  of the form

$$d(t', t) = \tilde{d}(t', t)\Theta(t' - t) + \sum_{i=0}^{+\infty} \tilde{d}_i(t', t)\delta^{(i)}(t' - t),$$

where  $\tilde{d}, \tilde{d}_i \in \mathcal{C}^\infty(I^2)$  are complex valued functions defined on  $I^2$ ,  $\Theta(\cdot)$  stands for the Heaviside theta function with the convention  $\Theta(0) = 1$  and  $\delta^{(i)}(t' - t)$  is the  $i$ th Dirac delta derivative in the sense of distributions evaluated in  $t' - t$ . Then we have:

<sup>3</sup>YES: the sum of all walks on a purely discrete graph is a resolvent  $\sum_n \mathbf{A}^n = (\mathbf{Id} - \mathbf{A})^{-1}$  but the sum of walks on a semi-continuous graph is a matrix exponential! This is seemingly little known.

**Theorem 3.1.1** (Ryckebusch2023 [175]). *The  $\star_I$ -product, defined by*

$$(f \star_I g)(x, y) := \int_I f(x, \tau)g(\tau, y)d\tau, \quad (3.1.1)$$

*is well defined on the weak closure  $\overline{\mathcal{C}^\infty(I^2)}$  of  $\mathcal{C}^\infty(I^2)$ , that is for any  $f, g \in \overline{\mathcal{C}^\infty(I^2)}$ ,  $f \star_I g$  exists and is in  $\overline{\mathcal{C}^\infty(I^2)}$ . Furthermore the  $\star_I$ -product is associative over  $\overline{\mathcal{C}^\infty(I^2)}$ ,  $\mathcal{D} \subset \overline{\mathcal{C}^\infty(I^2)}$  and for  $t', t, \in I^2$ ,  $1_\star := \delta(t' - t)$  is the unit of the  $\star_I$  product. The  $\star_{\mathbb{R}}$ -product is a well defined associative product on  $\mathcal{D}$ , that is for any  $d, e \in \mathcal{D}$ ,*

$$(d \star_{\mathbb{R}} e)(t', t) := \int_{-\infty}^{\infty} d(t', \tau)e(\tau, t)d\tau,$$

*is a distribution of  $\mathcal{D}$ .*

From now-on the  $\star_{\mathbb{R}}$  product will be generically designated as ‘the  $\star$ -product’. The above theorem is non-trivial and follows from a lengthy and careful sequential approach to distributions in the spirit of Mikusiski’s pioneering work [143]. From now on, we omit the  $t' - t$  arguments of the Heaviside  $\Theta$  functions and Dirac deltas  $\delta^{(i)}$  to alleviate the equations.

**Remark.** The  $\star$ -product extends directly to time-dependent matrices  $\mathbf{A}, \mathbf{B} \in \mathcal{D}^{n \times n}$  in the natural way,

$$(\mathbf{A} \star \mathbf{B})_{i,j}(t', t) = \sum_{k=1}^n (\mathbf{B}_{i,k} \star \mathbf{A}_{k,j})(t', t) = \int_{-\infty}^{\infty} (\mathbf{A}(t', \tau)\mathbf{B}(\tau, t))_{i,j} d\tau.$$

## Properties

The  $\star$ -product is non-commutative, induces the convolution  $f \star g \equiv f * g$  whenever both  $f$  and  $g$  depend only on the difference between their variables; but also the Volterra compositions of first and second kind; the pointwise product on  $\mathcal{C}^\infty(I^2)$ ; the Schwartz bracket on  $\overline{\mathcal{C}^\infty(I)}$  and can be seen as ‘continuum version of the matrix product.

Basic  $\star$ -multiplicative identities on  $\mathcal{D}$  include  $\Theta \star \delta' = \delta$ , which indicates that  $\delta'^{\star-1} = \Theta$  and equivalently  $\Theta^{\star-1} = \delta' = \delta^{(1)}$  since  $\delta \equiv 1_\star$  acts as the unit of the  $\star$ -product. In addition since, for  $n \in \mathbb{N} \setminus \{0\}$ ,  $\Theta^{\star n} = (t' - t)^{n-1}/(n-1)! \Theta$  then  $\Theta^{\star n} \propto \Theta$ , implying that all negative  $\star$ -powers of  $\delta'$  are included in  $\mathcal{D}$ . Conveniently, differentiation coincide with  $\star$ -powers of  $\delta'$ ,  $\delta^{(j)} = (\delta')^{\star j}$ . In view of our earlier remarks this in fact holds for  $j \in \mathbb{Z}$ , understanding that  $\delta^{(-|j|)} := (\delta')^{\star -|j|} = \Theta^{\star |j|}$ . This means that iterated integration also coincides with  $\star$ -powers. We may therefore summarily write, for all  $i, j \in \mathbb{Z}$ ,

$$\delta^{(i)} \star \delta^{(j)} = (\delta')^{\star i} \star (\delta')^{\star j} = \delta^{\star i+j} = \delta^{(i+j)}.$$

These results follow easily from the reduction of the  $\star$ -product to convolutions  $*$  but there are more general  $\star$ -multiplicative identities which cannot be obtained this way. Let  $\tilde{f} \in \mathcal{C}^\infty(I^2)$ , and denote  $\tilde{f}^{(k,\ell)}(\tau, \rho)$  the  $k$ th  $x$ -derivative and  $\ell$ th  $y$ -derivative of  $\tilde{f}$  evaluated at  $x = \tau, y = \rho$  with the conventions that  $k = 0$  or  $\ell = 0$  means no derivative is taken and  $k = -1$  or  $\ell = -1$  denotes integration. By associativity of the  $\star$ -product,  $(\delta^{(k)} \star \tilde{f}) \star \delta^{(\ell)} = \delta^{(k)} \star (\tilde{f} \star \delta^{(\ell)}) = \tilde{f}^{(k,\ell)}$  is well defined. We showed in [69] that, for any  $i, j \geq -1$ ,

$$\delta^{(j)} \star (\tilde{f}(t', t)\delta^{(i)}) = \tilde{f}^{(j,0)}(t', t)\delta^{(i)} + \sum_{k=1}^j \tilde{f}^{(j-k,0)}(t, t)\delta^{(i+k)}, \quad (3.1.2a)$$

$$(\tilde{f}(t', t)\delta^{(i)}) \star \delta^{(j)} = (-1)^j \tilde{f}^{(0,j)}(t', t)\delta^{(i)} + \sum_{k=1}^j (-1)^{j+k} \tilde{f}^{(0,j-k)}(t', t)\delta^{(i+k)}. \quad (3.1.2b)$$

Observe that the smooth function’s partial derivatives are evaluated in  $(t, t)$  and  $(t', t')$  in all but the first term.

**Remark.** The representation of  $\star$ -products between elements of  $\mathcal{D}$  can be deceptive. Consider for example  $\tilde{f} \in \mathcal{C}^\infty(I^2)$  such that all its derivative of order up to  $k$  are null whenever  $t' = t$ , i.e.  $\exists k \in \mathbb{N} : \forall j_1, j_2 \in \mathbb{N}, j_1 + j_2 \leq k, \tilde{f}^{(j_1, j_2)}(x, x) = 0$ . Then  $\tilde{f}(x, y)\delta^{(k)} \equiv 0_{\mathcal{D}}$  is null both as a linear functional  $\mathcal{C}^\infty(I^2) \rightarrow \mathbb{C}$  whose action is defined by the Schwarz bracket and as endomorphism of  $\overline{\mathcal{C}^\infty(I^2)}$ , something which is not readily apparent from the notation alone. To further illustrate the notational difficulties consider calculating  $(\tilde{f}(x, y)\delta') \star (\tilde{g}(x, y)\delta')$ . Relying on the  $\star$ -action of the leftmost  $\delta'$ , Eq. (3.1.2a) yields

$$(\tilde{f}(x, y)\delta') \star (\tilde{g}(x, y)\delta') = \tilde{f}^{(0,1)}(x, x)\tilde{g}(x, y)\delta' + \tilde{f}(x, x)\tilde{g}^{(1,0)}(x, y)\delta' + \tilde{f}(x, x)\tilde{g}(x, y)\delta^{(2)}. \quad (3.1.3)$$

But we could equally well calculate this relying on the  $\star$ -action of the rightmost  $\delta'$ . Then Eq. (3.1.2b) gives

$$(\tilde{f}(x, y)\delta') \star (\tilde{g}(x, y)\delta') = -\tilde{f}^{(0,1)}(x, y)\tilde{g}(y, y)\delta' - \tilde{f}(x, y)\tilde{g}^{(1,0)}(y, y)\delta' + \tilde{f}(x, y)\tilde{g}(y, y)\delta^{(2)}. \quad (3.1.4)$$

In spite of appearances the two results are equal: their action as linear functionals  $\mathcal{C}^\infty(I^2) \rightarrow \mathbb{C}$  are the same on any test function. This is because by [180, eqs. II,1; 57, p. 35] for any smooth function  $\tilde{h}$  and  $k \in \mathbb{N}$ ,

$$\tilde{h}(x)\delta^{(k)} = (-1)^k(\tilde{h}(y)\delta)^{(0,k)}, \quad \tilde{h}(y)\delta^{(k)} = (\tilde{h}(x)\delta)^{(k,0)},$$

so defining e.g.  $\tilde{h}(\tau) := \tilde{f}^{(0,1)}(x, \tau)\tilde{g}(\tau, y)$  and so on, one turns Eq. (3.1.4) into Eq. (3.1.3).

### On $\star$ -inverses

The calculation of  $\star$ -inverses of functions  $f(t', t)$  carries the gist of the difficulty inherent in obtaining explicit expressions for time-ordered exponentials. Contrary to  $\star$ -resolvents of elements of  $\text{Sm}_\Theta$  (see p. 24) which can be always represented by the Peano-Baker series; given an arbitrary smooth function  $\tilde{f}(t', t)$  and barring any further assumption, the  $\star$ -inverse of  $f(t', t) = \tilde{f}(t', t)\Theta(t' - t)$  cannot in general be given explicitly. In this section, we show that the  $\star$ -inverse  $f^{\star-1}$  exists and is accessible explicitly provided that  $\tilde{f}(t', t)$  is a separable function that is smooth in  $t, t'$  and not identically null. A function  $f(t', t)$  is separable if and only if there exist ordinary functions  $\tilde{a}_i$  and  $\tilde{b}_i$  with

$$\tilde{f}(t', t) = \sum_{i=1}^k \tilde{a}_i(t')\tilde{b}_i(t).$$

This result is of central importance because it implies two highly non-trivial results: i) that the  $\star$ -invertible elements of  $D$  are dense in  $D$ ; and ii) that the  $\star$ -Lanczos algorithm for the tridiagonalization of differential systems suffers from no further breakdowns than the classical non-Hermitian Lanczos algorithm.

We begin our results on  $\star$ -inverses with that of functions of a single time variable times a Heaviside function. These inverses are found by direct calculation of the solution of degree-one ordinary differential equations :

**Proposition 3.1.1.** *Let  $a(t', t) := \tilde{a}(t')\Theta(t' - t)$  and  $b(t', t) := \tilde{b}(t)\Theta(t' - t)$  so that  $\tilde{a}$  and  $\tilde{b}$  are differentiable, and not identically null over  $I$ . Then*

$$a^{\star-1}(t', t) = \frac{\partial}{\partial t'} \frac{\delta(t' - t)}{\tilde{a}(t')}, \quad b^{\star-1}(t', t) = -\frac{\partial}{\partial t} \frac{\delta(t' - t)}{\tilde{b}(t)}.$$

The method employed in the proof of the proposition above generalises to polynomials in at least one time variable, here taken to be  $t'$ . An analogous result can be given for functions that are polynomials in  $t$ .

**Proposition 3.1.2.** *Let  $p(t', t) = \tilde{p}(t', t)\Theta(t' - t)$  be so that  $\tilde{p}(t', t)$  is a polynomial of degree  $k \geq 1$  in  $t'$  and is smooth in  $t$ . If  $p(t, t)$  is not identically null over  $I$ , then*

$$p(t', t)^{\star-1} = x(t', t) \star \delta^{(k+1)}(t' - t),$$

where  $x(t', t) = \tilde{x}(t', t)\Theta(t' - t)$  is the solution of the linear homogeneous ordinary differential equation in  $t$   $\sum_{j=0}^k (-1)^j \tilde{p}^{(k-j,0)}(t, t)\tilde{x}^{(0,j)}(t', t) = 0$ , with the boundary conditions  $\tilde{x}^{(0,k-1)}(t', t') = (-1)^{k-1}\tilde{p}(t', t')^{-1}$ ,  $\tilde{x}^{(0,k-2)}(t', t') = 0, \dots, \tilde{x}(t', t') = 0$ .

**Remark.** The condition  $\tilde{p}(t, t) \neq 0$  for  $p^{\star-1}(t', t)$  to exist shortens the proof and facilitates the presentation of the results but can be relaxed. What is truly necessary is that  $p(t', t)$  itself must not be identically zero on  $I^2$ .

A technique similar to the one used in the proof of Proposition 3.1.2 can be applied to a more general class of functions. For instance, whenever differentiating leads to an expression like  $\delta^{(k)} \star f(t', t) = \tilde{h}(t)f(t', t) + g(t', t)$ , the expression can be rewritten as

$$(\delta^{(k)} - \tilde{h}(t)\delta) \star f(t', t) = g(t', t).$$

Then we can go on with a further combination of differentiations until there is no Heaviside function left on the right-hand side of the above equality. In particular, such a technique can be used when dealing with commonly encountered exponential or trigonometric functions.

The strategy used in the proof of Proposition 3.1.1 can be extended to give  $\star$ -inverses in the much more general case of functions which are separable and piecewise smooth in both time variables over the interval  $I$ . The proof is quite technical so it is omitted, see [68].

**Theorem 3.1.2.** *Consider a function  $f(t', t) := \tilde{f}(t', t)\Theta(t' - t)$  with  $\tilde{f}(t', t) \in \mathcal{C}^\infty[I^2]$  and so that  $\tilde{f}(t, t)$  is not identically null. Assume that there exists a distribution  $L(t', t) := \sum_{j=0}^{k+1} \tilde{g}_j(t')\delta^{(j)} \in \mathcal{D}$ , with  $\tilde{g}_j(t') \in \mathcal{C}^\infty[I]$  and  $\tilde{g}_{k+1} \neq 0$ , such that  $L \star \tilde{f} = 0$ . Then, if  $k > 0$ , the  $\star$ -inverse of  $f$  is*

$$f^{\star-1} = \tilde{r}_{-1}(t', t)\Theta + \sum_{m=0}^k \tilde{r}_m(t')\delta^{(m)},$$

with the separable smooth function  $\tilde{r}_{-1}(t', t) := \sum_{j=0}^{k+1} (-1)^j \tilde{y}_j^{(0,j)}(t', t)$ , and the smooth functions  $\tilde{r}_{m \geq 0}(t') := \sum_{j=m+1}^{k+1} (-1)^j \tilde{y}_j^{(0,j-1-m)}(t', t')$ , where  $\tilde{y}_j(t', t) := \tilde{x}(t', t) \tilde{g}_j(t)$  and  $\tilde{x}(t', t)$  is the solution of the linear homogeneous ordinary differential equation in  $t$ ,  $\sum_{m=0}^k \tilde{h}_m(t) \tilde{x}^{(0,m)}(t', t) = 0$ , with boundary conditions  $\tilde{x}^{(0,k-1)}(t', t) = -\tilde{h}_k(t')^{-1}$ ,  $\tilde{x}^{(0,k-2)}(t', t) = 0$ ,  $\dots$ ,  $\tilde{x}(t', t) = 0$ . In these expressions,  $\tilde{h}_m(t)$  are smooth functions given by

$$\tilde{h}_m(t) := \sum_{j=m+1}^{k+1} \sum_{\ell=m}^{j-1} \binom{\ell}{m} (-1)^\ell \tilde{f}^{(j-\ell-1,0)}(t, t) \tilde{g}_j^{(\ell-m)}(t).$$

If instead  $k = 0$ , the  $\star$ -inverse of  $f$  is trivially given by  $f^{\star-1}(t', t) = (\tilde{g}_1(t') \tilde{f}(t', t'))^{-1} L(t', t)$ .

Inverting the role of  $t'$  and  $t$ , a completely similar theorem is proven by changing all left  $\star$ -multiplications by  $\delta^{(j)}$  with right multiplications and vice-versa. In this situation,  $\tilde{x}$  satisfies a linear homogeneous ordinary differential equation in  $t'$ , and the boundary conditions involve the variable  $t$ .

**Remark.** The assumption  $f(t, t) = 0$  is not necessary. We can reformulate the theorem statement so that the condition is  $f$  not identically zero on  $I$ .

The most stringent condition imposed by Theorem 3.1.2 is the existence of the differential operator  $L$  with coefficients that depend only on  $t'$ . This condition can be made more transparent upon relating it to the class of separable functions. Let  $\tilde{y}_1(t'), \dots, \tilde{y}_{k+1}(t')$  be smooth functions of  $t'$ , and  $\tilde{a}_1(t), \dots, \tilde{a}_{k+1}(t)$  be functions of  $t$ . If  $\tilde{y}_1(t'), \dots, \tilde{y}_{k+1}(t')$  are linearly independent, equivalently, the related *Wronskian*  $W(\tilde{y}_1, \dots, \tilde{y}_{k+1})$  is not identically null, i.e.

$$W(\tilde{y}_1, \dots, \tilde{y}_{k+1}) := \begin{vmatrix} \tilde{y}_1 & \tilde{y}_2 & \dots & \tilde{y}_{k+1} \\ \tilde{y}'_1 & \tilde{y}'_2 & \dots & \tilde{y}'_{k+1} \\ \vdots & \vdots & & \vdots \\ \tilde{y}_1^{(k)} & \tilde{y}_2^{(k)} & \dots & \tilde{y}_{k+1}^{(k)} \end{vmatrix} \neq 0,$$

then there exist  $L$  as in Theorem 3.1.2 so that  $L \star \tilde{f} = 0$  for every separable function

$$\tilde{f}(t', t) = \tilde{a}_1(t) \tilde{y}_1(t') + \dots + \tilde{a}_{k+1}(t) \tilde{y}_{k+1}(t'). \quad (3.1.5)$$

Indeed, the conditions  $L \star \tilde{y}_j = 0$ , for  $j = 1, \dots, k+1$ , give the system

$$\begin{bmatrix} \tilde{y}_1 & \tilde{y}'_1 & \dots & \tilde{y}_1^{(k)} \\ \tilde{y}_2 & \tilde{y}'_2 & \dots & \tilde{y}_2^{(k)} \\ \vdots & \vdots & & \vdots \\ \tilde{y}_{k+1} & \tilde{y}'_{k+1} & \dots & \tilde{y}_{k+1}^{(k)} \end{bmatrix} \begin{bmatrix} \tilde{g}_0 \\ \tilde{g}_1 \\ \vdots \\ \tilde{g}_k \end{bmatrix} = -\tilde{g}_{k+1} \begin{bmatrix} \tilde{y}_1^{(k+1)} \\ \tilde{y}_2^{(k+1)} \\ \vdots \\ \tilde{y}_{k+1}^{(k+1)} \end{bmatrix},$$

whose solutions exist since the Wronskian is not identically null. In particular, at least one of the solutions has smooth coefficients. Theorem 3.1.2 thus yields the following corollary for separable functions:

**Corollary 3.1.1.** *Let  $f(t', t) := \tilde{f}(t', t) \Theta(t' - t)$  with  $\tilde{f}(t', t) \in C^\infty[I^2]$  so that  $\tilde{f}(t, t)$  is not identically null. Then  $f^{\star-1}$  exists and is given as in Theorem 3.1.2.*

Thanks to the previous results, we can also show that the set comprising all the separable distributions in  $\mathcal{D}$  is closed under  $\star$ -inversion. Here a distribution  $d = \sum_{i=-1}^N \tilde{a}_i(x, y) \delta^{(i)} \in \mathcal{D}$  is said to be separable if and only if all of its smooth coefficients  $\tilde{d}^{(i)}$  are separable. If  $N \in \mathbb{N} \cup \{+\infty\}$  is finite, we say that  $d$  is separable of order  $N$ .

**Corollary 3.1.2.** *Let  $d \in \mathcal{D}$  a separable distribution of order  $N$ . Then the  $\star$ -inverse of  $d$  exists and can be written as*

$$d^{\star-1}(t', t) = \Theta(t' - t)^{\star(N+1)} \star h^{\star-1}(t', t),$$

where  $h(t', t)$  is a separable, hence  $\star$ -invertible function. Furthermore,  $d^{\star-1}$  is a separable distribution.

Before we turn to the consequences of these results, let us present one example of  $\star$ -inverses since these are much less commonly encountered than the  $\star$ -resolvents.

**Example 3.1.1.** Let us determine the  $\star$ -inverse of  $f(t', t) = (t'^2 - t/t') \Theta(t' - t)$ . Since  $\tilde{f}(t', t)$  is separable, smooth in both variables, and  $\tilde{f}(t, t)$  is not identically null, Theorem 3.1.2 applies immediately. Setting  $L(t', t) := \tilde{g}_0(t') \delta + \tilde{g}_1(t') \delta' + \tilde{g}_2(t') \delta''$  with  $\tilde{g}_0(t') := 1$ ,  $\tilde{g}_1(t') := 0$  and  $\tilde{g}_2(t') := -t'^2/2$ , we have  $k = 1$  and  $L(t', t) \star \tilde{f}(t', t) = 0$ . This leads to

$$\tilde{h}_0(t) := 3t/2, \quad \tilde{h}_1(t) := (t^4 + t^2)/2,$$



which are the only non-identically null functions  $\tilde{h}_m$ . The function  $\tilde{x}$  is thus the solution of

$$3\tilde{x}(t', t) + t(1 + t^2)\tilde{x}^{(0,1)}(t', t) = 0, \quad \tilde{x}(t', t') \frac{t'^2}{2}(t'^2 + 1) = -1.$$

We find

$$\tilde{x}(t', t) = -\frac{2t'(t^2 + 1)^{3/2}}{(t'^2 + 1)^{5/2}t^3}.$$

We verify that

$$x \star L \star f = \tilde{h}_1(t)\tilde{x}(t', t')\delta = \frac{t^2(t^2 + 1)}{t'^2(t'^2 + 1)}\delta = \delta,$$

indicating that indeed

$$f^{\star-1} = x \star L = \left( \frac{2t'(t^2 + 1)^{3/2}}{(t'^2 + 1)^{5/2}t^3} \Theta \right) \star \left( \delta - \frac{t'^2}{2}\delta'' \right).$$

In conjunction with the Stone-Weierstrass theorem, study of the topology of  $\mathcal{D}$  as well as convergence arguments in  $\mathcal{D}$ , the result on  $\star$ -invertibility of separable distributions leads to:

**Theorem 3.1.3** (Ryckebusch2023 [175]). *The set  $\text{Inv}(\mathcal{D})$  of  $\star$ -invertible distributions of  $\mathcal{D}$  is a dense subset of  $\mathcal{D}$  that is made of automorphisms of  $\mathcal{C}^\infty(I^2)$ . Furthermore,  $(\text{Inv}(\mathcal{D}), \star)$  is a Fréchet Lie-group.*

### Properties of $\star$ -resolvents

As a case of special importance in applications is the subset  $\text{Sm}_\Theta \subset \mathcal{D}$  comprising those distributions of the form  $f(t', t) = \tilde{f}(t', t)\Theta(t' - t)$ ,  $\tilde{f} \in \mathcal{C}^\infty(I^2)$ . For  $f_1, f_2 \in \text{Sm}_\Theta$ , the  $\star$ -product between  $f_1, f_2$  simplifies to the Volterra composition of the second kind between  $\tilde{f}_1$  and  $\tilde{f}_2$ ,

$$(f_2 \star f_1)(t', t) = \int_{-\infty}^{\infty} \tilde{f}_2(t', \tau)\tilde{f}_1(\tau, t)\Theta(t' - \tau)\Theta(\tau - t) d\tau = \Theta(t' - t) \int_t^{t'} \tilde{f}_2(t', \tau)\tilde{f}_1(\tau, t) d\tau,$$

showing that  $(\text{Sm}_\Theta, \star)$  is a monoid. The primary role played by  $\text{Sm}_\Theta$  comes from  $\star$ -resolvents of elements of  $\text{Sm}_\Theta$ , which solve Volterra integral equations of the second kind.

Let  $f \in \text{Sm}_\Theta$ , the  $\star$ -resolvent of  $f$  is the distribution  $R_f := (1_\star - f)^{\star-1} \in \text{Sm}_\Theta \cup \{1_\star\}$ . The  $\star$ -resolvent of an element of  $\text{Sm}_\Theta$  is guaranteed to exist [84], as shown by the  $\star$ -Neumann series (also known as Peano-Baker series and Picard iteration)

$$(1_\star - f)^{\star-1} = \sum_{n=0}^{\infty} f^{\star n} = 1_\star + f + f \star f + f \star f \star f + \dots$$

Indeed, since  $\tilde{f} \in \mathcal{C}^\infty(I^2)$ ,  $\|\tilde{f}\|_{I^2}$  exists on any compact  $I^2$  of  $\mathbb{R}^2$ . Then  $\|f^{\star n}\| \leq \|\tilde{f}\|_\infty (t' - t)^n/n!$  and the  $\star$ -Neumann series converges. Let now  $\tilde{R}_f \Theta := R_f - 1_\star$ . Since  $f \star R_f = R_f - 1_\star$ , we find that  $\tilde{R}_f$  solves the inhomogenous linear Volterra integral equation of the second kind with kernel  $\tilde{f}$  [124, 88],

$$\tilde{f}(t', t) + \int_t^{t'} \tilde{f}(t', \tau)\tilde{R}_f(\tau, t) d\tau = \tilde{R}_f(t', t).$$

In general, such equations are usually solved indirectly through transformations mapping the equation into a system of non-autonomous ODEs [36, 84, 162]. The solutions of such systems are in fact themselves non-obvious since they involve time-ordered exponentials. To make matter worse this process is often circular in applications, as the ODEs are usually the equations meant to be solved! Restricting the problem to separable kernels, i.e. assuming  $\tilde{f}(t', t) = \sum_i^K \tilde{a}_i(t')\tilde{b}_i(t)$ , is unfortunately not sufficient. Indeed, the only available general result is for  $K = 1$ ,

**Proposition 3.1.3.** *Let  $\tilde{f}(t', t) = \tilde{a}(t')\tilde{b}(t) \in \mathcal{C}^\infty(I^2)$ . Then  $\tilde{R}_f = \tilde{a}(t')\tilde{b}(t)e^{\int_t^{t'} \tilde{a}(\tau)\tilde{b}(\tau) d\tau}$ .*

To the best of our knowledge, whenever  $K > 1$  there is no known closed-form expression for  $\star$ -resolvents with separable kernels, save in a few very special cases [162]. Examples where  $\tilde{R}_f$  is a higher transcendental function are known [203]. All that can be said in general is that if  $\tilde{f}$  is separable then  $\tilde{R}_f$  is separable as well [161]. Consequently, the best possible analytical approach is to provide a series representation of the solution with ‘good’ convergence and truncation properties. Taylor polynomial expansion have been proposed [182] but the  $\star$ -Neumann series gives a simpler starting point in this quest, as it is amenable to series acceleration [60]:

**Theorem 3.1.4** (Accelerated  $\star$ -Neumann series). *Let  $\tilde{f} := \sum_{i=1}^N \tilde{f}_i$  with  $\tilde{f}_i \in \mathcal{C}^\infty(I^2)$  and let  $\tilde{R}_i$  be the smooth part of the  $\star$ -resolvent of  $\tilde{f}_i$ . Then for any permutation  $\sigma \in S_N$ ,*

$$\tilde{R}_f = \sum_{n=0}^{\infty} T^{\star n} \star_{i=1}^N \tilde{R}_{\sigma(i)} - 1_\star = \star_{i=1}^N \tilde{R}_{\sigma(i)} + T \star \star_{i=1}^N \tilde{R}_{\sigma(i)} + T^{\star 2} \star \star_{i=1}^N \tilde{R}_{\sigma(i)} \dots$$

with

$$T := 1_\star - \star_{i=1}^d \tilde{R}_{\sigma(i)} \star (1_\star - \tilde{f})$$

This acceleration is particularly effective when one of the  $\tilde{f}_i$  dominates over the others or when  $T$  is very small for other reasons, see §4.2.

### On numerical computations of $\star$ -products

We turn to the question of evaluating  $\star$ -products and  $\star$ -resolvents numerically. Let  $I = ]a, b[$  be an interval of interest for computations and let  $\{t_i \in I\}_{0 \leq i \leq N-1}$  be the discrete values at which the numerical evaluations are to be made. For simplicity, suppose that the step  $\Delta t := |t_{i+1} - t_i|$  is the same for all  $0 \leq i \leq N-2$ . This assumption is not necessary but alleviates the notation. Now for  $f \in \text{Sm}_\Theta$ ,  $\tilde{f} \in \mathcal{C}^\infty(I^2)$ , define a matrix  $F$  with entries

$$F_{i,j} := f(t_i, t_j) = \tilde{f}(t_i, t_j) \Theta(t_i - t_j).$$

By construction  $F$  is lower *triangular* owing to the Heaviside step function. Now let  $f, l \in \text{Sm}_\Theta$  with  $F$  and  $L$  the corresponding matrices. Once  $I$  is discretised the  $\star$ -product—which is a Volterra composition of second kind on elements of  $\text{Sm}_\Theta$ —turns into an ordinary matrix product,

$$(f \star l)(t_i, t_j) = \int_{t_j}^{t_i} \tilde{f}(t_i, \tau) \tilde{l}(\tau, t_j) d\tau \Theta(t_i - t_j) \longrightarrow \sum_{t_j \leq t_k \leq t_i} \tilde{f}(t_i, t_k) \tilde{l}(t_k, t_j) \Delta t = (F.L)_{i,j} \Delta t,$$

since  $\lim_{\Delta t \rightarrow 0} (F.L)_{i,j} \Delta t = \int_{t_j}^{t_i} \tilde{f}(t_i, \tau) \tilde{l}(\tau, t_j) d\tau$ . This line of reasoning extends to  $\star$ -resolvents,

$$(1_\star - f)^{\star -1}(t_i, t_j) = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} (\text{Id} - \Delta t F)_{i,j}^{-1},$$

which in practice would mean taking  $\Delta t \ll 1$  and computing an ordinary matrix resolvent. We improve on the above by noting that these results correspond to using the rectangular rule of integration. Using the trapezoidal rule instead leads to more accurate results. To follow this rule, the usual matrix product  $F.L \Delta t$  representing  $f \star l$  must be replaced by

$$\frac{\Delta t}{2} (F - dF).L + \frac{\Delta t}{2} F.(L - dL),$$

where  $dF$  is the diagonal of  $F$ . Now the  $\star$ -resolvent of  $f$  becomes

$$(1_\star - f)^{\star -1}(t_i, t_j) \simeq R_f := \frac{1}{\Delta t} \left( \text{Id} - \Delta t F + \frac{\Delta t}{2} dF \right)_{i,j}^{-1}.$$

with an error scaling quadratically in  $O(\Delta t^2)$ . In applications the time-ordered exponential  $U$  is rarely necessary at all  $t', t \in I$ , rather only  $U(t, 0)$  is required. This means that only the first column of  $R_f$  is useful. This observation is profitably exploited numerically, as it avoids the need to even compute the matrix inverse in  $R_f$ , rather asking for the solution of the triangular system  $(\text{Id} - \Delta t F + \frac{\Delta t}{2} dF).\vec{x} = \vec{v}$ , where  $v = (1, 0, 0, \dots)^T$ , which is faster and requires less memory. From there further matrix multiplications can be implemented vectorially on  $\vec{x}$ .

Other, better, quadrature rules than the trapezoidal one can be implemented to improve the error scaling with  $\Delta t$ . Simpson's quadrature for example leads to an error scaling in  $O(\Delta t^3)$ . Taken together these results completely bypass the  $\star$ -Neumann series, which is not desirable numerically, rather evaluating directly what the series converges to. The entire complexity inherent in the calculation of  $\star$ -resolvent is reduced to multiplying and inverting triangular, well-conditioned matrices. For the latter assertion, consider the diagonal elements of  $\text{Id} - \Delta t F + (\Delta t/2)dF$ : these can be made as far from 0 as desired by tuning  $\Delta t$ .

While these ideas are intuitive and stem from the deeper view of the  $\star$ -product as a continuum matrix product, they are not the best way to proceed numerically. Instead it is better to express all functions to be manipulated in the basis of Legendre polynomials. In this basis, inherently discrete, a matrix representation for elements of  $\text{Sm}_\Theta$  also arises while the error scaling, stability and speed of the computations are profoundly improved. This now represents an extensive line of research conducted mainly by S. Pozza's group with ground-breaking performances. We refer the reader to [165, 164, 166, 167, 39, 25] and references therein.

### 3.2 Path-sum representation of the solution of systems of non-autonomous ODEs

In its most general form Theorem 2.4.1 stems from a fundamental algebraic property of the set of all walks on any graph. Consequently the representation of the formal series of all walks with fixed endpoints as a finite branched continued fraction is universal and continues to hold *mutatis mutandis* for series of weighted walks as well. It is therefore sufficient to show that the solution of a problem takes the form of a resolvent to imply the existence of path-sum formulation for it. This bypasses the space-time view sketched earlier but is equivalent to it [67].

In the case of non-autonomous systems of coupled linear ordinary differential equations this is a consequence of the  $\star$ -product formalism. Indeed consider the system

$$\frac{d}{dt}U(t) = \tilde{A}(t)U(t), \quad U(0) = \text{Id},$$

where  $\tilde{A}$  is a time-dependent matrix whose entries are smooth functions of time over some interval  $I$  of interest; and  $U$ , called the evolution operator, is the solution of the system. Now remark that the system above is equivalent to the two-variable system

$$\frac{d}{dt'}\{U(t')\}\Theta(t' - t) = A(t', t).U(t')\Theta(t' - t), \quad U(t, t) = \text{Id}.$$

where we introduced  $A(t', t) := \tilde{A}(t')\Theta(t' - t)$ . Now define the Green's function  $G := \delta' \star U\Theta = \frac{d}{dt'}\{U(t')\}\Theta(t' - t) + \text{Id}_\star$  with  $\text{Id}_\star := \text{Id} \star$ . Observe also that  $A.U\Theta = A \star G$ . Thus the Green's function obeys the equation

$$G - \text{Id}_\star = A \star G \Rightarrow G = (1_\star - A)^{\star-1}, \quad (3.2.1)$$

while  $U = \Theta \star G$ . This shows that the solution of non-autonomous systems of coupled linear ODEs stems from the  $\star$ -resolvent of  $A = \tilde{A}\Theta$ . This in turn entails the existence of a path-sum formulation for  $G$  and  $U$ .

#### Path-sum formulation of the time-ordered exponential

We consider  $\tilde{A}(t) \in \mathcal{C}^\infty[I]^{n \times n}$  a time-dependent matrix whose entries are smooth on an open neighborhood containing the compact  $I \subset \mathbb{R}$ . As earlier we denote  $A := \tilde{A}\Theta$ .

Let  $G = (V, E)$  be the graph with weighted adjacency matrix  $A$ , i.e. if there exists  $t \in I$  with  $A_{\beta\alpha}(t) \neq 0$ , then  $(\alpha, \beta) \in E$ . We designate  $G \setminus \{\alpha_1, \dots, \alpha_n\}$  the induced subgraph of  $G$  with vertex set  $V \setminus \{\alpha_1, \dots, \alpha_n\}$ . Recall that  $\Pi(G)_{\alpha\omega}$  and  $\Gamma(G)_\alpha$  are the set of simple paths from  $\alpha$  to  $\omega$  on  $G$  and the set of simple cycles from  $\alpha$  to itself on  $G$ , respectively. If  $G$  has finitely many vertices and edges, these two sets are finite.

**Theorem 3.2.1.** *The time-ordered exponential  $U$  of  $A(t)$  is given by*

$$U_{\omega\alpha} = \Theta \star \sum_{p \in \Pi(G)_{\alpha\omega}} G_{G \setminus \{\alpha, \nu_1, \dots, \nu_{\ell-1}\}; \omega} \star A_{\omega\nu_{\ell-1}} \star \dots \star A_{\nu_2\nu_1} \star G_{G \setminus \{\alpha\}; \nu_1} \star A_{\nu_1\alpha} \star G_{G; \alpha}, \quad (3.2.2a)$$

where  $p = (\alpha, \nu_1, \dots, \nu_{\ell-1}, \omega)$  is a simple path of length  $\ell$  from  $\alpha$  to  $\omega$  on  $G$  and  $G_{G; \alpha}$  is a Green's function given by

$$G_{G; \alpha} = \left[ \text{Id}_\star - \sum_{\gamma \in \Gamma(G)_\alpha} G_{G \setminus \{\alpha, \mu_1, \dots, \mu_{\ell'-2}\}; \mu_{\ell'-1}} \star \dots \star G_{G \setminus \{\alpha\}; \mu_1} \star H_{\mu_1\alpha} \right]^{\star-1}, \quad (3.2.2b)$$

with  $\gamma = (\alpha, \mu_1, \dots, \mu_{\ell'-1}, \alpha)$  is a simple cycle of length  $\ell'$  from  $\alpha$  to itself on  $G$ .

Note, in these expressions the time arguments  $(t', t)$  have been omitted for the sake of clarity.

**Remark.** As expected of a branched continued fraction, the Green's function  $G_{G; \alpha}$  is obtained recursively through Eq. (3.2.2b). Indeed,  $G_{G; \alpha}$  is expressed in terms of Green's functions such as  $G_{G \setminus \{\alpha, \mu_1, \dots, \mu_{\ell-2}\}; \mu_{j-1}}$ , which is in turn defined through Eq. (3.2.2b) but on the smaller subgraph  $G \setminus \{\alpha, \dots, \mu_{j-1}\}$  of  $G$ . The recursion stops when vertex  $\mu_j$  has no neighbour on this subgraph, in which case

$$G_{G \setminus \{\alpha, \mu_1, \dots, \mu_{\ell-2}\}; \mu_{j-1}} = \begin{cases} [\text{Id}_\star - A(t)_{\mu_j\mu_j}]^{\star-1} & \text{if } A(t)_{\mu_j\mu_j} \neq 0 \text{ for some } t \in I, \\ \text{Id}_\star & \text{otherwise,} \end{cases}$$

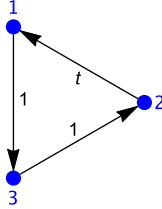
and  $\text{Id}_\star$  is the  $\star$ -algebra matrix identity of appropriate dimension.

**Example 3.2.1.** In this example, we consider the following system of differential equations on the interval  $I = [0, T]$ ,  $T > 0$ , for  $t \in I$

$$\tilde{A}(t)v(t) = \dot{v}(t), \quad \tilde{A}(t) = \begin{pmatrix} 0 & t & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad v(0) = v_0.$$

Matrix  $\tilde{A}(t)$  does not commute with itself at different times:  $[\tilde{A}(t'), \tilde{A}(t)] \neq 0$  for  $t' \neq t$ . Furthermore the Magnus series representation of the solution of this system is guaranteed to be convergent only for  $t < \sqrt{2\pi}$  [23] and indeed the path-sum solution reveals the appearance of a negative real eigenvalue in the time-ordered exponential of  $\tilde{A}$  at  $t \simeq 1.15\sqrt{2\pi}$ , implying the divergence of the Magnus series from that point on.

To present the path-sum formulation of the solution we first note that the graph corresponding to  $\tilde{A}$  is an *oriented* triangle, which we designate  $T$ :



Let us detail the calculation of entry  $U_{11}$  of the time-ordered exponential of  $\tilde{A}$ . There is a single simple cycle from vertex 1 to itself on  $T$ , namely  $1 \rightarrow 3 \rightarrow 2 \rightarrow 1$ . Furthermore  $T$  is acyclic as soon as a vertex is removed from it. Thus, following Theorem 3.2.1, the path-sum formulation for  $U_{11}$  is

$$U_{11} = \int_0^t G_{T;11}(\tau) d\tau, \quad G_{T;11}(\tau) = \left( 1_{\star} - \underbrace{\overbrace{t}^{\text{Edge } 1 \leftarrow 2} \star \overbrace{1}^{\text{Edge } 2 \leftarrow 3} \star \overbrace{1}^{\text{Edge } 3 \leftarrow 1}}}_{\text{Triangle}} \right)^{\star-1} (\tau, 0).$$

here we omitted writing the  $\Theta$  altogether to facilitate the identification of the edge weights but  $t$  above should be understood as  $t'\Theta(t'-t)$ , 1 and as  $1\Theta(t'-t)$ . The  $\star$ -resolvent of  $f(t', t) := (t \star 1 \star 1)(t', t) = (t-t)^2 t' / 2 \Theta(t'-t)$  is obtained from the  $\star$ -Neumann series  $\sum_n f^{\star n}$ , i.e. the Peano-Baker series for  $\hat{f}$ . This gives

$$G_{T;11}(t) = \delta(t) + \frac{1}{2} t^3 {}_0F_2 \left( ; \frac{5}{4}, \frac{3}{2}; \frac{t^4}{64} \right) \Rightarrow U_{11}(t) = \int_0^t G_{T;11}(\tau) d\tau = {}_0F_2 \left( ; \frac{1}{4}, \frac{1}{2}; \frac{t^4}{64} \right).$$

Similarly we get

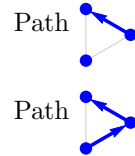
$$U_{22}(t) = {}_0F_2 \left( ; \frac{1}{2}, \frac{3}{4}; \frac{t^4}{64} \right), \quad U_{33}(t) = {}_0F_2 \left( ; \frac{1}{4}, \frac{3}{4}; \frac{t^4}{64} \right).$$

Note how these entries differ from  $U_{11}(t)$ , despite arising from circular permutations of the same triangle (cycles 1321, 2132 and 3213). This is because  $t$  and 1 do not  $\star$ -commute, that is  $t \star 1 \neq 1 \star t$ .

Since there is a single simple path between any two vertices of  $T$ , path-sum formulation for the off-diagonal elements is, for example,

$$U_{12}(t) = \left( \Theta \star \overbrace{t}^{\text{Edge } 2 \leftarrow 1} \star G_{T;22} \right)(t) = \int_0^t d\tau \int_0^\tau d\tau' \tau G_{T;22}(\tau'),$$

$$U_{13}(t) = \left( \Theta \star \overbrace{t}^{\text{Edge } 1 \leftarrow 2} \star \overbrace{1}^{\text{Edge } 2 \leftarrow 3} \star G_{T;22} \right)(t) = \int_0^t d\tau \int_0^\tau d\tau_1 \int_{\tau_1}^\tau d\tau_2 \tau G_{T;33}(\tau_1),$$



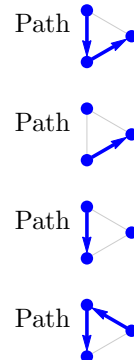
where again  $t \equiv t'\Theta(t'-t)$  etc. Similarly,

$$U_{21}(t) = \int_0^t d\tau \left( 1 \star 1 \star G_{T;11} \right)(\tau),$$

$$U_{23}(t) = \int_0^t d\tau \left( 1 \star G_{T;33} \right)(\tau),$$

$$U_{31}(t) = \int_0^t d\tau \left( 1 \star G_{T;11} \right)(\tau),$$

$$U_{32}(t) = \int_0^t d\tau \left( 1 \star t \star G_{T;22} \right)(\tau),$$



Calculating these (straightforward) integrals, the time-ordered exponential of  $\tilde{\mathbf{A}}$  is found to be

$$\mathbf{U}(t) = \begin{pmatrix} Q_{\frac{1}{4}, \frac{1}{2}}(t) & \frac{1}{2}t^2 Q_{\frac{3}{4}, \frac{3}{2}}(t) & \frac{1}{2}t^3 Q_{\frac{3}{4}, \frac{5}{4}}(t) - \frac{1}{6}t^3 Q_{\frac{1}{4}, \frac{7}{4}}(t) \\ t^2 Q_{\frac{1}{2}, \frac{5}{4}}(t) - \frac{1}{2}t^2 Q_{\frac{1}{4}, \frac{3}{2}}(t) & Q_{\frac{1}{2}, \frac{3}{4}}(t) & t Q_{\frac{3}{4}, \frac{5}{4}}(t) \\ t Q_{\frac{1}{2}, \frac{5}{4}}(t) & \frac{1}{2}t^3 Q_{\frac{3}{4}, \frac{3}{2}}(t) - \frac{1}{3}t^3 Q_{\frac{1}{2}, \frac{7}{4}}(t) & Q_{\frac{1}{4}, \frac{3}{4}}(t) \end{pmatrix},$$

where  $Q_{a,b}(t) := {}_0F_2(; a, b; t^4/64)$ . While the solution is closed form here, we emphasise that this very rarely the case as time-ordered exponentials typically produce hitherto undescribed transcendent functions. In the case of  $2 \times 2$  systems, Kovacic's algorithm allows for a rigorous a priori decision on the nature of the solution (transcendent versus non-transcendent) relying on Picard-Vessiot theory [110]. The question is non-trivial, profound difficulties must still be overcome before it can effectively be extended to larger systems.

**Example 3.2.2** (Time-dependent Dyson equation). Let  $\tilde{\mathbf{A}}(t) \in \mathcal{C}^\infty[I]^{n \times n}$ ,  $\mathbf{A} := \tilde{\mathbf{A}}(t')\Theta(t' - t)$  and consider a  $2 \times 2$  partition of  $\mathbf{A}$  into 4 blocks. Let  $\mathbf{A}_{\alpha\alpha}$  and  $\mathbf{A}_{\omega\omega}$  be the two diagonal blocks and  $G \equiv \mathcal{K}_2$  be the corresponding graph on vertices  $\alpha$  and  $\omega$ . This means that  $\mathbf{A}_{\alpha\alpha}$  and  $\mathbf{A}_{\omega\omega}$  are the time-dependent weights of the self-loops on vertices  $\alpha$  and  $\omega$ , respectively. Similarly,  $\mathbf{A}_{\omega\alpha}$  and  $\mathbf{A}_{\alpha\omega}$  designate the off-diagonal blocks and are the weights of the edges  $(\alpha\omega)$  and  $(\omega\alpha)$ , respectively. Then Theorem 3.2.1 states that the Green's function at  $\alpha$  is given by

$$\mathbf{G}_{\mathcal{K}_2; \alpha} = \left[ \text{Id}_* - \mathbf{A}_{\alpha\alpha} - \mathbf{A}_{\alpha\omega} \star \mathbf{G}_{\mathcal{K}_2 \setminus \{\alpha\}; \omega} \star \mathbf{A}_{\omega\alpha} \right]^{\star-1}, \quad (3.2.5)$$

and  $\mathbf{G}_{\mathcal{K}_2 \setminus \{\alpha\}; \omega} = (\text{Id}_* - \mathbf{A}_{\omega\omega})^{\star-1}$ . The above result is the celebrated Dyson equation. To see this, let  $\mathbf{G} := \mathbf{G}_{\mathcal{K}_2; \alpha}$ ,  $\mathbf{G}_0 := (\text{Id}_* - \mathbf{A}_{\alpha\alpha})^{\star-1}$  and  $\Sigma := \mathbf{A}_{\alpha\omega} \star \mathbf{G}_{\mathcal{K}_2 \setminus \{\alpha\}; \omega} \star \mathbf{A}_{\omega\alpha}$ . Then Eq. (3.2.5) indicates that the Green's function  $\mathbf{G}$  is  $\mathbf{G} = (\mathbf{G}_0^{\star-1} - \Sigma)^{\star-1}$ , or equivalently,

$$\mathbf{G} = \mathbf{G}_0 + \mathbf{G} \star \Sigma \star \mathbf{G}_0.$$

This is the time-dependent Dyson equation [6], which arises naturally from resummations of the Dyson series for the time-ordered exponential in the context of quantum many-body physics. This equation appears for example when considering a physical entity (for example a particle, or an ensemble of sites in a solid) in contact with a larger system. In this situation, the Hamiltonian driving the system + entity is naturally partitioned into four submatrices (blocks):  $\mathbf{A}_{\alpha\alpha}$ , which drives the isolated entity,  $\mathbf{A}_{\omega\omega}$  which drives the rest of the system without the entity and  $\mathbf{A}_{\omega\alpha}(t)$  and  $\mathbf{A}_{\alpha\omega}(t)$ , which represent the interactions system–entity. In this context,  $\Sigma$  is known as the self-energy.

Hence we see that the Dyson equation stems from Theorem 3.2.1 on the complete graph on two vertices. In general, Theorem 3.2.1 can be seen as extending the Dyson equation to an arbitrary number of systems/entities in contact with each other. It therefore provide an *explicit non-perturbative formula* for the self-energy that involves finitely many terms for finite systems.

## Decay properties of the time-ordered exponential

In the last 20 years, a number of significant results have established exponentially decaying bounds for the magnitude of the entries of holomorphic functions of sparse matrices [16, 17, 18]. These results have given rise to a flurry of applications in linear algebra and physics as they underlie efficient approximation techniques, see e.g. [16, 40, 183]. The techniques used to prove these results do not extend to the time-ordered exponential function however. Relying instead on  $\star$ -resolvent formalism, we establish super-exponential decaying bounds for the magnitude of the entries of the time-ordered exponential of sparse matrices.

We have seen that the time-ordered exponential  $\mathbf{U}$  of any-time-dependent matrix  $\mathbf{A}$  is  $\mathbf{U} = \Theta \star (\text{Id}_* - \mathbf{A})^{\star-1}$ . Furthermore, the Peano-Baker series for  $\tilde{\mathbf{A}}$  is unconditionally convergent so that  $(\text{Id}_* - \mathbf{A})^{\star-1} = \sum_{n \geq 0} \mathbf{A}^{\star n}$ . Using the Taylor series remainder theorem then leads to the following bound for the entries of the time-ordered exponential of a sparse matrix:

**Proposition 3.2.1.** *Let  $I \subset \mathbb{R}$ ,  $\tilde{\mathbf{A}}(t) \in \mathcal{C}^\infty[I]^{n \times n}$  and  $\mathbf{A} := \tilde{\mathbf{A}}\Theta$ . Let  $G$  be the graph encoding the sparsity structure of  $\mathbf{A}$ . Let  $d := d(\alpha, \omega)$  be the length of the shortest path from vertex  $\alpha$  to vertex  $\omega$  on  $G$ . Define  $h := \sup_{t \in I} \max_{\alpha, \beta} |\tilde{\mathbf{A}}_{\alpha\beta}(t)|$  and let  $|\mathcal{W}_{G; \alpha\omega; k}|$  be the number of walks of length  $k$  from  $\alpha$  to  $\omega$  on  $G$ . Then*

$$|\mathbf{U}_{\omega\alpha}(t', t)| \leq \sum_{k \geq d} \frac{h^k}{k!} (t' - t)^k |\mathcal{W}_{G; \alpha\omega; k}|, \quad (3.2.6a)$$

with equality when  $\tilde{\mathbf{A}}$  is a constant multiple of the ordinary adjacency matrix of  $G$ . Let  $\Delta$  be the maximum degree of any vertex of  $G$ . If  $\Delta$  is finite, we have

$$|\mathbf{U}_{\omega\alpha}(t', t)| \leq e^{\Delta h(t'-t)} \frac{(\Delta h(t'-t))^d}{d!}. \quad (3.2.6b)$$

The bound of Eq. (3.2.6b) demonstrates the super-exponential decay of the ordered-exponential function of any time-dependent sparse matrix, contingent on the assumption that  $\Delta$  is finite<sup>4</sup>. Furthermore, the result of the proposition is non-trivial only when the maximum distance  $D := \max_{\alpha, \omega} d(\alpha, \omega)$  between any two vertices  $\alpha$  and  $\omega$  on  $G$  is infinite. Otherwise, a super-exponentially decaying bound can always be found for any matrix, by choosing a large enough multiplying constant. We emphasise the validity of these results in the case of infinite matrices of finite norm. Indeed, convergence of the Peano-Baker series necessitates only  $\sup_{t \in I} \|\tilde{A}(t)\|$  to be finite.

### 3.3 Tridiagonalization of differential systems: $\star$ -Lanczos algorithm

The  $\star$ -resolvent formulation of the solution to systems of non-autonomous linear ODEs, Eq. (3.2.1), shows that the  $\star$ -algebra formed by matrices of  $\text{Sm}_{\Theta}^{N \times N}$  is the relevant algebraic context for dealing with such differential systems. This algebra allows for the import of linear algebraic methods in the differential context. In this section, we report on the first such method: an extension to differential systems of the celebrated Lanczos algorithm. Given a matrix  $M \in \mathbb{C}^{N \times N}$  and two vectors  $\mathbf{w}$  and  $\mathbf{v} \in \mathbb{C}^N$  as inputs and barring breakdowns, this algorithm outputs a tridiagonal matrix  $T_N \in \mathbb{C}^{N \times N}$  such that for all  $n \in \mathbb{N}$ ,  $(T_N^n)_{1,1} = \mathbf{w}^H A^n \mathbf{v}$ . Such moment matching property, if it could be extended from the ordinary matrix product to the  $\star$ -product, would allow for the computation of time-ordered exponentials from tridiagonal matrices.

Indeed, let  $A \in \text{Sm}_{\Theta}^{N \times N}$ . We have seen that the time-ordered exponential  $U(t', t)$  of  $A$  is  $U = \Theta \star G_A$ , where the Green's function  $G_A$  is the  $\star$ -resolvent of  $A$ , that is

$$G_A := (\text{Id}_{\star} - A)^{\star^{-1}} = \sum_{n \geq 0} A^{\star n}, \quad (3.3.1a)$$

the series on the right-hand side converging when  $\tilde{A}$  elements are bounded over  $I^2$ . Note that here we wrote  $\text{Id}_{\star}$  for  $\text{Id} \times 1_{\star}$ . In particular then the time-ordered exponential  $U$  of  $A$  obeys

$$\mathbf{w}^H \cdot U \cdot \mathbf{v} = \Theta \star \sum_{n \geq 0} \mathbf{w}^H \cdot A^{\star n} \cdot \mathbf{v}. \quad (3.3.1b)$$

This confirms that if a tridiagonal  $T_N$  could be found with a  $\star$ -moment matching property, then  $\mathbf{w}^H \cdot U \cdot \mathbf{v}$  could be evaluated from it. As with the original Lanczos method, this presents the major advantage that  $T_N$  is extremely sparse while  $A$  can be full.

Now we can present our results on the matter [70]: *barring breakdowns*—which we will characterise below—the  $\star$ -Lanczos algorithm presented in Table 3.1 produces a sequence of tridiagonal matrices  $T_n$ ,  $1 \leq n \leq N$ , of the form

$$T_n := \begin{bmatrix} \alpha_0 & \delta & & & \\ \beta_1 & \alpha_1 & \ddots & & \\ & \ddots & \ddots & \delta & \\ & & \beta_{n-1} & \alpha_{n-1} & \end{bmatrix}, \quad (3.3.2)$$

and such that the matching  $\star$ -moment property is achieved:

**Theorem 3.3.1.** *Let  $A$ ,  $\mathbf{w}$ ,  $\mathbf{v}$  and  $T_n$  be as described above, then*

$$\mathbf{w}^H (A^{\star j}) \mathbf{v} = \mathbf{e}_1^H (T_n^{\star j}) \mathbf{e}_1, \quad \text{for } j = 0, \dots, 2n - 1. \quad (3.3.3)$$

Combining this with Eqs. (3.3.1) we have, for  $n = N$ , the exact expression

$$\mathbf{w}^H U \mathbf{v} = \Theta \star (\text{Id}_{\star} - T_n)_{1,1}^{\star^{-1}},$$

while for  $n < N$ , the right-hand side yields an approximation to the time-ordered exponential. The path-sum theorem then gives,

$$(\text{Id}_{\star} - T_n)_{1,1}^{\star^{-1}} = \left( 1_{\star} - \alpha_0 - (1_{\star} - \alpha_1 - (1_{\star} - (\dots (1_{\star} - \alpha_{n-1})^{\star^{-1}} \dots)^{\star^{-1}} \star \beta_2)^{\star^{-1}} \star \beta_1)^{\star^{-1}} \right).$$

The  $\star$ -resolvents in the expression above are accessible either numerically or analytically from the  $\star$ -Neumann series.

<sup>4</sup>In [67] we give an example where  $\Delta$  infinite leads to 'only' exponential decay.

Input: A complex time-dependent matrix  $\mathbf{A}$ , and complex vectors  $\mathbf{w}, \mathbf{v}$  such that  $\mathbf{w}^H \mathbf{v} = 1$ .  
Output: Coefficients  $\alpha_0, \dots, \alpha_{n-1}$  and  $\beta_1, \dots, \beta_{n-1}$  defining the matrix  $\mathbf{T}_n$  of Eq. (3.3.2) which satisfies Eq. (3.3.3).

Initialize:  $\mathbf{v}_{-1} = \mathbf{w}_{-1} = 0$ ,  $\mathbf{v}_0 = \mathbf{v} \mathbf{1}_*$ ,  $\mathbf{w}_0^H = \mathbf{w}^H \mathbf{1}_*$ .  
 $\alpha_0 = \mathbf{w}^H \mathbf{A} \mathbf{v}$ ,  
 $\mathbf{w}_1^H = \mathbf{w}^H \mathbf{A} - \alpha_0 \mathbf{w}^H$ ,  
 $\widehat{\mathbf{v}}_1 = \mathbf{A} \mathbf{v} - \mathbf{v} \alpha_0$ ,  
 $\beta_1 = \mathbf{w}^H \mathbf{A}^* \mathbf{v} - \alpha_0^{*2}$ ,  
 If  $\beta_1$  is not  $\star$ -invertible, then stop, otherwise,  
 $\mathbf{v}_1 = \widehat{\mathbf{v}}_1 \star \beta_1^{\star-1}$ ,  
 For  $n = 2, \dots$   
 $\alpha_{n-1} = \mathbf{w}_{n-1}^H \star \mathbf{A} \star \mathbf{v}_{n-1}$ ,  
 $\mathbf{w}_n^H = \mathbf{w}_{n-1}^H \star \mathbf{A} - \alpha_{n-1} \star \mathbf{w}_{n-1}^H - \beta_{n-1} \star \mathbf{w}_{n-2}^H$ ,  
 $\widehat{\mathbf{v}}_n = \mathbf{A} \star \mathbf{v}_{n-1} - \mathbf{v}_{n-1} \star \alpha_{n-1} - \mathbf{v}_{n-2}$ ,  
 $\beta_n = \mathbf{w}_n^H \star \mathbf{A} \star \mathbf{v}_{n-1}$ ,  
 If  $\beta_n$  is not  $\star$ -invertible, then stop, otherwise,  
 $\mathbf{v}_n = \widehat{\mathbf{v}}_n \star \beta_n^{\star-1}$ ,  
 end.

Table 3.1: The  $\star$ -Lanczos algorithm.

**Remark.** The described tridiagonalization of the system of ODEs effected by Theorem 3.3.1 can also be seen as a  $\star$ -factorization of the matrix  $\mathbf{A}$ . Consider the matrices  $\mathbf{W}_N = [\mathbf{w}_0, \dots, \mathbf{w}_{N-1}]$  and  $\mathbf{V}_N = [\mathbf{v}_0, \dots, \mathbf{v}_{N-1}]$  composed of the vectors computed by the  $\star$ -Lanczos algorithm. Then

$$\mathbf{T}_N = \mathbf{W}_N^H \star \mathbf{A} \star \mathbf{V}_N, \quad \mathbf{W}_N^H \star \mathbf{V}_N = \mathbf{Id}_*, \quad (3.3.4)$$

and  $\mathbf{G}_A = \mathbf{V}_N \star (\mathbf{Id}_* - \mathbf{T}_N)^{\star-1} \star \mathbf{W}_N^H$

A crucial assumption underlying these results is that the algorithm suffers no breakdown. This is related to the nature of the  $\alpha_j$  and  $\beta_j$  distributions appearing in the  $\mathbf{T}_n$  matrices and which are produced by the  $\star$ -Lanczos procedure through recurrence relations. These necessitate the  $\star$ -inversion of the  $\beta_j$  without which the algorithm breaks down. If  $\beta_j$  is not identically null, the existence of  $\beta_j^{\star-1}$  is established by Corollary 3.1.1 assuming *ad minima* that  $\alpha_j, \beta_j \in \text{Sm}_\Theta$ . Proving that this assumption is always verified turns out to be surprisingly difficult. In the course of proof, we also established that the remaining breakdowns of the  $\star$ -Lanczos—arising when a  $\beta_j$  is identically null—coincide exactly with the breakdowns of the non-Hermitian Lanczos algorithm.

Before we state the main theorems on the tridiagonalization of systems of coupled linear differential equations with non-constant coefficients, we begin by exhibiting a relation between breakdowns in the  $\star$ -Lanczos procedure and breakdowns in the ordinary non-Hermitian Lanczos procedure. This shows that the feasibility of tridiagonalization does not depend on the nature of the entries of the original matrix nor on the kind of product between these entries. Rather breakdowns in tridiagonalization must be topological in origin, i.e. they depend on the structure and the edge weights of the graph whose adjacency matrix is  $\mathbf{A}$ . We recall that, given as inputs a time-independent matrix  $\mathbf{B}$  and time-independent vectors  $\mathbf{p}, \mathbf{q}$ , the ordinary non-Hermitian Lanczos algorithm aims to compute the (time-independent) vectors  $\mathbf{p}_0, \dots, \mathbf{p}_n$  and  $\mathbf{q}_0, \dots, \mathbf{q}_n$ , respectively biorthonormal bases of the Krylov subspaces

$$\text{span}\{\mathbf{p}, \mathbf{B} \mathbf{p}, \dots, \mathbf{B}^n \mathbf{p}\}, \quad \text{span}\{\mathbf{q}, \mathbf{B}^H \mathbf{q}, \dots, (\mathbf{B}^H)^n \mathbf{q}\}.$$

There is a *serious breakdown* at the  $n$ th iteration of the ordinary non-Hermitian Lanczos algorithm when  $\mathbf{q}_n^H \mathbf{p}_n = 0$  and  $\mathbf{p}_n, \mathbf{q}_n \neq 0$ ; see [155, Remark 3.2]. Assuming no breakdown arises before the  $n$ th iteration, the non-Hermitian Lanczos algorithm also gives the  $n \times n$  tridiagonal matrix

$$\mathbf{S}_n := [\mathbf{q}_0, \dots, \mathbf{q}_{n-1}]^H \mathbf{B} [\mathbf{p}_0, \dots, \mathbf{p}_{n-1}]. \quad (3.3.5)$$

The first key result relating breakdowns of the  $\star$ -Lanczos algorithm and of its classical non-Hermitian counterpart is the following Lemma:

**Lemma 3.3.1.** *Let  $T_n$  be the tridiagonal matrix (3.3.2) obtained by  $n$  iterations of the  $\star$ -Lanczos algorithm in Table 3.1 with inputs  $A = \tilde{A}\Theta, \mathbf{w}, \mathbf{v}$ , where  $\tilde{A} \in C^\infty[I]^{N \times N}$  and  $\mathbf{w}, \mathbf{v}$  are time-independent vectors with  $\mathbf{w}^H \mathbf{v} = 1$ . Assume that the  $\star$ -Lanczos coefficients  $\alpha_{j-1}, \beta_j$  are in  $\text{Sm}_\Theta$  and that  $\beta_j(t, t) \equiv 0$ , for every  $j = 1, \dots, n-1$ . Let us denote with  $\tilde{\beta}_j^{(1,0)}(t', t)$  and  $\tilde{\beta}_j^{(0,1)}(t', t)$  respectively the derivative with respect to  $t'$  and  $t$  of  $\tilde{\beta}_j(t', t)$ . Then the following statements are equivalent:*

1.  $\tilde{\beta}_1^{(1,0)}(t, t), \dots, \tilde{\beta}_{n-1}^{(1,0)}(t, t)$  are not identically null on  $I$ ;
2.  $\tilde{\beta}_1^{(0,1)}(t, t), \dots, \tilde{\beta}_{n-1}^{(0,1)}(t, t)$  are not identically null on  $I$ ;
3. There exists at least one  $\rho \in I$  so that the usual non-Hermitian Lanczos algorithm with inputs  $\tilde{A}(\rho), \mathbf{w}, \mathbf{v}$  has no serious breakdown in the first  $n-1$  iterations.

Note that statement 1 (or equivalently Statement 2) in Lemma 3.3.1 also implies that there cannot be a breakdown in the first  $n$  iterations of the  $\star$ -Lanczos algorithm in Table 3.1, meaning that  $\beta_1, \dots, \beta_{n-1}$  are  $\star$ -invertible almost everywhere on  $I$ . Hence Statement 3 in Lemma 3.3.1 is a sufficient condition for not having a breakdown in the  $\star$ -Lanczos Algorithm.

**Theorem 3.3.2.** *Let  $I \subset \mathbb{R}$  be compact and  $\tilde{A} \in C^\infty[I]^{N \times N}$  with  $U$  its time-ordered exponential. Let  $\mathbf{w}$  and  $\mathbf{v}$  be time-independent  $N \times 1$  vectors with  $\mathbf{w}^H \mathbf{v} = 1$ . Assume that the classical non-Hermitian Lanczos algorithm with inputs  $A, \mathbf{w}, \mathbf{v}$  has not a serious breakdown in the  $k$ th iteration for  $k = 1, \dots, N-1$ , for every  $t'$  in  $I$ .*

*Then the  $\star$ -Lanczos algorithm 3.1 does not breakdown, all  $\star$ -inverses  $\beta_{1 \leq i \leq N-1}^{\star-1}$  exist, are of the form  $\beta_i^{\star-1} = \delta^{(3)} \star b$ , with  $b \in \text{Sm}_\Theta$ , and Theorem 3.3.1 holds for the non-autonomous differential system with coefficients  $\tilde{A}$ .*

As a byproduct of the proof of Lemma 3.3.1, we get the following result, which establishes a connection between the  $\star$ -Lanczos and the ordinary non-Hermitian Lanczos algorithms.

**Theorem 3.3.3.** *Under the assumption and notation of Theorem 3.3.2, consider the matrix*

$$J_n(t) := \begin{bmatrix} \tilde{\alpha}_0(t, t) & 1 & & & \\ \tilde{\beta}_1^{(1,0)}(t, t) & \tilde{\alpha}_1(t, t) & \ddots & & \\ & \ddots & \ddots & & \\ & & & \ddots & 1 \\ & & & \tilde{\beta}_{n-1}^{(1,0)}(t, t) & \tilde{\alpha}_{n-1}(t, t) \end{bmatrix}, \quad t \in I.$$

*Let  $S_{n,\rho}$  be the tridiagonal matrix obtained by running the ordinary non-Hermitian Lanczos algorithm with inputs  $A(\rho), \mathbf{v}, \mathbf{w}$ , for a fixed  $\rho \in I$ ; see Eq. 3.3.5. Then there exists a regular diagonal matrix  $D_\rho$  so that*

$$J_n(\rho) = D_\rho S_{n,\rho} D_\rho^{-1}.$$

In other terms the  $\star$ -Lanczos algorithm produces the classical non-Hermitian Lanczos tridiagonalization at all times in  $I$ , at once.

**Remark.** When either the vector  $\mathbf{v}_n$  or  $\mathbf{w}_n$  are identically null over  $I$ , we say that the  $\star$ -Lanczos has a *lucky breakdown*, in analogy with the ordinary non-Hermitian Lanczos algorithm. We show in Proposition 2 of [70] that in the case of a lucky breakdown the  $\star$ -Lanczos algorithm gives  $\mathbf{w}^H U(t', t) \mathbf{v}$  exactly.



## Chapter 4

# Further applications of the path-sum theorem

As explained in §2.4, the first field of application of the path-sum theorem is in linear algebra, in particular for the representation of matrix functions. The most immediate generalizations stem from mathematical problems that are naturally mappable to graphs. This is for example the case of Gaussian Markov random fields (GMRF), discussed here briefly. We then summarise example of applications of path-sum in conjunction with  $\star$ -calculus in quantum mechanics and in the representation of transcendent functions.

### 4.1 Statistical inference

A GMRF is a random vector that follows a multivariate normal distribution and satisfies conditional independence assumptions. If  $X_1, X_2, X_3$  are random variables with a joint probability density function (or joint probability mass function in a discrete case), we say that  $X_1$  is conditionally independent of  $X_2$  given  $X_3$ , denoted  $X_1 \perp\!\!\!\perp X_2 | X_3$ , if  $f(x_1, x_2 | x_3) = f(x_1 | x_3) f(x_2 | x_3)$ . Here we use  $f$  as a generic symbol for the probability density function of the random variables corresponding to its arguments. GMRFs have a simple interpretation and find their applications, for example, in image analysis, spatial statistics, structural time series analysis and analysis of longitudinal and survival data [174].

Consider now a random vector  $\mathbf{X} = (X_1, X_2, \dots, X_n) \sim \mathbb{N}(\mu, \Sigma)$  following a multivariate normal distribution with mean  $\mu$  and covariance matrix  $\Sigma$ . The probability density function of  $\mathbf{X}$  is given as

$$f(x) = \frac{1}{\sqrt{(2\pi)^n \det(\Sigma)}} \exp \left[ -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] = g(x) \exp \left[ -\frac{1}{2} x^T J x + h^T x - k(\mu, \Sigma) \right]. \quad (4.1.1)$$

Here  $\Sigma$  is a symmetric and positive definite matrix,  $J = \Sigma^{-1}$  is called information matrix,  $h = J\mu$  is called the potential vector,  $g(x) = (2\pi)^{-\frac{n}{2}}$  and  $k(\mu, \Sigma) = \frac{1}{2} \mu^T J \mu - \frac{1}{2} \ln(\det(J))$ . We may now construct a graphical model for statistical inference on GMRF as follows.

Let  $G = (V, E)$  be a graph and denote  $\mathbf{X}_{\setminus ij}$  the set of variables with  $X_i$  and  $X_j$  removed from  $\mathbf{X}$ . If  $J = (J_{ij})_{i,j \in V}$  is positive definite, then for  $i, j \in V$ , where  $i \neq j$ , we have [114, Proposition 5.2]  $X_i \perp\!\!\!\perp X_j | \mathbf{X}_{\setminus ij} \Leftrightarrow J_{ij} = 0$ .

**Definition 4.1.1** ([174]). A random vector  $\mathbf{X}$  is called a GMRF with respect to a graph  $G = (V, E)$  with information matrix  $J$  and potential vector  $h$  if and only if its density has the form of (4.1.1) and  $J_{ij} \neq 0 \Leftrightarrow (i, j) \in E$ , for all  $i$  and  $j$ .

It is known that  $X$  satisfies the Markov property on  $G$  [174, Theorem 2.4]<sup>1</sup>. By definition there is a one-to-one correspondence between the structure of  $J$  and the structure of  $G$ . Most information matrices  $J$  for GMRFs are sparse with only  $O(n)$  non-zero entries in  $J$  a key property facilitating the simulation of GMRFs through their information matrix.

Estimations of  $\mathbf{X}$  given noisy observations  $\mathbf{Y}$  are also readily accessible in this framework. Assume that  $\mathbf{Y} = C\mathbf{X} + \varepsilon$ , where  $C$  is an  $n \times n$  real matrix and  $\varepsilon \sim \mathbb{N}(0, M)$ . Then the conditional distribution of  $\mathbf{X} | \mathbf{Y}$  is given by  $f(x|y) = \frac{f(y|x)f(x)}{f(y)} \propto \exp \left[ -\frac{1}{2} x^T \tilde{J} x + \tilde{h}^T x \right]$ , where  $\tilde{J} = J + C^T M^{-1} C$  and  $\tilde{h} = h + C^T M^{-1} y$ . Thus given noisy observations, one only needs to update the information matrix and the potential vector to construct a graphical model for  $f(x|y)$ . For simplicity, we shall still use  $J$  and  $h$  to denote the parameters after absorption of observations.

<sup>1</sup>For a GMRF, the pairwise Markov property, the local Markov property and the global Markov property are equivalent. This is proven by using [114, Proposition 3.8], in conjunction with the Hammersley-Clifford Theorem [114, Theorem 3.9].

As apparent from Eq. 4.1.1 one needs both the covariance matrix  $\Sigma = J^{-1}$  and the mean vector  $\mu = J^{-1}h$  to obtain the marginal distributions of  $\mathbf{X}$  or  $\mathbf{X}|\mathbf{Y}$ . Since knowing  $J^{-1}$  is sufficient to recover  $\mu$ , we focus our efforts on calculating  $J^{-1}$ . Direct inversion of  $J$  has complexity  $O(n^3)$  and does not exploit the sparsity of  $J$ .<sup>2</sup> In a simple situation where the graph  $G$  of a GMRF is a tree, belief propagation (BP) efficiently calculates the correct marginals [132, 158]. For graphs with cycles (also called loopy graphs), the method of Loopy Belief Propagation (LBP) can be used to efficiently approximate the marginals yet, estimates of the covariance matrices it provides are generally incorrect [200].

As earlier we denote  $G \setminus \{\alpha, \beta \dots\}$  the subgraph of  $G$  obtained by deleting from  $G$  the vertices  $\{\alpha, \beta \dots\} \subset V$  and the edges incident to them. The path-sum theorem immediately gives

**Theorem 4.1.1.** *Let  $J$  be a finite GMRF information matrix. Let  $\Pi(G)_{\alpha\omega}$  and  $\Gamma(G)_{\alpha}$  be the sets of simple paths from  $\alpha$  to  $\omega$  on  $G$  and the set of simple cycles from  $\alpha$  to itself on  $G$ , respectively. Then each entry of the covariance matrix  $\Sigma = J^{-1}$  admits the path-sum representation*

$$J_{\omega\alpha}^{-1} = \sum_{p \in \Pi_{G; \alpha\omega}} (-1)^{\ell(p)} \prod_{j=1}^{\ell(p)+1} \left\{ (J_{G \setminus \{\alpha, \nu_2, \dots, \nu_{j-1}\}})_{\nu_j \nu_j}^{-1} J_{\nu_{j+1} \nu_j} \right\} J_{\alpha\alpha}^{-1},$$

$$J_{\alpha\alpha}^{-1} = \left( \sum_{\gamma \in \Gamma_{G; \alpha\alpha}} (-1)^{\ell(\gamma)+1} J_{\mu_1 \mu_{\ell(\gamma)}} \prod_{j=2}^{\ell(\gamma)} \left\{ (J_{G \setminus \{\alpha, \mu_2, \dots, \mu_{j-1}\}})_{\mu_j \mu_j}^{-1} J_{\mu_j \mu_{j-1}} \right\} \right)^{-1},$$

where the products are right-to-left (i.e.  $\prod_{i=1}^m a_i = a_m \cdots a_1$ ),  $p = (\nu_1, \nu_2, \dots, \nu_{\ell(p)+1})$  is a simple path of length  $\ell(p)$  with  $\alpha \equiv \nu_1$  and  $\omega \equiv \nu_{\ell(p)+1}$  for convenience; and  $\gamma = (\mu_1, \mu_2, \dots, \mu_{\ell(\gamma)}, \mu_1)$  is a simple cycle of length  $\ell(\gamma)$  from  $\alpha \equiv \mu_1$  to itself.

**Remark.** The above path-sum formulation is valid for all matrix-partitions of  $J$ . For a GMRF  $\mathbf{X}$ , a partition of  $J$  is equivalent to a partition of the set of random variables  $\mathbf{X}$  into  $B > 1$  disjoint subsets  $\mathbf{X}_1, \dots, \mathbf{X}_B$ . Let  $\mathbf{X}' = (\mathbf{X}_1, \dots, \mathbf{X}_B)$  be a GMRF with respect to a new graph  $G' = (V', E')$  with information matrix  $J'$ . Note that each  $\mathbf{X}_i$  is now a random vector instead of a random variable. Following Definition 4.1.1 we define  $\mathbf{X}_i \perp\!\!\!\perp \mathbf{X}_j | \mathbf{X}'_{\setminus ij} \iff J'_{ij} = \mathbf{0} \iff (j, i) \notin E'$ , with  $\mathbf{X}'_{\setminus ij}$  the set of variables with  $\mathbf{X}_i$  and  $\mathbf{X}_j$  removed from  $\mathbf{X}'$ . Note that  $\mathbf{X}_i \perp\!\!\!\perp \mathbf{X}_j | \mathbf{X}'_{\setminus ij}$  implies the global Markov property (GMP), which, for GMRFs, is equivalent to the pairwise Markov property (PMP).

**Remark.** The authors of [132] provided a walk-based derivation for Gaussian belief propagation on trees. The equations they obtain follow immediately from an application of the above theorem under the assumption that  $G$  is a tree [63]. Another approach, presented in [102], proved that some entries of  $J^{-1}$  are sums over the simple paths of  $G$  with determinantal weights. This follows immediately from the above theorem on using the adjugate formula for the quantities  $(J_{G \setminus \{\alpha, \nu_2, \dots, \nu_{j-1}\}})_{\nu_j \nu_j}^{-1}$  when using the standard partition of  $J$  into its entries.

## 4.2 Quantum dynamics

A non-relativistic isolated quantum system evolves in time according to Schrödinger's equation, which we may synthesise as ( $\hbar = 1$ )

$$\dot{\mathbf{U}} = -i\mathbf{H}\mathbf{U}$$

Here  $\mathbf{H}$  is the possibly time-dependent Hamiltonian operator, which describes the system's energy. If the physical system's degrees of freedom are purely discrete then  $\mathbf{H}$  is a (possibly infinite) matrix. Then Schrödinger's equation is a system of non-autonomous linear ODEs. We may consequently use the  $\star$ -product formalism in conjunction with the path-sum theorem to solve this equation. These purely mathematical observations also make sense physically, as we now briefly discuss.<sup>3</sup>

### Quantum evolution, walks on graphs and scale invariance

Quantum systems with discrete degrees of freedom such as spin systems, obey a discrete analog to Feynman's path integrals. To illustrate this from a physical standpoint, define one history of a quantum system as a temporal succession of *orthogonal* quantum states  $h : |s_1\rangle \mapsto |s_2\rangle \mapsto |s_3\rangle \cdots$ , each transition  $|s_i\rangle \mapsto |s_{i+1}\rangle$  happening at a specified time  $t_i$ . Overall the history  $h$  acquires a complex weight which is the product of the

<sup>2</sup>Algorithms that compute some entries of a symmetric  $n \times n$  sparse matrix with complexity less than  $O(n^3)$  do exist. The path-sum representation achieves this as well, computing the covariance of a pair of variables with complexity  $O(n)$  whenever  $G$  is a tree [59].

<sup>3</sup>See also Chapter 4 of my PhD thesis for extended discussion and a physics-based proof of the walk-sum lemma, a weaker form of the path-sum theorem [59].

weights of all the transitions in the history. The weight of an individual transition  $|s_i\rangle \mapsto |s_{i+1}\rangle$  is dictated by the Hamiltonian as  $\langle s_{i+1} | H(t_i) | s_i \rangle$ .

A natural representation of such discrete histories is as walks on a graph. Define  $G_t$  the graph where each vertex  $v_i$  corresponds to one member  $|s_i\rangle$  of an orthonormal basis for the entire state-space and give the directed edge  $v_i \mapsto v_j$  the *time-dependent* weight  $\langle s_j | H(t) | s_i \rangle$ . In this picture, a system history as defined earlier is a walk on  $G_t$  and  $H(t)$  is the adjacency matrix of  $G_t$ . Because the Hamiltonian is time-dependent, the graph itself is dynamical.

Now just as for Feynman's path-integrals, the exact evolution of the system is obtained from the superposition of all its possible histories. Equivalently, every element  $\langle s_j | U(t) | s_i \rangle$  of the evolution operator  $U(t)$  is given by the sum over all walks from  $v_i$  to  $v_j$  on  $G_t$ , including all possible jumping times for each transition between vertices. While individual walks are the discrete counterpart of Feynman diagrams, their algebraic structure is better understood (Chapter 2). Since all walks are uniquely representable as nestings of simple cycles and paths, so walks series have a formulation involving only these: the path-sum. Then any  $\langle s_j | U(t) | s_i \rangle$  is given as branched continued fractions comprising only the weights of the simple cycles and paths of the graph. Because the graph  $G_t$  is finite, there are finitely many such cycles and paths and the fraction is *finite* in both depth and breadth. It is thus unconditionally convergent. As presented in Chapter 3, the same principles apply regardless of whether the Hamiltonian depends on time or not.

Combinatorially, path-sums stem from formal resummations of families of walks. This principle does not depend on what those walks represent. In particular, it remains unchanged by the nature of the evolving system. To exploit this observation, consider a more general type of system histories made of temporal successions of orthogonal vector spaces  $\tilde{h} : V_1 \mapsto V_2 \mapsto V_3 \cdots$ . Physically such histories can describe an evolving subsystem, such as a group of protons in a large molecule. Mathematically they correspond to walks on a coarse-grained representation of the quantum state space, a subgraph  $\tilde{G}_t$  of  $G_t$ . To see this, take a complete family of orthogonal spaces, i.e.  $\bigoplus_{i=1} V_i = V$ , where  $V$  is the entire quantum state space. To each  $V_i$  associate a vertex  $v_i$  and give the edge  $v_i \mapsto v_j$  the time-dependent weight  $P_{V_j} \cdot H(t) \cdot P_{V_i}$ . Here  $P_{V_k}$  is the projector onto  $V_k$ . Observe then that these edge weights are generally non-Abelian. Yet, because path-sums fundamentally retain the order and time of the transitions in histories when performing resummations of walks, this setup poses no further difficulty. It follows that the submatrix  $P_{V_j} \cdot U(t', t) \cdot P_{V_i}$  of the evolution operator is again given as a matrix-valued branched continued fraction of finite depth and breadth. While the shape of this fraction depends on the particular choice of vector spaces, its existence and convergence properties do not. If the vector spaces are chosen so that the shape of the fraction itself is unchanged, and such a choice is always possible, then the path-sum formulation is truly invariant under scale changes in the quantum state space.

An immediate consequence of scale-invariance is that there is always a path-sum calculation rigorously relating the global evolution of a system to that of any ensemble of its subsystems, such as clusters of spins in a large molecule. In this scheme, we can evolve each subsystem *separately* from one-another using any preferred method; only to then combine these isolated evolutions *exactly* via a path-sum to generate the true system evolution.

## Solutions for small non-autonomous systems

We give the explicit path-sum solutions for all  $2 \times 2$  and  $3 \times 3$  problems, solutions to an  $8 \times 8$  and  $14 \times 14$  problem are presented in [64] and [62], respectively.

### General $2 \times 2$ case

Consider the time-dependent matrix

$$\tilde{H}(t) = \begin{pmatrix} \tilde{H}_{11}(t) & \tilde{H}_{12}(t) \\ \tilde{H}_{21}(t) & \tilde{H}_{22}(t) \end{pmatrix},$$

where all  $\tilde{H}_{ij} \in \mathcal{C}^\infty[I]$  for some  $I \subset \mathbb{R}$  compact. In the standard partition of  $H$  into its entries, the corresponding graph  $G$  is the complete graph  $K_2$ . Thus, the path-sum theorem gives the time-ordered matrix exponential  $U$  of  $H := \dot{H}\Theta$ , solution of  $\dot{U} = H \cdot U$ , as

$$\begin{aligned} U_{ii} &= \Theta \star G_i, & G_i &:= \left( 1_\star - H_{ii} - H_{ij} \star (1_\star - H_{jj})^{\star-1} \star H_{ji} \right)^{\star-1}, \\ U_{ji} &= \Theta \star (1_\star - H_{jj})^{\star-1} \star H_{ji} \star G_i, \end{aligned}$$

where  $i, j = 1, 2$  and  $i \neq j$ . Furthermore  $(1_\star - H_{jj})^{\star-1} = 1_\star + H_{jj} \exp(\Theta \star H_{jj})$ ,  $j = 1, 2$  by virtue of Proposition 3.1.3, p. 24. This notably implies  $H_{ij} \star (1_\star - H_{jj})^{\star-1} = H_{ij} \exp(\Theta \star H_{jj})$  and  $\Theta \star (1_\star - H_{jj})^{\star-1} = \exp(\Theta \star H_{jj})$ . Since the graph comprises only two vertices, the path-sum theorem reduces to a use of the Schur complement in the  $\star$ -algebra  $(\mathcal{C}^\infty[I]^{2 \times 2}, \star)$ , as may be recognised above.

### General $3 \times 3$ case

We consider now a time-dependent matrix  $\tilde{H} \in \mathcal{C}^\infty[I]^{3 \times 3}$ . The corresponding graph is the  $K_3$  graph with self-loops. The path-sum representation of the time-ordered exponential of  $H := \tilde{H}\Theta$  is  $U = \Theta \star G$  with  $G$  a matrix whose entries  $G_{ij}(t', t)$ ,  $i, j, k \in \{1, 2, 3\}$ ,  $i \neq j \neq k$ , are explicitly given by

$$\begin{aligned} G_{ii} &= \left( 1_\star - H_{ii} - (H_{ij} + H_{ik} \star G_{K_3 \setminus \{i,j\};k} \star H_{kj}) \star G_{K_3 \setminus \{i\};j} \star H_{ji} \right. \\ &\quad \left. - (H_{ik} + H_{ij} \star G_{K_3 \setminus \{i,k\};j} \star H_{jk}) \star G_{K_3 \setminus \{i\};k} \star H_{ki} \right)^{\star-1}, \\ G_{ij} &= G_{K_3 \setminus \{j\};i} \star H_{ij} \star G_{jj} + G_{K_3 \setminus \{j,k\};i} \star H_{ik} \star G_{K_3 \setminus \{j\};k} \star H_{kj} \star G_{jj}. \end{aligned}$$

In these expressions,

$$\begin{aligned} G_{K_3 \setminus \{j\};i} &:= (1_\star - H_{ik} \star H_{ki} - H_{ik} \star G_{K_3 \setminus \{i,j\};k} \star H_{ki})^{\star-1}, \\ G_{K_3 \setminus \{i,j\};k} &= 1_\star + H_{kk} \exp(\Theta \star H_{kk}). \end{aligned}$$

### Bloch-Siegert dynamics

The Bloch-Siegert Hamiltonian, here denoted  $H_{BS}(t)$ , is possibly the simplest model to exhibit non-trivial physical effects (such as the Bloch-Siegert shifts [185]) due to time-dependencies in the driving radio-frequency fields. The detailed study of these effects is of paramount importance in the broad field of quantum computing, as they have a deleterious impact on qubit driving and stored quantum information [207]. The Hamiltonian reads, in the  $\{|\uparrow\rangle, |\downarrow\rangle\}$  basis,

$$\tilde{H}_{BS}(t) = \begin{pmatrix} \omega_0/2 & 2\beta \cos(\omega t) \\ 2\beta \cos(\omega t) & -\omega_0/2 \end{pmatrix}. \quad (4.2.1)$$

This is usually given in the interaction picture  $\tilde{H}_{BS}(t) = 2\beta \cos(\omega t) \cos(\omega_0 t) \sigma_x - 2\beta \cos(\omega t) \sin(\omega_0 t) \sigma_y$ . In these expressions, the coupling parameter  $\beta$  is the amplitude of the radio-frequency field. Beyond the rotating wave approximation—which omits the field's counter-rotating terms and is limited to near resonant  $\omega \sim \omega_0$  ultra-weak couplings  $\beta/\omega \ll 1$  and in spite of the much theoretical efforts [7, 8, 204, 208], a non-perturbative truly analytical solution at all orders over the entire coupling range, on and off resonance, is ultimately lacking.

### Path-sum solution

Since in the rotating frame,  $(H_{BS})_{11} = (H_{BS})_{22} = 0$ , the graph representing  $H_{BS}$  in its standard partition is  $K_2$  but with no self-loops. Then the general solution given above yields the time-ordered exponential of  $-iH_{BS}$

$$\begin{aligned} U(t)_{11} &= \int_0^t G_\uparrow(\tau, 0) d\tau, & U(t)_{22} &= \int_0^t G_\downarrow(\tau, 0) d\tau, \\ U(t)_{21} &= -2i\beta \int_0^t \int_0^{\tau_1} \cos(\omega\tau_1) e^{i\omega_0\tau_1} G_\uparrow(\tau_0, 0) d\tau_0 d\tau_1, & U(t)_{12} &= -2i\beta \int_0^t \int_0^{\tau_1} \cos(\omega\tau_1) e^{-i\omega_0\tau_1} G_\downarrow(\tau_0, 0) d\tau_0 d\tau_1, \end{aligned}$$

while  $G_\uparrow(t', t) = (1_\star - K_\uparrow \Theta)^{\star-1}$ ,  $G_\downarrow = (1_\star - K_\downarrow \Theta)^{\star-1}$  with

$$\begin{aligned} K_\uparrow(t', t) &= \frac{4\beta^2}{\omega^2 - \omega_0^2} \cos(\omega t') \left( k_\uparrow(t) e^{-i\omega_0(t'-t)} - k_\uparrow(t') \right), \\ K_\downarrow(t', t) &= \frac{i\beta^2}{\omega^2 - \omega_0^2} \left( 1 + e^{-2i\omega t'} \right) \left( k_\downarrow(t') - k_\downarrow(t) e^{i(\omega+\omega_0)(t'-t)} \right), \end{aligned}$$

where  $k_\uparrow(t) = i\omega_0 \cos(\omega t) + \omega \sin(\omega t)$  and  $k_\downarrow(t) = e^{2i\omega t}(\omega + \omega_0) - (\omega - \omega_0)$ . In spite of the apparent divergences in the resonant case  $\omega_0 \rightarrow \omega$ , the kernels  $K_\uparrow$  and  $K_\downarrow$  are actually well defined in this limit. The quantity  $G_\uparrow$  as obtained from  $K_\uparrow$  has no closed form, rather it is a hitherto unknown higher special function. It is nonetheless analytically available thanks to *unconditionally convergent*  $\star$ -Neumann expansion  $G_\uparrow = 1_\star + \sum_{k>0} K_\uparrow^{\star k}$ .<sup>4</sup> The  $\star$ -Neumann series is well suited to analytical computations, yielding (here displaying only the first two orders on resonance  $\omega_0 = \omega$ ),

$$\begin{aligned} G_\uparrow(t, 0) &= \delta(t) - \frac{\beta^2}{\omega} e^{-i\omega t} \cos(\omega t) (-ie^{2i\omega t} + 2\omega t + i) \\ &\quad + \frac{\beta^4}{24\omega^3} e^{-3i\omega t} \cos(\omega t) \left( 3ie^{6i\omega t} + 6e^{4i\omega t} (-2i\omega^2 t^2 + 2\omega t + i) + e^{2i\omega t} (8\omega^3 t^3 + 12i\omega^2 t^2 + 12\omega t - 15i) - 12\omega t + 6i \right) + \dots \end{aligned}$$

<sup>4</sup>This observation holds for all  $N \times N$  time-dependent Hamiltonians treated by path-sum.

Of particular interest for qubit-driving experiments is the evolution of the transition probability  $P_{\uparrow \rightarrow \downarrow}(t) := |U_{21}(t)|^2$  from state  $|\uparrow\rangle$  to state  $|\downarrow\rangle$  [4, 126, 206]. This quantity is usually found perturbatively in the weak coupling regime using Floquet theory [185] as Magnus series again suffer from divergences [136]. It is now easily accessible— $U_{21}$  being given above. We find that  $P_{\uparrow \rightarrow \downarrow}(t)$  takes on the form of a Fourier-like series

$$P_{\uparrow \rightarrow \downarrow}(t) = \sum_{k=0}^{\infty} \sin(2k\omega t) S_{2k}(\beta, t) + \cos(2k\omega t) C_{2k}(\beta, t), \quad (4.2.2)$$

with  $S_{2k}$  and  $C_{2k}$  functions of  $\beta$  and  $t$ , a representation of which is analytically available [62]. This form of  $P_{\uparrow \rightarrow \downarrow}(t)$  is due to the path-sum integral of  $U_{21}$ , which resembles a Fourier transform. We emphasise that this is not a general feature of path-sum nor of  $2 \times 2$  Hamiltonians, but solely of the present Hamiltonian with linearly polarised driving.

### Anomalous resonances and accelerated $\star$ -Neumann series

One of the striking effects related to Bloch-Siegert dynamics is an anomalous resonance known as Coherent Destruction of Tunneling (CDT) [82, 126]. Concretely this effect manifests itself when  $4\beta/\omega$  falls on a root of the 0th Bessel function  $J_0$ . At this point there is a strong suppression of the transition between states  $|\psi_{\pm}\rangle := \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm |\downarrow\rangle)$  in spite of a very strong coupling  $\beta/\omega_0 \gg 1$  between the  $|\uparrow\rangle$  and  $|\downarrow\rangle$  states in the Hamiltonian. In this situation we found it highly advantageous to see  $-iH_{BS}$  as comprising two parts,

$$K_1(t) = -2i\beta \begin{pmatrix} 0 & \cos(\omega t) \\ \cos(\omega t) & 0 \end{pmatrix}, \quad K_2 = -i\omega_0 \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}.$$

In the trivial partition where  $H_{BS}$  is a single block, the  $\star$ -resolvent formulation indicates that  $U = \Theta \star (\text{Id}_{\star} + iH_{BS}\Theta)^{\star-1}$ , which is also the path-sum formulation for the graph with a single vertex and a self-loop. We calculate the  $\star$ -resolvent of  $H$  directly with an accelerated  $\star$ -Neumann series (see §3.1), suitably truncated for approximations. We expect this to work well because in strong coupling regime  $\beta/\omega_0 \gg 1$ ,  $K_1$  dominates  $K_2$  and the  $\star$ -resolvents of  $K_{1,2}$  are both known exactly. *For reasons unknown* we found this scheme to work beyond well in that it gave exact expressions at order 0 as all subsequent orders of the accelerated series vanished when on the CDT resonance. We emphasise that this is *non-trivial and not understood*. Anyhow at the 0th order of the accelerated series, we get the  $\star$ -resolvent as  $G^{(acc,0)} = (\text{Id}_{\star} - K_1\Theta)^{\star-1} \star (\text{Id}_{\star} - K_2\Theta)^{\star-1}$  so that

$$U^{(acc,0)}(t) = \begin{pmatrix} \cos\left(\frac{2\beta}{\omega} \sin(\omega t)\right) + e^{-\frac{1}{2}i\omega_0 t} - 1 & -i \sin\left(\frac{2\beta}{\omega} \sin(\omega t)\right) \\ -i \sin\left(\frac{2\beta}{\omega} \sin(\omega t)\right) & \cos\left(\frac{2\beta}{\omega} \sin(\omega t)\right) + e^{\frac{1}{2}i\omega_0 t} - 1 \end{pmatrix} \\ + \int_0^t \begin{pmatrix} i\omega_0 e^{-\frac{1}{2}i\omega_0 \tau} \sin^2\left(\frac{2\beta}{\omega} (\sin(\omega \tau) - \sin(\omega t))\right) & -\frac{1}{2}\omega_0 e^{\frac{1}{2}i\omega_0 \tau} \sin\left(\frac{4\beta}{\omega} (\sin(\omega \tau) - \sin(\omega t))\right) \\ \frac{1}{2}\omega_0 e^{-\frac{1}{2}i\omega_0 \tau} \sin\left(\frac{4\beta}{\omega} (\sin(\omega \tau) - \sin(\omega t))\right) & -i\omega_0 e^{\frac{1}{2}i\omega_0 \tau} \sin^2\left(\frac{2\beta}{\omega} (\sin(\omega \tau) - \sin(\omega t))\right) \end{pmatrix} d\tau.$$

The integrals in  $U^{(acc,0)}(t)$  have no closed form as revealed by standard expansions over Bessel functions, e.g.

$$\sin(\alpha + z \sin(\phi)) = \sin(\alpha) \left( J_0(z) + 2 \sum_{n=1}^{\infty} J_{2n}(z) \cos(2n\phi) \right) + 2 \cos(\alpha) \sum_{n=0}^{\infty} J_{2n+1}(z) \sin((2n+1)\phi).$$

All physical quantities of interest are now accessible, for example, the return probability to the  $|\uparrow\rangle$  state is found to be

$$P_{\uparrow \rightarrow \uparrow}^{(acc,0)}(t) = \left| \cos\left(\frac{2\beta}{\omega} \sin(\omega t)\right) + e^{-\frac{1}{2}it\omega_0} - 1 + \int_0^t i\omega_0 e^{-\frac{1}{2}i\tau\omega_0} \sin^2\left(\frac{\beta}{\omega} (\sin(\omega \tau) - \sin(\omega t))\right) d\tau \right|^2, \quad (4.2.3)$$

This formula becomes exact when either  $\omega_0 \rightarrow 0$  or  $\beta \rightarrow 0$ , as expected from the acceleration procedure. In general, it provides excellent approximations when  $\beta/\omega_0$  is large, see Fig. (4.1 a, b, c). The time-average of the return probability is therefore found to be

$$\langle P_{\uparrow \rightarrow \uparrow}^{(acc,0)}(t) \rangle_t = \frac{1}{2} \left( 1 + J_0\left(\frac{4\beta}{\omega}\right) \right), \quad (4.2.4)$$

which is exactly 1/2 on CDT resonances where  $J_0(4\beta/\omega) = 0$ , consistent with the understanding of CDT offered by Floquet analysis. To be more precise let us study CDT directly by considering the states  $|\psi_{\pm}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm |\downarrow\rangle)$ .

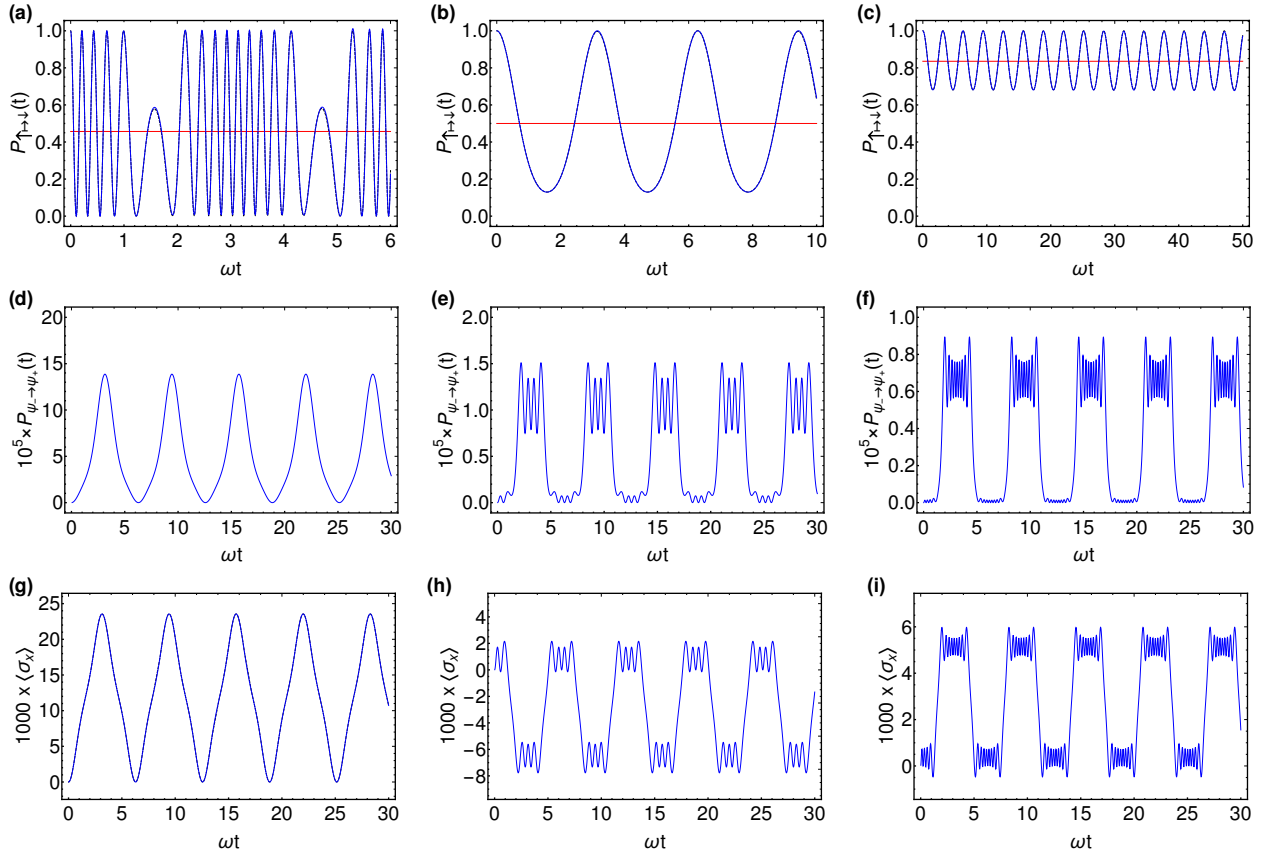


Figure 4.1: **Coherent destruction of tunneling:** Top line, return probability  $P_{\uparrow\rightarrow\uparrow}(t)$  in the ultra-strong coupling regime  $\beta/\omega_0 = 30$  for (a)  $\omega = 4\omega_0$ ; (b)  $\omega = 20\omega_0$ ; and (c)  $\omega = 100\omega_0$ . Shown here are  $P_{\uparrow\rightarrow\uparrow}(t)$  as given by Eq. (4.2.3) (solid blue line), the numerical solution (dashed black line), and its predicted time-average Eq. (4.2.4) (solid red straight line, indistinguishable from the numerically computed time-average). Middle line: transition probability  $P_{\psi_- \rightarrow \psi_+}(t)$  for a system starting in the  $|\psi_- \rangle$  state at  $t = 0$  with: (d)  $4\beta/\omega = 2.404\dots$ , first zero of  $J_0(4\beta/\omega)$ ; (e)  $4\beta/\omega = 11.79\dots$ , fourth zero of  $J_0(4\beta/\omega)$ ; and (f)  $4\beta/\omega = 27.49\dots$ , ninth zero of  $J_0(4\beta/\omega)$ . Note the changes of scales. Shown here are the formula of Eq. (4.2.5) (solid blue line) and the numerical solution (dashed black line), these two being completely indistinguishable. Bottom line: far off-resonance  $\omega = 100\omega_0$  expectation value of  $\sigma_x$  for a system starting in the  $|\uparrow \rangle$  state at  $t = 0$  with: (g)  $4\beta/\omega = 2.404\dots$ , first zero of  $J_0(4\beta/\omega)$ ; (h)  $4\beta/\omega = 11.79\dots$ , fourth zero of  $J_0(4\beta/\omega)$ ; and (i)  $4\beta/\omega = 27.49\dots$ , ninth zero of  $J_0(4\beta/\omega)$ . Note the changes of scales in  $\langle \sigma_x \rangle$ . Shown here are the formula of Eq. (4.2.6) (solid blue line) and the numerical solution (dashed black line), these two being indistinguishable.

The probability of transition between these states, denoted  $P_{\psi_- \rightarrow \psi_+}(t)$ , is found from  $U^{(acc,0)}(t)$  in the situation where  $\omega_0 \ll (\beta/\omega)^{1/2}$ , as

$$P_{\psi_- \rightarrow \psi_+}^{(acc,0)}(t) = \frac{\omega_0^2}{4} \left( \int_0^t \sin\left(\frac{4\beta}{\omega}(\sin(\omega t) - \sin(\omega \tau))\right) d\tau \right)^2 + \frac{\omega_0^2}{4} \left( \int_0^t \cos\left(\frac{4\beta}{\omega}(\sin(\omega t) - \sin(\omega \tau))\right) d\tau \right)^2. \quad (4.2.5)$$

This expression *flawlessly* reproduces the numerical solution in its finest details, details which had hitherto not been captured with such accuracy [126]. Minimizing the time-average of this formula confirms that the CDT condition is exactly  $J_0(4\beta/\omega) = 0$ , i.e. this is not changed by the non-perturbative corrections. Mathematically, the reason for this is simple: the  $J_0$  function is quadratically dominant over the other terms of the Bessel-series expansion of Eq. (4.2.5) because it stems from the sole term of that expansion which does not depend on  $\tau$  in both integrals.

While these results are as expected from the standard theory of CDT, it is not so for all physical quantities. Consider for example, the expectation value of the observable  $\sigma_x$  for a system initially prepared in the  $|\uparrow \rangle$  state. As observed by [191],  $\langle \sigma_x \rangle$  presents anomalous fluctuations on CDT resonances, a fact that was interpreted as a hallmark of and resulting from a crossing Floquet states. This interpretation is in fact not correct. Indeed,

at order 0 of the accelerated expansion of the path-sum solution we get,

$$\begin{aligned} \langle \sigma_x \rangle^{(acc,0)} &= \omega_0 \int_0^t \cos\left(\frac{1}{2}\omega_0\tau\right) \sin\left(\frac{2\beta}{\omega} \sin(\omega\tau)\right) d\tau \\ &\quad + 2\omega_0 \sin\left(\frac{1}{4}\omega_0 t\right) \int_0^t \sin\left(\frac{1}{4}\omega_0(t-2\tau)\right) \sin\left(\frac{2\beta}{\omega}(\sin(\omega t) - \sin(\omega\tau))\right) d\tau. \end{aligned}$$

In the regime  $\omega_0 \ll \omega$ , both  $\cos(\omega_0 t/2)$  and  $\sin(\omega_0 t/4)$  are essentially equal to their initial  $t = 0$  values, leading to the simpler

$$\langle \sigma_x \rangle^{(acc,0)} = \omega_0 \int_0^t \sin\left(\frac{4\beta}{\omega} \sin(\omega\tau)\right) d\tau. \quad (4.2.6)$$

This simple expression fits once again absolutely flawlessly with the numerically computed expectation  $\langle \sigma_x \rangle$ , see Fig. (4.1 d, e, f). Now evaluating the integral remaining in Eq. (4.2.6) via Bessel functions shows that the time average of  $\langle \sigma_x \rangle$  is

$$\langle \langle \sigma_x \rangle^{(acc,0)} \rangle_t = \frac{2\omega_0}{\omega} \sum_{n=0}^{\infty} J_{2n+1}\left(\frac{4\beta}{\omega}\right) \frac{1}{2n+1},$$

whose extrema are reached whenever

$$1 - \frac{\pi}{2} H_1\left(\frac{4\beta}{\omega}\right) = 0, \quad (4.2.7)$$

with  $H_1(\cdot)$  the first Struve function. Remarkably, the difference  $\Delta_n$  between the location of the  $n$ th zero of  $J_0(\cdot)$  and of the  $n$ th zero of Eq. (4.2.7) tends asymptotically to 0 as  $\Delta_n \sim 1/(2\pi n)$  for  $n \gg 1$ . This asymptotics develops quite quickly: while  $\Delta_1 \simeq 0.4$ , already  $\Delta_2 \simeq 0.03$ . The fact that the anomalous fluctuations in the expectation value of  $\sigma_x$  peak at the zeroes of Eq. (4.2.7) rather than on CDT resonances is confirmed by the numerical simulations. This analysis indicates that while  $\langle \sigma_x \rangle$  does indeed seem to fluctuate the most on CDT resonances, it is in fact not true and the phenomenon driving these fluctuations is subtly different from that behind CDT.

These results demonstrate the power of various expansions of the path-sum solution, enabling very precise and hitherto unequaled analytical analysis of subtle phenomena, e.g.  $P_{\psi_- \rightarrow \psi_+}(t)$  is on the order of  $10^{-5}$  on CDT resonances and reproduced exactly by the formulae provided. This is not because of special features of the Bloch-Siegert Hamiltonian. Rather, the path-sum approach and acceleration of  $\star$ -Neumann series are both generally valid as shown on p. 34. In particular the same treatment is valid for dissipative non-Hermitian operators.

### 4.3 Representation of Heun functions

Heun differential equations are the most general second order Fuchsian equations with four regular singularities. Series representations for the Heun functions have finite radiuses of convergence causing difficulties notably for black hole perturbation theory [135], where conditions at the black hole horizon ( $z = 1$ ) cannot easily be inferred from Earth-bound observations ( $z = +\infty$ ). These issues were noted in the recent review [97] on Heun's functions and are well-understood mathematically to be inherently tied with the use of series representations. This has been clearly identified as a major obstacle when extracting physical meaning in areas of black holes astrophysics [97], yet remains unaddressed in the mathematical literature. The quest for an unconditionally-convergent representation has led physicists to seek integral transformations relating Heun functions with other functions, all of which are transcendent. In spite of these efforts, [97] observes that: “*No example has been given of a solution of Heun's equation expressed in the form of a definite integral or contour integral involving only functions which are, in some sense, simpler.[...] This statement does not exclude the possibility of having an infinite series of integrals with 'simpler' integrands*”.

Thanks to the path-sum theorem and  $\star$ -algebra, we provide such elementary integral representations of the solutions of all equations of the Heun class: general, confluent, bi-confluent, doubly-confluent and triconfluent. For brevity's sake we here only state the results in the general Heun function case. Our results lead to the first representation of the solution to the Teukolsky radial equation<sup>5</sup> governing the metric perturbations of rotating black holes that is convergent everywhere from the black hole horizon up to spatial infinity.

<sup>5</sup>The Teukolsky Equation [189] is a gauge invariant equation that governs the curvature perturbations of the Kerr black hole [147].

## Heun's equation

In its canonical form, the General Heun Equation (GHE) is given as follows:

$$\frac{d^2 y(z)}{dz^2} + \left[ \frac{\gamma}{z} + \frac{\delta}{z-1} + \frac{\epsilon}{z-t} \right] \frac{dy(z)}{dz} + \frac{\alpha\beta z - q}{z(z-1)(z-t)} y(z) = 0. \quad (4.3.1)$$

In this equation,  $q \in \mathbb{C}$  while the other parameters satisfy the Fuch's condition:  $1 + \alpha + \beta = \gamma + \delta + \epsilon$ . The GHE has four singular points at  $z = 0, 1, t, \infty$ . Concerning its solutions, Maier—completing a task initiated by Heun [96] himself—has shown that there are 192 solutions that can be generated using the symmetries of  $D_4$  [131]. For specific parameter values the GHE reduces to other well-known equations of importance: e.g. setting  $\epsilon = 0, \gamma = \delta = 1/2$  yields the Mathieu equation [42].

In order to produce an integral representation for Heun's functions, remark that the GHE (and, in fact, all other Heun equations) take the form

$$y''(z) - B_1(z)y'(z) - B_2(z)y(z) = 0, \quad (4.3.2)$$

We may thus focus on obtaining the integral representation of the solution of the above equation in terms of integrals involving  $B_1$  and  $B_2$ . To this end, remark that we may transform the ODE Eq. (4.3.2) into a matrix equation:

**Proposition 4.3.1.** *Let  $y(z)$  be a solution of Eq. (4.3.2) with initial conditions  $y(z_0) = y_0$  and  $y'(z_0) = y'_0$ . Let*

$$\mathbf{M}(z) = \begin{pmatrix} 1 & 1 \\ B_1(z) + B_2(z) - 1 & B_1(z) - 1 \end{pmatrix}, \quad (4.3.3)$$

and let  $\mathbf{U}(z, z_0) := \mathcal{P}e^{\int_{z_0}^z \mathbf{M}(\zeta) d\zeta}$  be the path-ordered exponential of  $\mathbf{M}$ , that is the solution of  $\dot{\mathbf{U}}(z, z_0) = \mathbf{M}(z)\mathbf{U}(z, z_0)$ . Then

$$y(z) = y_0 \mathbf{U}_{11}(z, z_0) + (y'_0 - y_0) \mathbf{U}_{12}(z, z_0).$$

Hence the problem of determining any Heun function is equivalent with that of determining the path-ordered exponential of a (rather simple) matrix. Using the results of Chapter 3 and the path-sum theorem, one gets as a consequence:

**Corollary 4.3.1.** *Let  $H_G(z)$  be solution of the General Heun Equation,*

$$\frac{d^2 H_G(z)}{dz^2} + \left[ \frac{\gamma}{z} + \frac{\delta}{z-1} + \frac{\epsilon}{z-t} \right] \frac{dH_G(z)}{dz} + \frac{\alpha\beta z - q}{z(z-1)(z-t)} H_G(z) = 0,$$

with initial conditions  $H_G(z_0) = H_0$  and  $\dot{H}_G(z_0) = H'_0$ , assuming that  $z_0 \in \mathbb{R}$  is not a singular point of  $H_G$ . Denote  $I$  the largest real interval that contains  $z_0$  and does not contain any singular point of  $H_G$ . Then, for any  $z \in I$ ,

$$H_G(z) = H_0 + H_0 \int_{z_0}^z G_1(\zeta, z_0) d\zeta + (H'_0 - H_0) \left( e^{z-z_0} - 1 + \int_{z_0}^z (e^{z-\zeta} - 1) G_2(\zeta, z_0) d\zeta \right),$$

where  $G_i = (1_\star - \tilde{K}_i \Theta)^\star{}^{-1} = \sum_{n=1}^{\infty} \tilde{K}_i^{\star n} \Theta$  and

$$\begin{aligned} \tilde{K}_1(z, z_0) &:= 1 + e^{-z} \int_{z_0}^z \frac{\zeta_1^\gamma (\zeta_1 - 1)^\delta (t - \zeta_1)^\epsilon}{z^\gamma (z-1)^\delta (t-z)^\epsilon} e^{\zeta_1} \left( \frac{q - \alpha\beta\zeta_1}{(\zeta_1 - 1)\zeta_1(\zeta_1 - t)} - \frac{\epsilon}{t - \zeta_1} - \frac{\gamma}{\zeta_1} - \frac{\delta}{\zeta_1 - 1} - 1 \right) d\zeta_1, \\ \tilde{K}_2(z, z_0) &:= \left( \frac{q - \alpha\beta z}{(z-1)z(z-t)} - \frac{\epsilon}{t-z} - \frac{\gamma}{z} - \frac{\delta}{z-1} - 1 \right) e^{z-z_0} - \frac{q - \alpha\beta z}{(z-1)z(z-t)}. \end{aligned}$$

In particular both  $\tilde{K}_1$  and  $\tilde{K}_2$  are bounded over  $I$ , implying convergence of the  $\star$ -Neumann series for  $G_1$  and  $G_2$  for all  $z \in I$ .

**Example 4.3.1** (Elementary integral series converging to a general Heun function). In order to illustrate concretely the above corollary, consider the following General Heun equation (here with arbitrary parameters),

$$\frac{d^2 H_G(z)}{dz^2} + \left[ \frac{2}{z} + \frac{7}{z-1} + \frac{(-1)}{z-4} \right] \frac{dH_G(z)}{dz} + \frac{(3/2)z - 1}{z(z-1)(z-4)} H_G(z) = 0, \quad (4.3.4)$$

with initial conditions  $H_G(6) = H'_G(6) = 1$ . Here, the largest real interval containing 6 and none of the singular points 0, 1 and  $t = 4$  is  $I = ]4, +\infty[$ . Thus Corollary 4.3.1 indicates that for any  $z \in ]4, +\infty[$ ,

$$H_G(z) = (\Theta \star G_1)(z, z_0) = 1 + \int_{z_0}^z G_1(\zeta, z_0) d\zeta$$



with  $G_1 = (1_\star - \tilde{K}_1\Theta)^{\star-1}$  and the kernel  $\tilde{K}_1$  given by

$$\tilde{K}_1(z, z_0) = 1 - e^{-z} \frac{(z-4)}{z^2(z-1)^7} \int_{z_0}^z e^{\zeta_1} \frac{\zeta_1(\zeta_1-1)^6}{2(\zeta_1-4)^2} (2\zeta_1^3 + 10\zeta_1^2 - 67\zeta_1 + 14) d\zeta_1.$$

All the other types of Heun functions are treated similarly [75]. Of particular importance is the solution of the Confluent Heun equation which is that modelling the event horizon of a Kerr black-hole. Since the singular points of this equation are located at  $z = 0, 1, +\infty$ , given any initial conditions for  $H(z_0)$  and  $\dot{H}(z_0)$  at  $z_0 \in ]1, +\infty[$ , the  $\star$ -Neumann series representation for the confluent Heun function resulting from the path-sum theorem is guaranteed to converge on the entire domain  $]1, +\infty[$ , that is from the black hole horizon up to spatial infinity. This crucial property stands in stark contrast with the hypergeometric and Coulomb series, which converge close to 1 and to  $+\infty$ , respectively. Algorithmic implementations of the novel representations of the Heun function reported are discussed in [20].

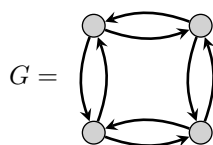
## **Part 2: Extending number theory to walks on graphs**

## Chapter 5

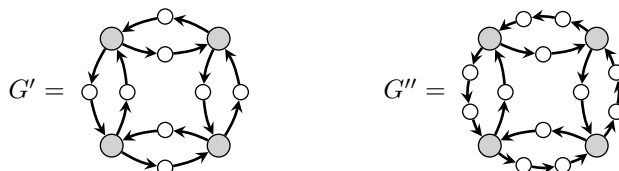
# Walk theory: combinatorics on hike monoids

### 5.1 On the necessity of a theory of walks

The precise nature of the relation between graphs and their walks has, to the best of our knowledge, not yet been thoroughly scrutinised. It seems to be often assumed that walks are slave objects to graphs, in that once the graph is specified its walks can be studied and, in principle, be perfectly known. As a corollary it is expected that properties of the graph leave indelible imprints on its walks, from which the former can thus be inferred. These simple arguments mask the subtle nature of the relation between walks and graphs. For example, consider the following bidirected, vertex-transitive, hence regular, bipartite graph



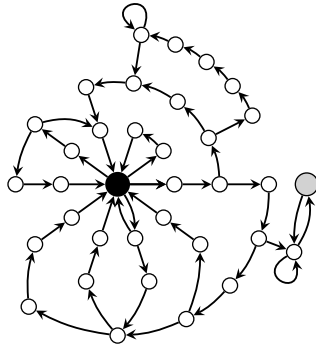
and let  $W_{G:\circ\rightarrow\circ'}$  be the set of all walks from any vertex  $\circ$  to any vertex  $\circ'$  on  $G$ . Now consider the following two digraphs



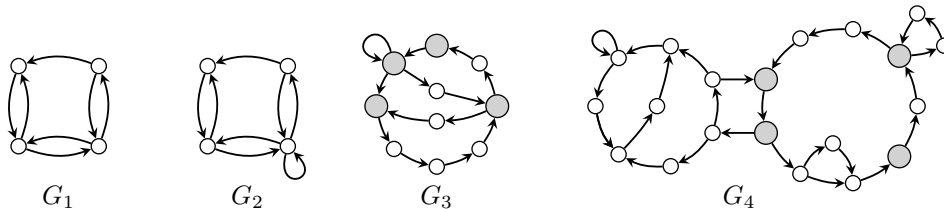
Remark that  $G'$  is directed and neither vertex-transitive nor regular. Yet, the set of all walks from any gray vertex to any gray vertex on  $G'$  is in bijection with the corresponding set  $W_{G:\circ\rightarrow\circ'}$  on  $G$ . The correspondence between both walk sets is simple: the white transient vertices of  $G'$  do not add any new cycle to the digraph as compared to  $G$  and so only cause the lengths of all of these walks to be multiplied by 2. The structure of every individual walk, i.e. the way it is composed of cycles and of at most one open simple path, is clearly preserved. Rigorously, this makes the bijection into an isomorphism between monoids on walks and walk-like objects, called hikes, something we discuss in details later. Similarly, sets of walks between gray vertices on  $G''$  are in bijection with the corresponding sets on  $G$ . In this case however the bijection does not act plainly on the length of individual walks but it continues to be a monoid isomorphism preserving the internal structure of walks. Remarkably here,  $G''$  is not even bipartite. That is, from the point of view of graph theory the transformations from  $G$  to  $G'$  and from  $G$  to  $G''$  are nontrivial and subtle. They correspond to the loss of respectively three and four fundamental graph properties namely bidirectedness, vertex-transitivity, regularity and bipartiteness. Yet walks sets are essentially unchanged by these alterations.

At the very least, these observations suggest a rather loose relationship between graph properties and walk properties. It raises the question of whether there are more graph transformations—excluding graph automorphisms—that preserve walk sets, and if so are they all somewhat trivial, as above with the addition of transient vertices? This question indirectly sprung up in the fields of applied network analysis and machine learning. For example it was noted that vertex centralities, mathematical quantities designed to grasp the relative importance of nodes in a graph, sometimes fail to do so meaningfully [169, 153]. They can for instance

predict that an outlying vertex is just as ‘central’ as another one which appears to be at the heart of a graph:



On this digraph with adjacency matrix  $A$ , the gray and black vertices are deemed to be equally central by the subgraph centrality measure  $(e^A)_\circ = (e^A)_\bullet$ , a widely used index of vertex importance in real-world networks [50]. Similarly, measures aimed at grasping the degree of “similarity” between networks are prone to failures. In the field of machine learning these measures, called graph-kernels, are used primarily for tasks of automatic graph classification. In particular it is known that walk-based graph-kernels suffer from the existence of differing graph structures with similar walk counts or arrangement of walks, hindering the automatic distinction of these graph structures, see e.g. [170, 130, 113] and references therein. To illustrate this observation, consider the following four directed graphs



While digraphs  $G_1$  and  $G_2$  might seem most similar with one another among all four, sets of walks between any pairs of gray vertices on graphs  $G_3$  and  $G_4$  are in bijection with sets of walks on  $G_1$ . As in the earlier example, this bijection preserves the structure of individual walks. At the opposite, there is no such correspondence between the set of all walks on graph  $G_2$  and those on  $G_1$ .

When questioned, these failures have at times been put down to the underlying non-rigorous notions of “importance of a node” and of “similarity between graphs” as we *intuitively* understand them. It is argued that such an understanding, imprecise and fraught with preconceptions, is difficult to express rigorously in mathematical terms thus leading to seemingly absurd results. But the failures could also run deeper and be yet more manifestations of the misappreciated mathematical relation between graphs and walks. Indeed almost all of the measures proposed so far for quantifying such notions as network centrality and graph similarity are algebraic quantities which translate into statements about closed walks. If indeed the cause of the problem is that graphs and their walks give relatively little or at least indirect information about one another, then this issue should be made mathematically rigorous. Considering in particular the case of closed walks on strongly connected digraphs, is perfect knowledge of the former sufficient to determine fundamental properties of the later, possibly up to some triviality?

We answer the preceding question in the negative: not only are there many transformations between strongly connected digraphs that profoundly alter their properties yet leave their sets of closed walks invariant, but these transformations are diverse and far from trivial. Some produce bijective mappings between walk sets that not only preserve their monoidal structure as in the above examples, but also the length of *all* closed walks. Algebraic quantities routinely used to characterise graphs are left invariant under such mappings. A complete classification of all walk-preserving graph transformations seems to be particularly arduous. The problem finds a wider context in the assertion that a digraph can be reconstructed based solely on structural information about its simple cycles, something which, we find, fails to hold in many a strange way. The complementary question, namely deciding whether a digraph exhibiting certain structural relations between simple cycles exists at all turns out to be unexpectedly difficult. We show at least that this question is decidable and give a meaning for and examples of algebraically closed sets of walks and walk-like objects that cannot, by themselves, be drawn on digraphs. In one more unexpected result we find that these ‘undrawable’ walks do exist on larger digraphs where they are accompanied by a host of algebraically unrelated walks.

In order to talk about closed walks and digraphs in a clearly separate manner so as to untangle their thorny relationship, it is necessary to have a mathematical language for describing sets of closed walks and walk-like objects independently from the digraphs that sustain them.

## 5.2 Hike monoids and number theory

Several schools of thoughts have emerged from the literature concerned such a task, aiming at studying walks as algebraic objects. Among the numerous structures proposed over the years are those based on walk concatenation such as the path-algebra [29] and later, nesting [76] or the cycle space [43]. A promising approach using the theory of partially commutative monoids (also called trace monoids), consists in viewing the arcs (i.e. the directed edges) of a graph as letters forming an alphabet and walks as words on this alphabet. A crucial idea in this approach, proposed by [32], is to define a specific commutation rule on the alphabet: two arcs commute if and only if they initiate from different vertices. This construction yields a semi-commutative monoid which allows for a great flexibility in the walk structure while preserving the ability to distinguish between different walks composed of the same arcs. A remarkable consequence of this construction is the existence of a stable subset of traces, formed by collections of cycles: the hikes. More specifically, hikes constitute a simplified trace monoid that carries most of the information pertaining to the graph structure and, in the case of undirected graphs, all the information. In this trace monoid, the simple cycles form the alphabet while the independence relation is characterised by vertex-disjointness.

Of fundamental importance for the trace monoid of hikes is the hitherto underappreciated prime-property satisfied by the simple cycles. Recall that an element of a monoid is prime if and only if, whenever it is factor of the product of two elements, then it is a factor of at least one of the two. The importance of the prime property lies in that because of it, the partially ordered set formed by the hikes ordered by divisibility is host to a plethora of algebraic relations in direct extension to number theory. This includes identities involving many more objects beyond the well-studied Möbius function [32, 173], such as the von Mangoldt and Liouville functions. In this respect hikes are natural objects to consider, as most of their algebraic properties follow from analytical transformations of the weighted adjacency matrix. The study of the algebraic structures associated with hikes is the main subject of the present work. These structures provide an extended semi-commutative framework to number theory from which both well-known and novel relations in general combinatorics are derived as particular consequences.

### Notations for graphs and walks

While we begin by recalling standard definitions for graphs, we introduce somewhat less common concepts for walks, of which we advise the reader to take special notice.

A *graph*  $G = (V, E)$  is a finite set of vertices  $V$  and a finite set  $E$  of distinct paired vertices, called edges or arcs, denoted  $\{i, j\}$ ,  $i, j \in V$ . A *digraph*  $G = (V, E)$  is a finite set of vertices  $V$  and a finite set  $E \subseteq V^2$  of *directed edges* (or *arcs*), denoted  $(i, j)$  for the arc from  $i$  to  $j$ . A *directed multigraph* (or *multidigraph*) is defined the same way as a digraph, except that  $E$  is a multiset. An edge of  $E$  is then denoted  $(i, j)_k$ , the integer  $k$  specifying which edge from  $i$  to  $j$  we consider. We denote by  $A_G$  or simply by  $A$  the adjacency matrix of  $G$  defined as  $A_{ij} := n$  with  $n \geq 0$  the number of directed edges  $(i, j)_k \in E$  from vertex  $i \in V$  to vertex  $j \in V$ .

The *labeled adjacency matrix*  $W = (w_{ij})_{i,j=1,\dots,N}$  of the graph  $G$  is built by attributing a formal variable  $w_{ij}$  to every pair  $(v_i, v_j) \in V^2$  and setting  $w_{ij} = 0$  whenever there is no arc from  $v_i$  to  $v_j$  in  $G$ . In the sequel, we identify each arc of a digraph  $G$  to the corresponding non-zero variable  $w_{ij}$ .

We say that  $G' = (V', E')$  is a *subgraph* of a multidigraph  $G$ , denoted by  $G' \subseteq G$ , if  $V' \subseteq V$  and  $E' \subseteq E$ . We say that  $G'$  is an *induced subgraph* of a digraph  $G$  if furthermore we have  $E' = V'^2 \cap E$ , that is  $G'$  is obtained from  $G$  by deleting some of its vertices and only the edges adjacent to them.

A *rooted walk*, or *rooted path*, of length  $\ell$  from vertex  $i$  to vertex  $j$  on a multi directed graph  $G$  is a contiguous sequence of  $\ell$  arcs starting from  $i$  and ending in  $j$ , e.g.  $w = (i, i_1)_{k_1} (i_1, i_2)_{k_2} \cdots (i_{\ell-1}, j)_{k_\ell}$  (a sequence of arcs is said to be contiguous if each arc but the first one starts where the previous ended). The rooted walk  $w$  is *open* if  $i \neq j$  and *closed* otherwise, in which case it is also called *rooted cycle*. A rooted cycle  $(i_0, i_1)_{k_1} (i_1, i_2)_{k_2} \cdots (i_{\ell-1}, i_0)_{k_\ell}$  of non-zero length for which all vertices  $i_t$  are distinct is said to be *simple* or *self-avoiding*. A self-loop  $(i, i)_k$  is considered a rooted simple cycle of length one. On digraphs we may also represent walks unambiguously as ordered sequences of vertices  $w = i, i_1, \dots, i_{\ell-1}, j$ .

Discarding the piece of information regarding the position of the root turns rooted simple cycles into *simple cycles*. An *induced cycle* is a simple cycle for which no pair of visited vertices is linked by an arc that does not belong to the cycle.

A *strongly connected component* of a digraph  $G$  is a maximal digraph  $G' \subseteq G$  such that for every pair of vertices  $v_1, v_2$  in  $G'$ , there is a rooted path in  $G'$  from  $v_1$  to  $v_2$ . A digraph  $G$  is then said to be *strongly connected* if it is its sole strongly connected component.

### Partially commutative structure on the arcs

Let  $\Sigma$  be an alphabet then its Kleene star  $\Sigma^*$  designates the set of all finite words on the letters of  $\Sigma$ . Now let  $\mathcal{I} \subseteq \Sigma^2$  be a set of pairs of letters. This set defines a rule, called independence relation, which affirms that pairs of letters in  $\mathcal{I}$  are independent and can be commuted when they occur next to each other in a word. Thus  $\mathcal{I}$  induces an equivalence relation  $\sim_{\mathcal{I}}$  between words  $w_1, w_2 \in \Sigma^*$  with  $w_1 \sim_{\mathcal{I}} w_2$  if and only if it is possible to pass from  $w_1$  to  $w_2$  by commuting adjacent pairs of independent letters. Then the *trace monoid*  $\mathcal{T} = \Sigma^*/\sim_{\mathcal{I}}$ , is the free partially commutative monoid formed by the  $\sim_{\mathcal{I}}$  equivalence classes on  $\Sigma^*$ . These classes are generically called *traces*. Different elements of an equivalence class, i.e. trace  $t \in \mathcal{T}$  will be referred to as *representations* of a trace.

At the heart of the trace monoid  $\mathcal{T}$  is the partially commutative structure induced by  $\mathcal{I}$ . This structure is best represented as a graph, called the *dependency graph*  $H$  of  $\mathcal{T}$ . It is the graph for which vertices represent all letters of the alphabet  $\Sigma$  and two vertices  $v_i$  and  $v_j$  are joined by an undirected edge if and only if letters  $i, j \in \Sigma$  are *not* allowed to commute per  $\mathcal{I}$ . Formally,  $H$  is the complement graph of  $(\Sigma, \mathcal{I})$ .

Trace monoids were introduced by Pierre Cartier and Dominique Foata in their quest for a purely combinatorial proof of MacMahon’s master theorem [32, 127]. They considered more specifically the trace monoid  $\mathcal{T}_{CF}$  on the alphabet of labeled directed edges  $\Sigma = E$  of a digraph  $G = (V, E)$  with independence relation

$$\mathcal{I}_{CF} := \{ \{(i, j), (k, l)\} : i \neq k \},$$

where  $(i, j) \in E$  and  $(k, l) \in E$  are arcs of  $G$ . This rule implies that two directed edges with different starting points are allowed to commute. For example, words  $(1, 2)(2, 3)(1, 4)$  and  $(2, 3)(1, 2)(1, 4)$  belong to the same Cartier-Foata trace, while  $(2, 3)(1, 4)(1, 2)$  belongs to a distinct trace due to the forbidden commutation of  $(1, 4)$  with  $(1, 2)$  required to pass from the former trace to the latter. The trace monoid  $\mathcal{T}_{CF}$  is sometimes called the *Cartier-Foata monoid*. In this monoid, a walk (that is a sequence of contiguous arcs) may have non-contiguous representations. For instance, the walk  $w_{12}w_{23}$  from  $v_1$  to  $v_3$  can be rewritten as  $w_{23}w_{12}$  since  $w_{23}$  and  $w_{12}$  start from different vertices. In fact, an open walk always has a unique contiguous representation, as any allowed permutations of arcs would break the contiguity. Surprisingly, the uniqueness of the contiguous representation no longer holds for closed walks. This consequence is an important feature of the partially commutative structure on the arcs: two closed walks starting from different vertices define the same object if they can be obtained from one another by permuting arcs with different starting points.

To illustrate this statement, consider the example pictured in Figure 5.1. The only closed walk starting from  $v_1$  that covers every arc exactly once is  $c_1 := w_{12}w_{23}w_{34}w_{45}w_{53}w_{31}$ . Since the only non-commuting arcs are  $w_{31}$  and  $w_{34}$ , the cycle can be rewritten as starting from  $v_3$  by  $c_1 = w_{34}w_{45}w_{53}w_{31}w_{12}w_{23}$ . On the other hand, there are two closed walks starting from  $v_3$  covering every arc once, one is  $c_1$  and the other is  $c_2 := w_{31}w_{12}w_{23}w_{34}w_{45}w_{53}$ . One cannot go from  $c_1$  to  $c_2$  without permuting  $w_{31}$  and  $w_{34}$ , thus  $c_1$  and  $c_2$  are different elements in  $\mathcal{T}_{CF}$ . Here,  $w_{12}w_{23}w_{31}$  and  $w_{31}w_{12}w_{23}$  are equivalent representations of the same cycle since the permutations of the arcs to go from one to the other are allowed. More generally, the starting vertex of a simple cycle never influences its value.

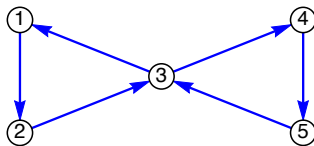


Figure 5.1: The closed walks  $c_1 = w_{34}w_{45}w_{53}w_{31}w_{12}w_{23}$  and  $c_2 = w_{31}w_{12}w_{23}w_{34}w_{45}w_{53}$  are different although composed of the same arcs. Both are achievable starting from  $v_3$  but only  $c_1$  is achievable from  $v_1$ .

### Multiplication and factorization of hikes

A closed walk can be characterised as a contiguous sequence of arcs comprising the same number of ingoing and outgoing arcs for each vertex. A hike is obtained upon relaxing the contiguity condition:

**Definition 5.2.1.** A hike is a trace  $h = w_{i_1 j_1} \cdots w_{i_\ell j_\ell} \in \mathcal{M}$  for which the numbers of outgoing and ingoing arcs for each vertex are equal. Formally, the indices  $i_k, j_k, k = 1, \dots, \ell$  of the arcs of  $h$  satisfy,

$$\forall i = 1, \dots, N, \quad \#\{k : i_k = i\} = \#\{k : j_k = i\}, \tag{5.2.1}$$

where  $\#$  stands for the cardinality.

**Remark.** Hikes have been studied in various forms in the literature. They originated under the name "circuits" in the seminal paper [32], written in french. We here use a different term to avoid confusion, as circuit may refer to other common objects in graph theory. Hikes can also be defined as the particular heaps of pieces formed from the simple cycles of the graph, see [196].

We denote by  $\mathcal{H}$  the set of hikes, which is a subset of  $\mathcal{T}_{\text{CF}}$ . By convention, the trivial walk 1 viewed as the empty sequence is considered to be a hike. We emphasise that, since hikes are elements of  $\mathcal{T}_{\text{CF}}$ , they obey the partially commutative structure on the arcs: two hikes  $h$  and  $h'$  are equal if, and only if,  $h'$  can be obtained from  $h$  by permuting arcs in  $h$  with different starting point. In particular, while every closed walk is a hike, a hike is a closed walk only if it has a contiguous representation. Moreover, we say that a hike is self-avoiding if all its arcs are different and commute.

The multiplication of two hikes  $h, h'$ , simply defined as the concatenation, yields a hike and shall be denoted by  $h.h'$  or simply  $hh'$  in the sequel. We define hike division as the reverse operation:  $d \in \mathcal{H}$  divides  $h \in \mathcal{H}$ , which we write  $d|h$ , if there exists  $h' \in \mathcal{H}$  such that  $h = d.h'$ . We shall use the standard division notation

$$h = d.h' \iff h' = \frac{h}{d}.$$

Here the choice of left-division, rather than right-division, is only a matter of convention. Remark that because the multiplication of hikes is not commutative,  $d|h$  does not necessarily imply that  $h/d$  divides  $h$ .

A main concern of this chapter is to treat the decomposition of a hike into simple cycles as a *prime decomposition*, seeing the simple cycles as prime factors. Rigorously, an element  $p$  of a monoid is prime if and only if, whenever  $p$  is a factor of  $a.b$ , then  $p$  is a factor of  $a$  or  $b$ . Thus, in this context, the primes are indeed given by the simple cycles. We emphasise that, because of the lack of commutativity, the prime factors of  $h$ , i.e. the elements of the prime decomposition, are different from its prime divisors.

An important consequence of the commutation rule on the arcs is that the prime decomposition  $h = c_1 \cdots c_k$  is unique up to permutations of consecutive vertex-disjoint simple cycles. Indeed, switching two different consecutive cycles in the prime decomposition  $h = c_1 \cdots c_k$  violates the commutation rule as soon as  $V(c_i) \cap V(c_{i+1}) \neq \emptyset$ . This property highlights that  $\mathcal{H}$  forms a sub-monoid of  $\mathcal{T}_{\text{CF}}$ , whose alphabet is the set of prime hikes (the simple cycles)  $\Sigma_{\mathcal{H}} := \{c_1, \dots, c_k\}$  and with independence relation defined by

$$I_{\mathcal{H}} = \{(c_i, c_j) : V(c_i) \cap V(c_j) = \emptyset\}. \quad (5.2.2)$$

A geometric interpretation of the prime decomposition can be found in Viennot's theory of *heaps of pieces* [196]. In this case, the simple cycles are pieces "piled up" in such a way that two simple cycles can only be put to the same level if they share no vertex in common. In fact, heaps of pieces provide a geometric construction for the Cartier-Foata clique decomposition of a trace.

**Definition 5.2.2.** The independence graph of  $\mathcal{H}$  is the undirected graph whose vertices are the simple cycles of  $G$  and with an edge between two simple cycles  $c, c' \in \Sigma_{\mathcal{H}}$  if they share no vertex in common. The *hike dependency graph* of a hike monoid is the complement of its independence graph.

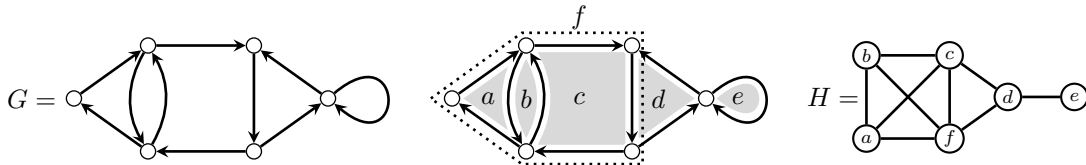


Figure 5.2: An example of a digraph  $G$  (left), the simple cycles on  $G$  (middle) and the corresponding hike dependency graph  $H$  (right).

A clique of the independence graph of  $\mathcal{H}$  can be identified with a product of pairwise non-intersecting simple cycles, that is, a self-avoiding hike. The Cartier-Foata clique decomposition of a hike  $h$  can then be built as follows.

- i) The maximal self-avoiding divisor of a hike  $h$  (i.e. the product  $s(h)$  of its prime divisors), is the first clique in the Cartier-Foata decomposition of  $h$ .
- ii) If  $h$  is self-avoiding, then  $s(h) = h$  and  $h$  is its own Cartier-Foata decomposition. All simple cycles composing  $h$  are vertex disjoint so that they can be put to the same level, forming a heap of height 1.
- iii) Otherwise, consider a collection of self-avoiding hikes  $s_k$ , initiated by  $s_1 = s(h)$ , and setting

$$s_{k+1} = s\left(\frac{h}{s_1 \cdots s_k}\right)$$

until all simple cycles of  $h$  are made part of a clique  $s_k$ . Each clique of the Cartier-Foata decomposition defines a layer in the heap of pieces.

We refer to [111] for a detailed explanation of the representation of heaps of pieces and its equivalence with Cartier-Foata monoids.

In the sequel,  $\ell(h)$  represents the length of a closed hike  $h$  while the number of elements in its prime-decomposition (counted with multiplicity) is denoted by  $\Omega(h)$ . By convention, the trivial hike 1 is not prime and thus  $\Omega(1) = 0$ .

## Hikes incidence algebra

The hikes ordered by division form a locally finite partially ordered set, or *poset*, which we denote  $P_G$ . The reduced incidence algebra on this poset is the set  $\mathcal{F}$  of real-valued functions on  $\mathcal{H}$  endowed with the Dirichlet convolution

$$f * g(h) := \sum_{d|h} f(d)g\left(\frac{h}{d}\right), \quad h \in \mathcal{H}.$$

Here, the sum is taken over all left-divisors  $d$  of  $h$ , including  $h$  itself and the trivial hike 1. One verifies easily that the Dirichlet convolution is associative and distributive over addition. However, it is not commutative since  $d$  can divide  $h$  without it being the case for  $h/d$ .

**Proposition 5.2.1.** *The reduced incidence algebra  $(\mathcal{F}, *)$  is isomorphic to the algebra of formal series*

$$\sum_{h \in \mathcal{H}} f(h)h, \quad f \in \mathcal{F}$$

*endowed with hike multiplication.*

Important functions of the reduced incidence algebra include the identity  $\delta(\cdot)$  equal to one for  $h = 1$  and zero otherwise, the constant function  $1(h) = 1$ ,  $\forall h \in \mathcal{H}$  or the Möbius function, the inverse of 1 through the Dirichlet convolution. We refer to [173] for a more comprehensive study. It is one of the main results of the present work that many more number-theoretic functions beyond 1 and  $\mu$  have generalised analogs in the reduced incidence algebra  $(\mathcal{F}, *)$  and that these analogs satisfy the same relations as their number-theoretic counterparts, see §5.3.

The next theorem gives the expression of the Möbius function on  $\mathcal{H}$ . This result is discussed in Remark 3.6 in [32].

**Proposition 5.2.2.** *The Möbius function on  $\mathcal{H}$  is given by*

$$\mu(h) := \begin{cases} 1 & \text{if } h = 1 \\ (-1)^{\Omega(h)} & \text{if } h \text{ is self-avoiding} \\ 0 & \text{otherwise.} \end{cases} \quad (5.2.3)$$

Proposition 5.2.2 confirms the characterization of  $\mathcal{H}$  as the trace monoid generated by the alphabet of simple cycles  $\Sigma_{\mathcal{H}} = \{c_1, \dots, c_k\}$  with independence relation defined in Equation (5.2.2) (see Eq. (56), Chapter 2.5 in [177]). The formal series associated to the Möbius function for  $\mathcal{H}$  then appears in the identity

$$\det(\text{Id} - W) = \sum_{h \in \mathcal{H}} \mu(h)h, \quad (5.2.4)$$

where we recall that  $W$  denotes the labelled adjacency matrix of  $G$ . A proof of this identity can be found in Theorem 1 of [163] on noting that for self-avoiding hikes, the concatenation of arcs coincides with the ordinary multiplication. Proposition 5.2.2 thus provides a determinant formula for the Möbius function of  $\mathcal{H}$  and the formal series associated to 1 (i.e. the analogue of the zeta function) is obtained via the formal inversion

$$\det(\text{Id} - W)^{-1} = \frac{1}{\sum_{h \in \mathcal{H}} \mu(h)h} = \sum_{h \in \mathcal{H}} h.$$

**Remark (Coprimalty).** The Möbius function is multiplicative on vertex-disjoint hikes,

$$V(h) \cap V(h') = \emptyset \implies \mu(hh') = \mu(h)\mu(h'). \quad (5.2.5)$$

This identity is reminiscent of the multiplicative property of the number-theoretic Möbius function  $\mu_{\mathbb{N}}$  for which  $\mu_{\mathbb{N}}(nm) = \mu_{\mathbb{N}}(n)\mu_{\mathbb{N}}(m)$  whenever  $n$  and  $m$  are coprime integers. The fact that (5.2.5) only holds for vertex-disjoint hikes suggests a more general notion of coprimality on  $\mathcal{H}$ : two hikes are coprime if they share no vertex in common. In particular, coprime hikes have different prime factors, but contrary to natural integers, this condition is in general not sufficient. The two notions of coprimality coincide on a class of graphs where  $\mu_{\mathbb{N}}$  is recovered from  $\mu$ , see §5.3.



### 5.3 Algebraic relations between hikes series

In this section we show that a plethora of number theoretic relations find natural extensions on the trace monoid of hikes. These provide powerful algebraic tools in a novel graph theoretic context and yield further insights into well established results. For example, we find in §5.3 that MacMahon's master theorem and the Dirichlet inverse of totally multiplicative functions over the integers both originate from the same general result about series of hikes. Throughout this section,  $G$  designates a digraph and  $P_G$  is the poset of hikes on  $G$  ordered by divisibility.

**Definition 5.3.1.** The formal series associated to a function  $f \in \mathcal{F}$  is defined as

$$\mathcal{S}f(s) := \sum_{h \in \mathcal{H}} e^{-s\ell(h)} f(h)h$$

for  $s$  a complex variable. The particular case  $f = 1$  is the zeta function  $\zeta(s) := \mathcal{S}1(s)$ .

Recall that because of the lack of commutativity between hikes, Dirichlet convolution typically acts non-commutatively on functions on hikes  $g * f \neq f * g$  and thus hike-series also multiply non-commutatively, i.e.  $\mathcal{S}f.\mathcal{S}g = \mathcal{S}(f * g) \neq \mathcal{S}g.\mathcal{S}f = \mathcal{S}(g * f)$ . For convenience, we write  $\mathcal{S}f/\mathcal{S}g$  for the *right* multiplication with the inverse:  $\mathcal{S}f/\mathcal{S}g = \mathcal{S}f.(\mathcal{S}g)^{-1}$ . We begin with two simple relations counting the left divisors and left prime divisors of a hike.

**Proposition 5.3.1.** *Let  $\tau(h)$  be the number of left divisors of  $h \in \mathcal{H}$ . Then  $\mathcal{S}\tau(s) = \zeta^2(s)$ . Let  $1_p$  be the indicator function on primes and  $\omega(h)$  the number of prime divisors of  $h$ . Then  $\mathcal{S}\omega(s) = \mathcal{S}1_p(s) \cdot \zeta(s)$ .*

The results follow immediately from combinatorial arguments on the reduced incidence algebra of  $P_G$ . The functions  $\Omega$  and  $\omega$  coincide over self-avoiding hikes, unlike their number theoretic counterparts for which  $\Omega(n) = \omega(n)$  if and only if  $n$  is a square-free integer. This is due to the stronger characterization of the coprimality for hikes, which requires that the prime factors be not only different but also vertex-disjoint. Indeed, if two different prime factors of a hike  $h$  do intersect, then at least one of them is not a left-divisor, resulting in  $\Omega(h)$  being greater than  $\omega(h)$ . The parallel with number theory is however accurate if all the simple cycles commute, in which case a prime factor is always a divisor.

#### Walk von Mangoldt function

We begin with a hike version of the number theoretic von Mangoldt function.

**Definition 5.3.2.** The walk von Mangoldt function  $\Lambda : \mathcal{H} \rightarrow \mathbb{N}$  is defined as the number of contiguous representations of a hike that is,  $\Lambda(h)$  is the number of possible contiguous rearrangements of the arcs in  $h$ , obtained without permuting two arcs with the same starting point.

By convention, we set  $\Lambda(1) = 0$ . Remark that by this definition,  $\Lambda(h) = 0$  whenever  $h$  is not a walk. Since different contiguous representations of the same walk start from different vertices, the series associated to  $\Lambda$  is obtained by

$$\mathcal{S}\Lambda(s) = \sum_{h \in \mathcal{H}} e^{-s\ell(h)} \Lambda(h)h = \text{Tr}(e^{-s}\mathbf{W} + e^{-2s}\mathbf{W}^2 + \dots) = \text{Tr}((\text{Id} - e^{-s}\mathbf{W})^{-1}) - N. \quad (5.3.1)$$

The heaps of pieces point of view provides a remarkable characterization of closed walks as heaps of cycles with a unique high-most element (such heaps are called pyramids). Using our terminology, this translates into a (non-trivial) closed walk being a hike with a unique prime right-divisor, whose length is precisely the von Mangoldt function. To go even further, Viennot remarked that each piece in a heap can be associated to the pyramid formed by the pieces below it, including itself, thus revealing the bijection existing between the pieces composing a heap and its sub-heaps containing only one maximal element (this fact is discussed in the proof of Proposition 6 in [196]). In the context of hikes, this signifies that the prime factors a hike  $h$  can be put in bijection with the non-trivial walks dividing it. In particular, summing the von Mangoldt function over all divisors of a hike  $h$  reduces to summing the length of its prime factors:

$$\forall h \in \mathcal{H}, \sum_{d|h} \Lambda(d) = \ell(h) \iff \Lambda * 1 = \ell \iff \Lambda = \ell * \mu.$$

This powerful observation yields the following result as an immediate consequence.

**Proposition 5.3.2.** *The von Mangoldt function is linked to the zeta function by the following relation*

$$s\Lambda(s) = \sum_{h \in \mathcal{H}} e^{-s\ell(h)} \Lambda(h)h = -\frac{\zeta'(s)}{\zeta(s)} \quad (5.3.2)$$

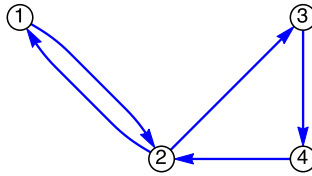
where  $\zeta'(s) := d\zeta(s)/ds = -\sum_{h \in \mathcal{H}} e^{-s\ell(h)} \ell(h)h$ .

Equation (5.3.2), which is none other than the series version of the identity  $\Lambda = \ell * \mu$ , coincides with the number theoretic formula of the von Mangoldt series obtained as the logarithmic derivative of the zeta function. The indefinite integral with respect to  $s$  yields the logarithmic identity,

$$\log \zeta(s) := \int \frac{\zeta'(s)}{\zeta(s)} ds = \sum_{h \in \mathcal{H}} e^{-s\ell(h)} \frac{\Lambda(h)}{\ell(h)} h, \quad (5.3.3)$$

also reminiscent of its number theoretic counterpart, with the length of a hike playing the role of the logarithm of an integer. Further analogies with number theory are discussed in Section 5.3.

**Example 5.3.1.** To illustrate the relation  $\Lambda = \ell * \mu$ , consider the following graph on 4 vertices:



Let  $p_1$  be the backtrack and  $p_2$  the triangle and let us calculate  $\Lambda(p_1 p_2)$  and  $\Lambda(p_2 p_1)$  from  $\ell * \mu$ . Since the left divisors of  $p_1 p_2$  are 1,  $p_1$  and  $p_1 p_2$ , we have

$$\Lambda(p_1 p_2) = \ell(1)\mu(p_1 p_2) + \ell(p_1)\mu(p_2) + \ell(p_1 p_2)\mu(1) = 0 \times 0 + 2 \times (-1) + 5 \times 1 = 3.$$

We proceed similarly for  $\Lambda(p_2 p_1)$ :

$$\Lambda(p_2 p_1) = \ell(1)\mu(p_2 p_1) + \ell(p_2)\mu(p_1) + \ell(p_2 p_1)\mu(1) = 0 \times 0 + 3 \times (-1) + 5 \times 1 = 2.$$

Let us now compare these results with a direct calculation of  $\Lambda$ , by way of counting all the contiguous sequences in the equivalence classes  $p_1 p_2$  and  $p_2 p_1$ . We find

$$\begin{aligned} w_{21}w_{12}w_{23}w_{34}w_{42} &\simeq p_1 p_2, & w_{12}w_{23}w_{34}w_{42}w_{21} &\simeq p_2 p_1, \\ w_{42}w_{21}w_{12}w_{23}w_{34} &\simeq p_1 p_2, & w_{23}w_{34}w_{42}w_{21}w_{12} &\simeq p_2 p_1, \\ w_{34}w_{42}w_{21}w_{12}w_{23} &\simeq p_1 p_2, \end{aligned}$$

This confirms that  $\Lambda(p_1 p_2) = 3$  and  $\Lambda(p_2 p_1) = 2$ , as expected.

## Totally additive functions on hikes

The von Mangoldt identity is a particular case of a more general result concerning totally additive functions over hikes. A function  $f : \mathcal{H} \rightarrow \mathbb{R}$  is said to be totally additive if

$$\forall h, h' \in \mathcal{H}, \quad f(h.h') = f(h) + f(h').$$

If the totally additive function  $f$  also respects the divisibility order, i.e.  $h \leq h' \Rightarrow f(h) \leq f(h')$ , then we say that  $f$  is a rank function.

**Proposition 5.3.3.** *Let  $f$  be a totally additive function over hikes, then*

$$f * \mu(h) = \begin{cases} f(c) & \text{if } h \text{ is a non-trivial walk, with } c \text{ its unique prime right-divisor,} \\ 0 & \text{otherwise.} \end{cases}$$

The proof of this result is similar to that effected in number-theory, relying on properties of Mbius inversion and the totally additive property, see [71]. Now the von Mangoldt identity can be obtained as an application of Proposition 5.3.3 to the length function  $\ell : \mathcal{H} \rightarrow \mathbb{N}$ , which is obviously totally additive. Another notable application concerns a relation between the prime factors counting function  $\Omega$  and the indicator function over walks.

**Corollary 5.3.1.** *For all  $h \in \mathcal{H}$ ,  $\Omega * \mu(h) = 1_w(h)$  where  $1_w$  is the indicator function over non-trivial walks.*

The proof is omitted as it is a direct application of Proposition 5.3.3 to the totally additive function  $\Omega$ . Alternatively, it follows from the fact that the number of prime factors of a hike  $h$  (counted with multiplicity) equals the numbers of non-trivial walks dividing it, i.e.  $\Omega = 1_w * 1$ .

Observe that a similar relation holds in number theory, namely that for  $n \in \mathbb{N}$ ,

$$\Omega_{\mathbb{N}} * \mu_{\mathbb{N}}(n) = \sum_{d|n} \Omega_{\mathbb{N}}(d) \mu_{\mathbb{N}}\left(\frac{n}{d}\right) = \begin{cases} 1 & \text{if } n = p^k \text{ with } p \text{ prime and } k \in \mathbb{N}, \\ 0 & \text{otherwise.} \end{cases}$$

Here,  $\Omega_{\mathbb{N}}(n)$  equals the number of prime factors (counted with multiplicity) of  $n \in \mathbb{N}$  and  $\mu_{\mathbb{N}}$  is the number theoretic Möbius function. This parallel indicates that powers of primes are in fact the “walks” of number theory, being the only numbers with a unique prime divisor, ergo a unique prime right-divisor.

### Totally multiplicative functions on hikes

A consequence of the Möbius inversion between  $\Lambda$  and  $\ell$ ,  $\Lambda = \ell * \mu$ , concerns totally multiplicative functions on hikes  $f \in \mathcal{F}$ . We say that  $f$  is totally multiplicative if

$$\forall h, h' \in \mathcal{H}, f(h.h') = f(h)f(h').$$

**Lemma 5.3.1.** *Let  $f$  be a totally multiplicative function. The inverse of  $f$  through the Dirichlet convolution is given by*

$$f^{-1} = \mu f : h \mapsto \mu(h)f(h), \quad h \in \mathcal{H}. \quad (5.3.4)$$

The proof is obtained by direct calculation. Lemma 5.3.1 is a semi-commutative extension of the number-theoretic result on the inverse of totally multiplicative functions,  $f^{-1}(n) = \mu_{\mathbb{N}}(n)f(n)$ ,  $n \geq 0$ , with  $\mu_{\mathbb{N}}$  the number-theoretic Möbius function, see below for a rigorous statement on the relation between both results. In a similar vein, the above Lemma leads to another result with a strong number-theoretic flavor:

**Corollary 5.3.2.** *Let  $f$  be a totally multiplicative function on hikes,  $F(s) = \mathcal{S}f(s)$  and  $F'(s) = dF(s)/ds$ . Then,*

$$\frac{F'(s)}{F(s)} = - \sum_{h \in \mathcal{H}} e^{-s\ell(h)} \Lambda(h) f(h) h.$$

An important extension to MacMahon’s master theorem stems from the formal series version of Lemma 5.3.1:

$$\mathcal{S}f(s) = \sum_{h \in \mathcal{H}} e^{-s\ell(h)} f(h) h = \frac{1}{\sum_{h \in \mathcal{H}} e^{-s\ell(h)} \mu(h) f(h) h}.$$

To see this, consider first a weighted version of the graph  $G$  where all arcs pointing to a vertex  $i$  are given a formal weight  $t_i$ . The weighted adjacency matrix of this weighted graph is  $\mathbf{TW}$ , with  $\mathbf{T}$  the diagonal matrix where  $\mathbf{T}_{ii} = t_i$ . Now observe that a totally multiplicative function on hikes is completely determined by its value on the primes (since  $f(hh') = f(h)f(h')$  regardless of the commutativity of  $h$  and  $h'$ ). We may therefore consider the totally multiplicative function which associates any prime  $p$  with its weight,

$$f(p) = \text{weight}(p) = t_{i_2} \cdots t_{i_{\ell(p)}} t_{i_1}. \quad (5.3.5)$$

where  $\{i_1, \dots, i_{\ell(p)}\}$  is the set of vertices visited by  $p$ . Then, Lemma 5.3.1 yields

$$\mathcal{S}f(0) = \sum_{h \in \mathcal{H}} f(h) h = \frac{1}{\sum_{h \in \mathcal{H}} \mu(h) f(h) h} = \frac{1}{\det(\mathbf{Id} - \mathbf{TW})}. \quad (5.3.6)$$

This is the non-commutative generalization of MacMahon’s theorem discovered by Cartier and Foata [32]. MacMahon’s original result [127] is then recovered upon replacing  $\mathbf{W}$  by the adjacency matrix  $\mathbf{A}$ , thus attributing the value 1 to every hike.

In general, totally multiplicative functions on hikes do not have to take on the extremely restricted form of Eq. (5.3.5). In these cases Lemma 5.3.1 goes beyond even the non-commutative generalization of MacMahon’s theorem. A striking example of this observation is given by the Liouville function. In number theory, this function is defined as  $\lambda(n) = (-1)^{\Omega(n)}$ , where we recall  $\Omega(n)$  is the number of prime factors of the positive integer  $n$ , counted with multiplicity. We define the walk Liouville function similarly.

**Definition 5.3.3.** The walk Liouville function  $\lambda(h) : \mathcal{H} \rightarrow \{-1, 1\}$  is defined by  $\lambda(h) := (-1)^{\Omega(h)}$ , where  $\Omega(h)$  is the number of prime factors of  $h$ , counted with multiplicity.

The series  $\mathcal{S}\lambda(s) := \sum_{h \in \mathcal{H}} e^{-s\ell(h)} \lambda(h)h$  associated to the walk Liouville function has a remarkably simple expression showing that calculating it is #P-complete on arbitrary graphs.

**Proposition 5.3.4.** *The formal series of the walk Liouville function  $\lambda$  satisfies*

$$\mathcal{S}\lambda(s) = \sum_{h \in \mathcal{H}} e^{-s\ell(h)} (-1)^{\Omega(h)} h = \frac{1}{\text{perm}(\text{Id} + e^{-s}\mathbf{W})},$$

where  $\text{perm}$  designates the permanent.

The permanent of  $\text{Id} + e^{-s}\mathbf{W}$  is the series associated to the indicator function on self-avoiding hikes, that is, the absolute value of  $\mu$ :

$$\text{perm}(\text{Id} + e^{-s}\mathbf{W}) = \sum_{h \in \mathcal{H}} e^{-s\ell(h)} |\mu(h)|h = \mathcal{S}|\mu|(s).$$

Hence, the walk Liouville function  $\lambda$  is the inverse of  $|\mu|$  through the Dirichlet convolution, similarly as its number theoretic counterpart.

## Relation to number theory

The unique factorization of hikes into products of hikes satisfying the prime property is reminiscent of the fundamental theorem of arithmetic. The difference between these two results stems from the non-commutativity of the product operation between hikes. Unsurprisingly then, on a graph where all prime cycles commute, the prime factorization of hikes identifies with that of the integers and the poset  $P_G$  becomes isomorphic to the poset of integers ordered by divisibility, which we denote  $P_{\mathbb{N}}$ .

**Theorem 5.3.1.** *Let  $G$  be an infinite directed graph formed by a countable union of vertex-disjoint oriented cycles. Then, the hike poset  $P_G$  is isomorphic to the poset  $P_{\mathbb{N}}$  of natural integers ordered by divisibility. In particular, the reduced incidence algebra of  $P_G$ ,  $(\mathcal{F}, *)$ , is isomorphic to the algebra of Dirichlet series equipped with ordinary multiplication.*

The theorem follows from the existence of a bijection between the simple cycles of  $G$  and a family of prime numbers. Then *all results* obtained earlier on hike series and their relations yield valid number theoretic results when applied to the infinite digraph  $G$  composed of a countable union of vertex-disjoint simple cycles. For example, on such digraph  $G$ :

- Two simple cycles are vertex-disjoint if, and only if, they are different. Thus, the Möbius function on  $\mathcal{H}$  coincides with the number theoretic Möbius function. More generally, the notion of co-primality which extends over hikes to vertex-disjointness is here equivalent to the usual definition of co-primality over  $\mathbb{N}$ .
- All prime factors of a hike are also divisors. It follows that  $\tau(h) := 1 * 1(h)$  and  $\omega(h) := 1_p * 1(h)$  (where  $1_p$  is the prime indicator function) give respectively the number of divisors and the number of prime factors of  $h$ , similarly as for the arithmetic versions of these functions.
- Closed walks take the form  $h = p^k$ , for  $p$  a prime hike (i.e. a simple cycle) and  $k \in \mathbb{N}$ . Thus, Definition 5.3.2 yields the von Mangoldt function

$$\Lambda(h) = \begin{cases} \ell(p), & \text{if } h = p^k, p \text{ prime} \\ 0, & \text{otherwise.} \end{cases}$$

This recovers the number-theoretic von Mangoldt function, provided we identify the length of a hike with the logarithm of an integer.

- More generally, Proposition 5.3.3 shows that, for any totally additive function  $f$ ,  $f * \mu$  has its support on non-trivial walks. On a digraph  $G$  where all primes commute, the walks are the powers of primes thus recovering the number theoretic version of the result: for all  $f : \mathcal{H} \rightarrow \mathbb{R}$  totally additive,

$$f * \mu(h) = \sum_{d|h} f(d) \mu\left(\frac{h}{d}\right) = \begin{cases} f(p) & \text{if } h = p^k, p \text{ prime} \\ 0 & \text{otherwise.} \end{cases}$$

# Chapter 6

## Number-theoretic sieves on hikes

The “widely open problem of counting Self-Avoiding Walks (SAWs) and Self-Avoiding Polygons (SAPs) on lattices” (quoting Flajolet & Sedgewick [55]) was first conceived from the study of polymer chemistry in 1947 [154]. Mathematically speaking, SAWs are walks that do not self-intersect, which mimic well actual polymer molecules. As the formal study of SAWs and their closed counterpart the SAPs started in earnest, it was quickly realised that self-avoiding objects arise in a wide range of physical and mathematical problems; e.g. as phase boundaries [186] and in percolation clusters [201, 120, 15] or, as B. Mandelbrot observed [134], from the outer frontier of Brownian motion [117]. Because in such models SAWs and SAPs are invariably realised through a random process, the problem of studying and counting them has so far only been attacked with tools from statistical physics and probability theory. Works along these directions have yielded deep insights into renormalisation and conformal mappings such as the relation between self-avoiding curves and the Schramm-Loewner Evolution (SLE) [118, 14], and the result of H. Duminil-Copin and S. Smirnov who proved the value of the connective constant of the honeycomb lattice [46]. One of the most active subfield of this research concerns loop-erased random walks (LERWs) [121, 119, 116], of which walk theory is the deterministic pendant.

We have seen in the preceding chapter that walks obey a semi-commutative extension of number theory where hikes extend the natural integers, self-avoiding hikes extend the square-free integers, walks extend prime powers, i.e. integers of the form  $p^k$  with  $p$  prime and  $k \in \mathbb{N}$  and finally simple paths and simple cycles extend the primes themselves. This last observation implies that in the framework of walk theory, *the extension of the Prime Number Theorem (PNT) describes the asymptotic growth of the number of SAPs on regular lattices* as their length goes to infinity. It therefore appears possible to work out an alternative deterministic approach to the 70-year old problem of SAP counting by using extending to a semi-commutative setting the number-theoretic tools originally developed for proving the PNT.

In this spirit, we use combinatorial sieves to prove an exact, explicit and compact formula for the asymptotic fraction of all closed walks on any finite or infinite vertex-transitive graph whose last erased loop is any chosen SAP. In stark contrast with approaches based on probability theory, we proceed via purely deterministic arguments relying on Viennot’s theory of heaps of pieces seen as a semi-commutative extension of number theory. Our approach sheds light on the origin of the discrepancies between exponents stemming from loop-erased walk and self-avoiding polygon models, and suggests a natural route to bridge the gap between both. Our results are illustrated by calculations on the infinite square lattice.

### 6.1 Asymptotic enumeration of walks by their last erased loop

The main result, which we prove in the remainder of this work is as follows:

**Infinite sieve theorem.** *Let  $G$  be an infinite vertex transitive graph of bounded degree  $\lambda$ . Let  $p$  be a self-avoiding polyong on  $G$ . Let  $\{G_N^{Tor}\}$  be a sequence of vertex-transitive graphs on  $N$  vertices converging to  $G$  as  $N \rightarrow \infty$ . Then the fraction of all hikes, i.e. heaps of cycles, which are closed walks whose last erased loop is  $p$  is given asymptotically for  $N \gg 1$  by*

$$\frac{\alpha^N F_p}{N \lambda^{\ell(p)}}.$$

*In this expression  $\alpha := \lim_{z \rightarrow 1/\lambda^-} \exp\left(\int \frac{1}{z}(R(z) - 1)dz\right)$ ,  $\alpha \in ]0, 1[$ , is well defined and  $F_p \lambda^{-\ell(p)}$  designates the fraction of all closed walks defined up to translation on  $G$  which are multiples of  $p$ . This fraction is explicitly given by*

$$\frac{F_p}{\lambda^{\ell(p)}} = \frac{1}{\lambda^{\ell(p)+1}} \deg^T \cdot \text{adj}\left(\text{Id} + C_G|_p \cdot B_p\right) \cdot \mathbf{1}, \quad (6.1.1)$$

*where  $\text{adj}(\cdot)$  designates the adjugate operator,  $B_p$  is the adjacency matrix of the graph  $G_p$  induced by  $p$  and its immediate neighbours on  $G$ ,  $\mathbf{1}$  designates the vector full of 1 and  $\deg = \text{diag}(B_p^2)$  is the vector of vertex-degrees*

on  $G_p$ . Finally,  $C_G|_p$  is the restriction to  $G_p$  of the matrix  $C_G := \lim_{z \rightarrow 1/\lambda^-} (\text{Id} - P_\lambda)R(z)$ , with  $P_\lambda$  the projector onto the eigenspace associated with the dominant eigenvalue.

Remarks and illustrations are in order before we sketch the proof of this theorem:

- The error terms generated by the sieve on infinite graphs are given in the full publication [61] and omitted here owing to length concerns.
- The lattice constant  $\alpha$  relates the *densities* of walks and of hikes on the infinite lattice  $G$ . On the square lattice,  $\alpha = \frac{1}{4}e^{\frac{4C}{\pi}} \simeq 0.8025\dots$  with  $C$  Catalan's constant.
- The matrix  $C_G$  is easy to obtain on regular graphs because its entries obey the same recursion relations as the graph resolvent. More precisely, let  $(C_G)_{m,n}$  designate the entry of the matrix corresponding to jumping from vertex  $m$  to vertex  $n$ . Then  $\lambda(C_G)_{m,n} = \sum_{i \in \mathcal{N}(n)} (C_G)_{m,i} + \sum_{j \in \mathcal{N}(m)} (C_G)_{j,n}$ , where  $\mathcal{N}(n)$  et  $\mathcal{N}(m)$  designate the set of vertices that are neighbours to  $n$  and  $m$  on  $G$ , respectively. On the square lattice this implies that  $C_G$  has the following explicit expression:

$$(C_G)_{ij} = -\frac{1}{\pi} \int_0^\infty \frac{1}{\tau} \left( 1 - \left( \frac{\tau - \mathbf{i}}{\tau + \mathbf{i}} \right)^{x_{ij} - y_{ij}} \left( \frac{\tau - 1}{\tau + 1} \right)^{x_{ij} + y_{ij}} \right) d\tau$$

where  $\mathbf{i}^2 = -1$ ,  $x_{ij}$  and  $y_{ij}$  are the distance along  $x$  and  $y$  between vertices  $i$  and  $j$  of  $G_p$ , respectively. In particular if  $x_{ij} = y_{ij} = m$  then

$$(C_G)_{ij} = -\frac{4}{\pi} \sum_{k=1}^{m-1} \frac{1}{2k+1} = -\frac{2}{\pi} \left( H_{m-\frac{1}{2}} + \log(4) \right),$$

with  $H_m$  the  $m$ th harmonic number. Explicit expressions for  $C_G$  have already been determined on many more lattices owing to its relation with lattice Green's functions and the resistor problem [9, 41].

Thanks to the last remark, the infinite sieve theorem gives the following corollary on the fraction of closed walk multiples of any SAP on certain vertex-transitive lattices:

**Corollary 6.1.1.** *Let  $G$  be an infinite vertex-transitive lattice of degree  $\lambda$ . Let  $p$  be a self-avoiding polygon on  $G$  and let  $F_p \lambda^{-\ell(p)}$  be the fraction of all closed walks which are walk multiples of  $p$ .*

- If  $G$  is a  $d$ -dimensional hypercubic lattice, then  $F_p \in \mathbb{Q}[1/\pi^{d-1}]$ .
- If  $G$  is the triangular, hexagonal or Kagomé lattice, then  $F_p \in \mathbb{Q}[\sqrt{3}/\pi]$ .

## Illustrations on the square lattice

We illustrate the infinite sieve theorem with a few examples on the square lattice.

- The fraction of closed walks which are multiples of a given edge  $e$  is

$$\frac{F_e}{4^2} = \frac{1}{8} = 0.125.$$

Since a point is connected to 4 edges, this means that 1/2 of all closed walks on the square lattice are multiples of an edge. In other terms, an edge is the last erased loop of 1/2 of all closed walks on the square lattice.

- The fraction of closed walks which are multiples of a  $1 \times 1$  square is

$$\frac{F_{1 \times 1}}{4^4} = \frac{128(\pi - 2)}{4^4 \pi^3} \simeq 0.0184. \quad (6.1.2)$$

See Fig. (6.1) for an illustration of the convergence of the fraction of closed walks on the infinite square lattice which are multiples of a  $1 \times 1$  square to the above number. Here the extension of Viennot's lemma to infinite graphs yields the ordinary generating function of closed walks multiple of a  $1 \times 1$  square as

$$\begin{aligned} R_{1 \times 1}(z) &= \frac{1}{256 \pi^4 z^4} \left( (16z^2 - 1) K(16z^2) + E(16z^2) \right)^2 \times \\ &\left( (1 - 16z^2) K(16z^2)^2 + 2K(16z^2) (8\pi z^2 - E(16z^2)) - 4\pi^2 z^2 + E(16z^2)^2 \right), \\ &= z^4 + 12z^6 + 144z^8 + 1804z^{10} + 23464z^{12} + \dots, \end{aligned} \quad (6.1.3)$$

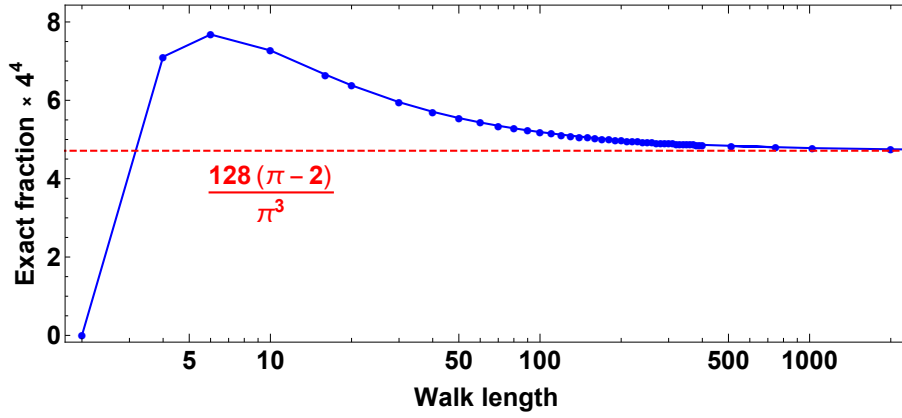


Figure 6.1: Exact fraction of closed walks of length  $\ell$  on the infinite square lattice which are multiples of a  $1 \times 1$  square as a function of the length of these walks. The exact fraction was obtained from the extension of Viennot's lemma to infinite graphs and Eq. (6.1.3). The exact fraction converges to its asymptotic value proportionally with the inverse of the walk length, as dictated by an analysis of the error terms associated with the infinite sieve theorem.

where  $K(x) := \int_0^{\pi/2} (1-x \sin^2(\theta))^{-1/2} d\theta$  and  $E(x) := \int_0^{\pi/2} (1-x \sin^2(\theta))^{1/2} d\theta$  are the complete elliptic integrals of the first and second kind, respectively. Here Eq. (6.1.2) establishes that asymptotically

$$R_{1 \times 1}(z)[2n] \sim \frac{128(\pi-2)}{4^4 \pi^3} \binom{2n}{n}^2, \text{ as } n \rightarrow \infty.$$

- The fraction of closed walks which are multiples of a  $1 \times 2$  rectangle is

$$\frac{F_{1 \times 2}}{4^6} = \frac{32(\pi-8)(\pi-4)(3\pi-8)(3\pi-4)}{4^6 \pi^4} \simeq 0.002585.$$

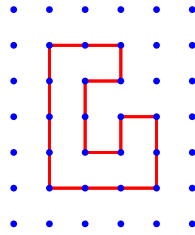
- The fraction of closed walks which are multiples of a  $1 \times 3$  rectangle is

$$\frac{F_{1 \times 3}}{4^8} = \frac{1024(16-3\pi)(64+3(\pi-12)\pi)(64+27(\pi-4)\pi)(128+\pi(27\pi-124))}{4^8 \times 81\pi^7} \simeq 0.00035499.$$

- The fraction of closed walks which are multiples of a  $2 \times 2$  square is

$$\frac{F_{2 \times 2}}{4^8} = \frac{32768(\pi-8)^2(\pi-4)(3\pi-8)^3(9\pi-32)}{4^8 \times 81\pi^7} \simeq 0.00044623.$$

- Consider the following SAP  $p$ :



Then the fraction of all closed walks which are multiples of this SAP is

$$\begin{aligned} \frac{F_p}{4^{18}} &= \frac{8388608}{4^{18} \times 8303765625 \pi^{12}} \left( 1721510367131231944781594624 \right. \\ &\quad - 6733029120634416611029155840\pi + 12001725045126647537146527744\pi^2 \\ &\quad - 12895675745638007921939841024\pi^3 + 9303982639359984674575220736\pi^4 \\ &\quad - 4748903115679537036020154368\pi^5 + 1758418560456019196044640256\pi^6 \\ &\quad - 475910723284488375970037760\pi^7 + 93430267561362281294131200\pi^8 \\ &\quad - 12973459941155225172708000\pi^9 + 1209211981439562793530000\pi^{10} \\ &\quad \left. - 67906363349663583525000\pi^{11} + 1736896666805181140625\pi^{12} \right), \\ &\simeq 7.7644 \times 10^{-9}. \end{aligned}$$

This result is well beyond what has been achievable when computing  $F_p$  from conformally invariant measures via Abelian sandpile models. Overall, thanks to computer codes by J. Fromentin we computed the fractions  $F_p/\lambda^{\ell(p)}$  for over 100,700,000 SAPs *analytically*, and for more than 3,480,000,000 SAPs numerically on the square lattice. Values of  $F_p$  of much longer SAPs are easily obtained numerically, costing no more than  $O(\ell(p)^3)$  to compute as outlined earlier. For example, the fraction of closed walks which are multiples of the  $70 \times 70$  square is

$$\frac{F_{70 \times 70}}{4^{280}} \simeq 1.5236 \times 10^{-108}. \quad (6.1.4)$$

Analytically speaking these fractions become very involved very quickly as a function of SAP length and there is no reason to believe that there exists a simpler expression for them than that given by Eq. (6.1.1) of the infinite sieve theorem. For example, the analytical expression for the fraction of closed walks which are multiples of the  $6 \times 6$  square already involves sums and products of up to 16-digits prime integers. In fully expanded form this fraction involves a 67-digits prime integer (!).

## 6.2 Proof of the infinite sieve theorem

### Asymptotic enumeration on finite graphs

We begin by wielding the sieving tools offered by number theory to asymptotically count hikes satisfying certain properties on finite graphs. The main results here will be the Finite Sieve Theorem and its length corollary. Before we state these results, there is an important precedent to be found in Viennot's work [195, 196], which provides the ordinary generating functions of hikes which are closed walk multiples of any chosen prime  $p$ , i.e. whose last erased loop is the SAP  $p$ . Since this result is conceptually important for the following we start with it:

**Viennot's lemma [196].** *Let  $G$  be a finite graph. Let  $p$  be a prime on this graph and let  $\Sigma_p := \sum_{w: p|_r w} w$  be the formal series of closed walks whose unique right prime divisor is  $p$ . Then*

$$\Sigma_p = \frac{\det(\text{Id} - W_{G \setminus p})}{\det(\text{Id} - W_G)} p.$$

where  $W_{G \setminus p}$  and  $W_G$  designate the labelled adjacency matrices of  $G \setminus p$  and  $G$ , respectively.

The semi-commutative extension of the Eratosthenes-Legendre sieve provides the asymptotic expansion of Viennot's result on  $\Sigma_p$ :

**Finite sieve theorem.** *Let  $G$  be a finite (weighted di)graph with adjacency matrix  $A$ . Let  $H$  be an induced subgraph of  $G$  and let  $\mathcal{P}_H$  be the set of primes on  $H$ . Let  $\rho : \mathcal{H} \mapsto \mathbb{R}$  be a rank function on hikes such that  $|\mathcal{H}_\rho| = \lambda^\rho f(\rho)$  with  $\lambda$  a real constant and  $f(\cdot)$  a bounded function such that  $\lim_{\rho \rightarrow \infty} f(\rho)$  exists. Then the number (weight)<sup>1</sup>  $S(\mathcal{H}_\rho, \mathcal{P}_H)$  of hikes of rank  $\rho$  which are not multiples of primes on  $H$  is asymptotically given by*

$$\frac{S(\mathcal{H}_\rho, \mathcal{P}_H)}{|\mathcal{H}_\rho|} \sim \sum_{d \in \mathcal{P}_H^{s,a}} \mu(d) \lambda^{-\rho(d)}, \quad \text{as } \rho \rightarrow \infty.$$

The finite sieve theorem's most important application here will be with the length rank-function and sieving subgraph  $H = G \setminus p$  for  $p$  a prime.

**Length corollary.** *Let  $G$  be a finite (weighted di)graph with adjacency matrix  $A$  and dominant eigenvalue  $\lambda$ , which we assume to be unique.<sup>2</sup> Let  $p$  be a simple cycle or a simple path on  $G$  of length  $\ell(p)$  and let  $S(\mathcal{H}_\ell, \mathcal{P}_{G \setminus p})$  be defined as in the finite sieve theorem. Then  $S(\mathcal{H}_\ell, \mathcal{P}_{G \setminus p})$  is equal to the number (weight) of closed walks of length  $\ell$  on  $G$  whose unique right prime divisor is  $p$  and is asymptotically given by*

$$\frac{S(\mathcal{H}_\ell, \mathcal{P}_{G \setminus p})}{|\mathcal{H}_\ell|} \sim \frac{1}{\lambda^{\ell(p)}} \det \left( \text{Id} - \frac{1}{\lambda} A_{G \setminus p} \right) \quad \text{as } \ell \rightarrow \infty.$$

Let  $\text{Err}(\mathcal{H}_\ell, \mathcal{P}_{G \setminus p})$  be the difference between the two terms above. Let  $f(\ell) := \zeta(z/\lambda)[\ell]$  be the coefficient of  $z^\ell$  in the expansion of  $\zeta(z/\lambda)$ . Then  $f$  is bounded,  $\lim_{\ell \rightarrow \infty} f(\ell)$  exists, and

$$\text{Err}(\mathcal{H}_\ell, \mathcal{P}_{G \setminus p}) = \frac{1}{\lambda^{\ell(p)}} \sum_{k \geq 0} \left( \frac{\nabla^k [f](\ell - \ell(p))}{f(\ell) \lambda^k k!} - \delta_{k,0} \right) \det^{(k)} \left( \text{Id} - \frac{1}{\lambda} A_{G \setminus p} \right).$$

with  $\delta_{k,0}$  the Kronecker delta. Here,  $\det^{(k)}(\text{Id} - \frac{1}{\lambda} A_{G \setminus p})$  stands for the  $k$ th derivative of  $\det(\text{Id} - z A_{G \setminus p})$  evaluated in  $z = 1/\lambda$ .

<sup>1</sup>The notation  $S(\mathcal{H}_\rho, \mathcal{P}_H)$  for this quantity is employed in keeping with conventions from sieve theory.

<sup>2</sup>The theorem extends if  $\lambda$  is not unique upon replacing  $\lambda^{-1}$  by  $\lambda^{-g}$  with  $g$  its multiplicity.



*Proof of the finite sieve theorem.* The proof relies on an inclusion-exclusion principle in the poset of the hikes ordered by right-divisibility. As such it is a limpid example of the usability of number-theoretic techniques in the context of hike monoids. For this reason we have kept most of the proof in this report.

Let  $\mathcal{P} \subsetneq \mathcal{H}$  be a set of primes and  $\mathcal{P}^{\text{s.a.}}$  the set of all self-avoiding hikes constructible from  $\mathcal{P}$ . Let  $S(\mathcal{H}_\rho, \mathcal{P})$  be the number (weight) of hikes in  $\mathcal{H}_\rho$  which are not right-divisible by any prime of  $\mathcal{P}$ . The inclusion-exclusion principle—here the extension to hikes of the sieve of Erathostenes–Legendre—yields

$$S(\mathcal{H}_\rho, \mathcal{P}) = \sum_{d \in \mathcal{P}^{\text{s.a.}}} \mu(d) |\mathcal{M}_d|,$$

with  $|\mathcal{M}_d|$  the number of multiples of  $d$  in  $\mathcal{H}_\rho$  and  $\mu(d)$  is the Möbius function on hikes.

In order to progress, we seek a multiplicative function  $\text{prob}(\cdot)$  such that  $|\mathcal{M}_d| = \text{prob}(d) |\mathcal{H}_\rho| + r(d)$ . In this expression,  $\text{prob}(d)$  approximates the probability that a hike taken uniformly at random in  $\mathcal{H}_\rho$  is right-divisible by  $d$ . If edge-weights are present, the hikes are not all uniformly probable but follow a distribution dependent on these weights. No knowledge of this distribution is required here. Similarly,  $m(d) = \text{prob}(d) |\mathcal{H}_\rho|$  is the expected number of multiples of  $d$  in  $\mathcal{H}_\rho$ . Finally,  $r(d)$  is the associated error term, arising from the fact that  $|\mathcal{M}_d|$  is not truly multiplicative. Supposing that we can identify the  $m(\cdot)$  function, we would obtain

$$S(\mathcal{H}_\rho, \mathcal{P}) = \sum_{d \in \mathcal{P}^{\text{s.a.}}} \mu(d) m(d) + \sum_{d \in \mathcal{P}^{\text{s.a.}}} \mu(d) r(d).$$

Contrary to number theory, the first term does not admit any simpler form without further assumptions on  $\mathcal{P}$ . This is because of the possible lack of commutativity between some elements of  $\mathcal{P}$ . We note however that since  $\mu(d)$  is non-zero if and only if  $d$  is self-avoiding, and since we have required that  $m(\cdot)$  be multiplicative,<sup>3</sup> then it follows that the first term is determined solely from the values of  $m(\cdot)$  over the primes of  $\mathcal{P}$ .

We therefore turn to determining  $m(p)$  for  $p$  prime. The set of left-multiples of  $p$  in  $\mathcal{H}$  is  $\mathcal{M}_p := \{hp, h \in \mathcal{H}\}$ , hence in bijection with the set  $\mathcal{H}$ . Thus, the number of left-multiples of  $p$  in  $\mathcal{H}_\rho$ , is exactly  $|\mathcal{H}_{\rho-\rho(p)}|$ . Then

$$\text{prob}(p) + \frac{r(p)}{|\mathcal{H}_\rho|} = \frac{|\mathcal{H}_{\rho-\rho(p)}|}{|\mathcal{H}_\rho|}.$$

Seeking the best possible probability function  $\text{prob}(\rho)$ , let us suppose that we can choose this function such that the error term of the above equation vanishes in the limit  $\rho \rightarrow \infty$ . If this is true, then we obtain

$$\text{prob}(\rho) = \lim_{\rho \rightarrow \infty} \frac{|\mathcal{H}_{\rho-\rho(p)}|}{|\mathcal{H}_\rho|}.$$

In order to progress, we have to make an important assumption regarding the cardinality of the set  $\mathcal{H}_\rho$ :

**Assumption 1.** There exists a scaling constant  $\lambda$  and bounded function  $f : \mathbb{R} \mapsto \mathbb{R}$  such that  $\lim_{\rho \rightarrow \infty} f(\rho)$  exists and for  $\rho \in \mathbb{N}^*$

$$|\mathcal{H}_\rho| = \lambda^\rho f(\rho).$$

In the case of the length function, this assumption is actually a proposition:

**Proposition 6.2.1.** *Let  $G$  be a finite (weighted di)graph with dominant eigenvalue  $\lambda$  of multiplicity  $g$ . Let  $\mathcal{H}_\ell := \{h \in \mathcal{H} : \ell(h) = \ell\}$  be set of all hikes on  $G$  of length  $\ell$ . Then, there exists a bounded function  $f : \mathbb{N} \mapsto \mathbb{R}$  such that  $\lim_{\ell \rightarrow \infty} f(\ell)$  exists and for  $\ell \in \mathbb{N}^*$  we have exactly*

$$|\mathcal{H}_\ell| = \lambda^{g\ell} f(\ell).$$

This follows from expanding the ordinary zeta function on hikes  $\zeta(z) = \det(\text{Id} - zA)^{-1}$  on the spectrum of  $G$ . Proceeding with Assumption 1. or Proposition 6.2.1, the existence of the limit for  $f$  gives

$$\text{prob}(p) = \lim_{\rho \rightarrow \infty} \frac{\lambda^{\rho-\rho(p)} f(\rho - \rho(p))}{\lambda^\rho f(\rho)} = \lambda^{-\rho(p)}.$$

The  $\text{prob}(\cdot)$  function is multiplicative over the primes as desired and yields  $m(p) = |\mathcal{H}_\rho| \lambda^{-\rho(p)}$ . The associated error term is

$$r(\rho) = |\mathcal{H}_{\rho-\rho(p)}| - |\mathcal{H}_\rho| \lambda^{-\rho(p)} = \lambda^{\rho-\rho(p)} \left( f(\rho - \rho(p)) - f(\rho) \right).$$

<sup>3</sup>But not necessarily totally multiplicative.

To establish the validity of these results, we need only verify that they are consistent with our initial supposition concerning the error term, namely that  $r(p)/|\mathcal{H}_\rho|$  vanishes in the limit  $\rho \rightarrow \infty$ . The existence of the limit of  $f$  implies  $\lim_{\rho \rightarrow \infty} |f(\rho - \rho(p)) - f(\rho)| = 0$  and therefore that

$$\lim_{\rho \rightarrow \infty} \frac{r(p)}{|\mathcal{H}_\rho|} = \lim_{\rho \rightarrow \infty} \lambda^{-\rho(p)} \left( f(\rho - \rho(p)) - f(\rho) \right) = 0,$$

as required.

We are now ready to proceed with general self-avoiding hikes. Let  $d = p_1 \cdots p_{\Omega(d)}$  be self-avoiding. Since  $m$  is multiplicative and the rank function is totally additive over  $\mathcal{H}$ ,  $m(d) = \prod_i m(p_i) = \lambda^{-\sum_i \rho(p_i)} = \lambda^{-\rho(d)}$ . The associated error term follows as

$$r(d) = |\mathcal{H}_{\rho-\rho(d)}| - |\mathcal{H}_\rho| \lambda^{-\rho(d)} = \lambda^{\rho-\rho(d)} (f(\rho - \rho(d)) - f(\rho)).$$

Inserting these forms for  $m(d)$  and  $r(d)$  in the sieve yields

$$S(\mathcal{H}_\ell, \mathcal{P}) = |\mathcal{H}_\rho| \sum_{d \in \mathcal{P}^{\text{s.a.}}} \mu(d) \lambda^{-\rho(d)} + \lambda^\rho \sum_{d \in \mathcal{P}^{\text{s.a.}}} \mu(d) \lambda^{-\rho(d)} (f(\rho - \rho(d)) - f(\rho)). \quad (6.2.1)$$

We can now progress much further on making an additional assumption concerning the nature of the prime set  $\mathcal{P}$ . We could consider two possibilities: i) that  $\mathcal{P}$  is the set of all primes on an induced subgraph  $H \prec G$ ; or ii) that  $\mathcal{P}$  is a cut-off set, e.g. one disposes of all the primes of length  $\ell(p) \leq L$ . Remarkably, in number theory, if i) is true then ii) is true as well, and the sieve benefits from the advantages of both situations. In general however, i) and ii) are not compatible and while ii) could be used to obtain direct estimates for the number of primes of any length, a problem of great interest, this actually makes the sieve NP-hard to implement. We therefore focus on the first situation.

Let  $H \prec G$  be an induced subgraph of the graph  $G$  and let that  $\mathcal{P} \equiv \mathcal{P}_H$  be the set of all primes (here simple cycles) on  $H$ . To conclude the proof we need only show that the error term of Eq. (6.2.1) is asymptotically dominated by the first term  $\sum_{d \in \mathcal{P}_H^{\text{s.a.}}} \mu(d) \lambda^{-\rho(d)}$ . To this end, we note that since  $H$  is finite<sup>4</sup>

$$\lambda^\rho \sum_{d \in \mathcal{P}_H^{\text{s.a.}}} \mu(d) \lambda^{-\rho(d)} (f(\rho - \rho(d)) - f(\rho)),$$

is a sum involving finitely many self-avoiding hikes  $d$ . In addition, given that  $\lim_{\rho \rightarrow \infty} f(\rho)$  exists (either by Assumption 1. or by Proposition 6.2.1 for the length rank function),  $\lim_{\rho \rightarrow \infty} f(\rho - \rho(d)) - f(\rho) = 0$  as long as  $\rho(d)$  is finite, which is guaranteed by the finiteness of  $H$ . We have consequently established that the error term comprises finitely many terms, each of which vanishes in the  $\rho \rightarrow \infty$  limit. As a corollary, the first term is asymptotically dominant:

$$\frac{S(\mathcal{H}_\rho, \mathcal{P}_H)}{|\mathcal{H}_\rho|} \sim \sum_{d \in \mathcal{P}_H^{\text{s.a.}}} \mu(d) \lambda^{-\rho(d)} \quad \text{as } \rho \rightarrow \infty,$$

where we assume that  $|\mathcal{H}_\rho| \neq 0$ .

We now turn to establishing the length corollary of the finite sieve theorem. We are specifically looking for the number of closed walks which are multiples of a prime  $p$ . To this end, we need only choose  $H$  correctly. Let  $h$  be a hike, for  $w = hp$  to be a walk of length  $\ell$ , then  $h$  must have length  $\ell - \ell(p)$  and be such that none of its right-prime divisor commutes with  $p$ . The sieve must thus eliminate all hikes  $h$  which are left-multiples of primes *commuting* with  $p$ . Observe that all such primes are on  $H = G \setminus p$ . Consequently the finite sieve theorem yields, for  $|\mathcal{H}_{\ell-\ell(p)}| \neq 0$ ,

$$\begin{aligned} S(\mathcal{H}_\ell, \mathcal{P}_{G \setminus p}) &= |\mathcal{H}_{\ell-\ell(p)}| \sum_{d \in \mathcal{P}^{\text{s.a.}}} \mu(d) \lambda^{-\ell(d)} \\ &+ \lambda^{\ell-\ell(p)} \sum_{d \in \mathcal{P}^{\text{s.a.}}} \mu(d) \lambda^{-\ell(d)} (f(\ell - \ell(p) - \ell(d)) - f(\ell - \ell(p))), \end{aligned}$$

where  $\lambda$  is now the graph dominant eigenvalue per Proposition 6.2.1. The asymptotically dominant term is a sum over all the self-avoiding hikes on  $G \setminus p$ , each with coefficient  $\mu(d) \lambda^{-\ell(d)}$  and is equal to  $\det(\text{Id} - \lambda^{-1} \mathbf{A}_{G \setminus p})$ . Since furthermore  $|\mathcal{H}_{\ell-\ell(p)}| = |\mathcal{H}_\ell| \lambda^{-\ell(p)} f(\ell - \ell(p)) / f(\ell)$ , we have asymptotically for  $\ell \gg 1$

$$\frac{S(\mathcal{H}_\ell, \mathcal{P}_{G \setminus p})}{|\mathcal{H}_\ell|} \sim \lambda^{-\ell(p)} \det \left( \text{Id} - \frac{1}{\lambda} \mathbf{A}_{G \setminus p} \right),$$

<sup>4</sup> $G$  is finite and so are all its induced subgraphs.

while the error terms is

$$\begin{aligned} \text{Err}(\mathcal{H}_\ell, \mathcal{P}_{G \setminus p}) &:= \frac{S(\mathcal{H}_\ell, \mathcal{P}_{G \setminus p})}{|\mathcal{H}_\ell|} - \lambda^{-\ell(p)} \det \left( \text{Id} - \frac{1}{\lambda} \mathbf{A}_{G \setminus p} \right), \\ &= \lambda^{-\ell(p)} (f(\ell - \ell(p)) / f(\ell) - 1) \det \left( \text{Id} - \frac{1}{\lambda} \mathbf{A}_{G \setminus p} \right) + \frac{\lambda^{-\ell(p)}}{f(\ell)} \sum_{d \in \mathcal{P}^{\text{s.a.}}} \mu(d) \lambda^{-\ell(d)} (f(\ell - \ell(p) - \ell(d)) - f(\ell - \ell(p))). \end{aligned}$$

The last line can be brought in determinantal form as well, since

$$\begin{aligned} \frac{\lambda^{-\ell(p)}}{f(\ell)} \sum_{d \in \mathcal{P}^{\text{s.a.}}} \mu(d) \lambda^{-\ell(d)} (f(\ell - \ell(p) - \ell(d)) - f(\ell - \ell(p))) &= \lambda^{-\ell(p)} \sum_{d \in \mathcal{P}_H^{\text{s.a.}}} \mu(d) \lambda^{-\ell(d)} \sum_{k \geq 1}^{\ell(d)} \frac{\nabla^k [f](\ell - \ell(p))}{f(\ell) k!} (\ell(d))_{(k)}, \\ &= \lambda^{-\ell(p)} \sum_{k \geq 1}^{\infty} \frac{\nabla^k [f](\ell - \ell(p))}{f(\ell) \lambda^k k!} \det^{(k)} \left( \text{Id} - \frac{1}{\lambda} \mathbf{A}_{G \setminus p} \right). \end{aligned}$$

Now setting  $k = 0$  in the above recovers  $\lambda^{-\ell(p)} (f(\ell - \ell(p)) / f(\ell) - 1) \det \left( \text{Id} - \frac{1}{\lambda} \mathbf{A}_{G \setminus p} \right)$  with the exception of the  $-1$  in the parenthesis, which can be introduced as  $-\delta_{k,0}$ . This establishes the finite sieve theorem and its length corollary.  $\square$

## Infinite graphs

We are now in position to sketch the proof of Theorem 6.1 for the fraction of walks that are multiple of any chosen self-avoiding polygon on any infinite vertex-transitive graph. The first difficulty in extending the finite sieve theorem to infinite graphs comes from the proliferation of hikes on such graphs: there are either exactly 0 or infinitely many hikes of any given length. Furthermore, the number of hikes increases uncontrollably with the length as there are also infinitely many more hikes of any length  $L' > L$  than of length  $L$ . These observations continue to be true even when hikes are considered up to translation. To make matters worse, the fraction of all hikes which are walks is exactly 0; and even with edge weights uniformly set to  $1/\lambda$ , the total weight carried by all walk multiples of any SAP  $p$  is still divergent. To resolve these serious difficulties requires us to separate the finite sieve results into two contributions, the first of which relates hikes to walks and the second relates closed walks to walks multiples of  $p$ . This second contribution must itself be dealt with carefully to cure divergences stemming from the non-meromorphic nature of the generating functions involved. We illustrate every step of the proof with explicit results on the square lattice.

Let us consider a sequence of finite graphs  $G_N^{\text{Tor}}$  converging to the desired lattice as  $N \rightarrow \infty$  (for an explicit construction of such a sequence and accompanying notions of convergence, see [61]). Fixing  $N$ , consider  $p$  a self-avoiding polygon on  $G_N^{\text{Tor}}$ . Then we can transform the asymptotic fraction of hikes of length  $\ell$  that are walks multiples of  $p$  as  $\ell \rightarrow \infty$  given by the finite sieve theorem into

$$\frac{S(\mathcal{H}_\ell, \mathcal{P}_{G_N^{\text{Tor}} \setminus p})}{|\mathcal{H}_\ell|} \sim \lambda^{-\ell(p)} \det \left( \text{Id} - \frac{1}{\lambda} \mathbf{A}_{G_N^{\text{Tor}} \setminus p} \right) = \lambda^{-\ell(p)} \lim_{z \rightarrow 1/\lambda^-} \zeta_N(z)^{-1} \det (\text{Id} + z \mathbf{R}_N(z) \mathbf{B}_{N,p}).$$

Here  $\mathbf{R}_N(z) := (\text{Id} - z \mathbf{A}_{G_N^{\text{Tor}}})^{-1}$  and  $\mathbf{B}_{N,p} := \mathbf{A}_{G_N^{\text{Tor}}} - \mathbf{A}_{G_N^{\text{Tor}} \setminus p}$ . Since  $\mathbf{B}_{N,p}$  is zero everywhere but on the few edges touching vertices of  $p$ , the determinant on the right-hand side is reducible to that of a finite matrix and thus will be well-defined under  $N \rightarrow \infty$ . This suggests a strategy consisting of proving separate convergence in  $z \rightarrow 1/\lambda^-$  of the two terms in the limit above. This naive strategy ultimately fails, but the procedure that works is best understood once the nature of this failure is made apparent and several results we will obtain along the way are necessary to implement the correct proof strategy. In this spirit, we pretend to follow the naive approach and thus first examine the behaviour of the limit  $\lim_{z \rightarrow \lambda^{-1}} \zeta_N(z)^{-1}$  asymptotically in  $N$ . We find [61],

**Lemma 6.2.1.** *Let  $\{G_N^{\text{Tor}}\}_{N \in \mathbb{N}}$  be a sequence of vertex-transitive graphs converging to the infinite bounded-degree vertex-transitive graph  $G$  with maximum eigenvalue  $\lambda$ . Let  $\zeta_N(z)$  be the zeta function of hikes on  $G_N^{\text{Tor}}$  and let  $R(z) = R(z)_{ii}$  be the ordinary generating function of closed walks on  $G$ . Then,*

$$\lim_{N \rightarrow \infty} \zeta_N(z)^{1/N} = \tilde{\zeta}(z) = \exp \left( \int \frac{1}{z} (R(z) - 1) dz \right). \quad (6.2.2)$$

Furthermore  $\alpha := \lim_{z \rightarrow 1/\lambda^-} \tilde{\zeta}^{-1}(z)$  is well defined.

All the coefficients  $\tilde{\zeta}(z)[n]$  are positive integers, while the coefficients  $\tilde{\zeta}^{-1}(z)[n]$  are integers. To see this, consider  $h$  a hike and let  $w_1, \dots, w_n$  be vertex-disjoint walks making up hike  $h$ , i.e.  $h = w_1 w_2 \dots w_n$  modulo

the fact that all these walk commute with one another. A *rooted hike*  $h_{\text{root}}$  is the object obtained from  $h$  on translating all walks  $w_i$  so that the origin lies on their unique right prime divisor but retaining the fact that they commute. Then  $\tilde{\zeta}(z)[n]$  counts the number of rooted hikes of length  $n$ ,  $\tilde{\zeta}(z)$  is the zeta function of rooted hikes, while  $\tilde{\mu}(z) := \tilde{\zeta}^{-1}(z)$  is the Möbius function on rooted hikes.

Lemma 6.2.1 implies that asymptotically, when  $N \gg 1$ ,  $\lim_{z \rightarrow 1/\lambda^-} \zeta_N(z)^{-1} \sim \alpha^N$  is well defined. We will see later on that  $\alpha^N$  relates the density of hikes to that of walks on an infinite graphs.

**Lemma 6.2.2.** *Let  $G$  be an infinite vertex-transitive graph of bounded degree. Let  $\{G_N^{\text{Tor}}\}_{N \in \mathbb{N}}$  be the small tori sequence of vertex-transitive graphs converging to  $G$ . Let  $\bullet$  be any vertex of  $G$ . Then the fraction  $F_\bullet$  of hikes which are closed walks from  $\bullet$  to itself is asymptotically given by  $F_\bullet \sim \alpha^N/N$ , as  $N \rightarrow \infty$ . In this expression  $\alpha$  is the constant defined in Lemma 6.2.1.*

The  $1/N$  factor in  $F_\bullet$  originates from that we have fixed the vertex  $\bullet$ . If instead we consider translation invariant quantities, i.e. we consider all closed walks irrespectively of their starting point, then the fraction of hikes which are closed walks is asymptotically  $\alpha^N$ ,  $N \gg 1$ . This important technical Lemma is proven on expanding the determinantal expression for  $F_\bullet$  as given by the finite sieve theorem perturbatively, developing  $A_G \setminus \bullet$  around  $A_G$ .

**Lemma 6.2.3.** *Let  $G$  be an infinite vertex-transitive graph of bounded-degree and let  $\lambda$  be the supremum of its spectrum. Let  $\{G_N^{\text{Tor}}\}_{N \in \mathbb{N}}$  be the small tori sequence of vertex-transitive graphs converging to  $G$ . Then the asymptotic fraction of closed walks which are walk multiples of  $p$  is well defined and given by*

$$\frac{F_p}{\lambda^{\ell(p)}} = \lim_{N \rightarrow \infty} \lim_{z \rightarrow 1/\lambda^-} z^{\ell(p)} \frac{\det(\text{Id} + zR_N(z)B_p)}{\det(\text{Id} + zR_N(z)B_\bullet)} = \frac{1}{\lambda^{\ell(p)+1}} \text{deg}^T \cdot \text{adj} \left( \text{Id} + C_G|_p \cdot B_p \right) \cdot \mathbf{1},$$

where  $C_G|_p$  is the restriction to  $G_p$  of  $C_G := \lim_{z \rightarrow 1/\lambda^-} (\text{Id} - P_\lambda)R(z)$ .

According to the finite sieve theorem, the asymptotic fraction of hikes which are closed walks multiples of  $p$  on  $G_N^{\text{Tor}}$  is  $\lim_{z \rightarrow 1/\lambda^-} z^{\ell(p)} \det(\text{Id} - zA_{G_N^{\text{Tor}} \setminus p})$ . Since all the limits taken here are finite and well defined (as everything takes place on  $G_N^{\text{Tor}}$ ), the asymptotic fraction of closed walks which are multiples of  $p$  on these finite graphs is

$$\begin{aligned} \frac{\lim_{z \rightarrow 1/\lambda^-} z^{\ell(p)} \det(\text{Id} - zA_{G_N^{\text{Tor}} \setminus p})}{\lim_{z \rightarrow 1/\lambda^-} z^0 \det(\text{Id} - zA_{G_N^{\text{Tor}} \setminus \bullet})} &= \lim_{z \rightarrow 1/\lambda^-} z^{\ell(p)} \frac{\zeta_N(z) \det(\text{Id} - zA_{G_N^{\text{Tor}} \setminus p})}{\zeta_N(z) \det(\text{Id} - zA_{G_N^{\text{Tor}} \setminus \bullet})}, \\ &= \lim_{z \rightarrow 1/\lambda^-} z^{\ell(p)} \frac{\det(\text{Id} + zR_N(z)B_p)}{\det(\text{Id} + zR_N(z)B_\bullet)}. \end{aligned}$$

We now turn to studying the behaviour of the right hand side as  $N \rightarrow \infty$ . To this end, we expand  $\text{Id} + zR_N(z)B_p$  around  $1/\lambda$  with  $z < 1/\lambda$ .

We need to distinguish behaviours based on the dimensionality  $d > 1$  of the lattice under study. We ignore the trivial 1D case (for which the only SAP is the edge, and the fraction of closed walk multiples of the left or right edge attached to any vertex is  $1/2$ ). On  $d > 1$  dimensional lattices we have,

$$\text{Id} + zR_N(z)B_p = C_N B_p - \frac{1}{\lambda\pi} P_{N,\lambda} B_p \text{Li}_{d/2}(1 - z\lambda) + O(1 - z\lambda), \quad (6.2.3)$$

with  $C_N := \lim_{z \rightarrow 1/\lambda^-} (\text{Id} - P_{N,\lambda})R_N(z)$  and  $\text{Li}_a(x) := \sum_{n>1} \frac{x^n}{n^a}$  is the  $a$ -polylogarithm function. Combinatorially, it arises here from summations over closed walks weighted by  $\lambda^{-\ell}$ , which leaves a residual total weight asymptotically given by  $\ell^{-d/2}$  for all closed walks of length  $\ell \gg 1$ . The generic nature of the behaviour exhibited by  $\text{Id} + zR_N(z)B_p$  is now readily apparent: 1) divergence occurs only on 2D lattices, where it is logarithmic; 2) it is the same for all SAPs; and 3) it is also the same for all closed walks (which are readily recovered upon taking  $p$  to be length 0, i.e.  $B_p \equiv B_\bullet$  is a corolla). Thanks to these observations, the determinant expansion at  $1/\lambda^-$  is

$$\begin{aligned} \det(\text{Id} + zR_N(z)B_p) &= \det \left( C_N B_p - \frac{1}{\lambda\pi} P_{N,\lambda} B_p \text{Li}_{d/2}(1 - z\lambda) + O(1 - z\lambda) \right), \\ &= -\frac{1}{\pi N} \text{Li}_{d/2}(1 - z\lambda) \frac{1}{\lambda} \text{deg}^T \cdot \text{adj}(\text{Id} + C_N \cdot B_p) \cdot \mathbf{1} + o(\text{Li}_{d/2}(1 - z\lambda)), \end{aligned}$$

where we used the matrix-determinant lemma and the QR decomposition

$$-\frac{1}{\lambda\pi} P_{N,\lambda} B_p = -\frac{1}{\pi N} \times \frac{1}{\lambda} \times \mathbf{1} \cdot \text{deg}^T.$$

This decomposition relies on the observation that  $P_{N,\lambda}$  is the projector onto  $\mathbf{1}$ , i.e. that all  $G_N^{\text{Tor}}$  are regular. We recall that in the above expression,  $\deg = B_p \cdot \mathbf{1} = \text{diag}(B_p^2)$  is the degree of vertices on  $G_p$ . Similarly, at  $1/\lambda^-$ ,

$$\det(\text{Id} + zR_N(z)B_\bullet) = -\frac{1}{\pi N} \text{Li}_{d/2}(1 - z\lambda) + o(\text{Li}_{d/2}(1 - z\lambda)),$$

and finally

$$z^{\ell(p)} \frac{\det(\text{Id} + zR_N(z)B_p)}{\det(\text{Id} + zR_N(z)B_\bullet)} = \frac{1}{\lambda^{\ell(p)+1}} \deg^T \cdot \text{adj}(\text{Id} + C_N \cdot B_p) \cdot \mathbf{1} + o(1),$$

which yields the result after taking the limits  $z \rightarrow 1/\lambda^-$  and  $N \rightarrow \infty$  now both clearly well-defined, even when  $d = 2$ . Combinatorially, the divergence curing on 2D lattices effected here comes from relating walk multiples of a SAP to all closed walks rather than directly to the hikes. The relation between closed walks and hikes is performed separately through Lemma 6.2.2.

### 6.3 Relation with the self-avoiding polygons counting problem

We recall that  $R(z)$  and  $R_p(z)$  are the ordinary generating functions of closed walks and of walk multiples of a SAP  $p$ , respectively. The research presented here suggests a natural strategy to tackle the open problem of asymptotically counting SAWs and SAPs. First, observe that we know the exact number  $R(z)[L]$  of closed walks of length  $L$  defined up to translation. Then, if we could determine the exact number  $R_p(z)[L]$  of closed walks of length exactly  $L$  that are multiples of a SAP  $p$ , it would be sufficient to sum this over all SAPs of length strictly less than  $L$  and subtract the result from  $R(z)[L]$  to determine the number  $\pi(L)$  of SAPs of length exactly  $L$ :

$$\pi(L) = R(z)[L] - \sum_{\substack{p: \text{SAP} \\ \ell(p) < L}} R_p(z)[L].$$

While such a precise count is not feasible in practice as  $L \rightarrow \infty$ , an asymptotic estimate of the number of walk multiples of SAPs may seem, at first, to be sufficient to gain an insight into the number of SAPs themselves. Following this idea, we would rather write

$$\frac{\pi(L)}{R(z)[L]} = 1 - \sum_{\substack{p: \text{SAP} \\ \ell(p) < L}} \frac{R_p(z)[L]}{R(z)[L]}. \quad (6.3.1)$$

and use  $R_p(z)[L]/R(z)[L] \sim F_p \lambda^{-\ell(p)}$  for  $L \gg 1$ . Thus, we would only need to estimate sums like

$$S(L) := \sum_{\substack{p: \text{SAP} \\ \ell(p) \leq L}} \frac{F_p}{\lambda^{\ell(p)}},$$

for  $L \gg 1$ , in order to work out an asymptotic expansion for  $\pi(L)$ . Such an estimate can already be determined from Kenyon's seminal results [104], we find  $S(L) = 1 - L^{-3/5} + O(L^{-3/5})$ . See also Fig 6.2 for a numerical illustration. This result of course wildly differs from the  $(\mu/\lambda)^L L^{-1/2}$  expected here from the numerically conjectured scaling for  $\pi(L)$ .<sup>5</sup> From the point of view of probability theory, the origin of this discrepancy is clear: the law governing Lawler's loop erased random walks essentially converges to SLE<sub>2</sub> rather than the conjectured SLE<sub>8/3</sub> for SAP and SAW models. From the point of view of sieve techniques however, the chasm between these results originates from an uncontrolled accumulation of error terms affecting the estimate  $R_p(z)[L]/R(z)[L] \sim F_p \lambda^{-\ell(p)}$ .<sup>6</sup>

It is important to recall that  $F_p \lambda^{-\ell(p)}$  is only the first, asymptotically dominant term of the asymptotic expansion of the number of walk multiples of  $p$ . In particular  $F_p \lambda^{-\ell(p)}$  is a good approximation to  $R_p(z)[L]/R(z)[L]$  only when  $L \gg \ell(p)$ . Yet, when we subtract walks multiples of SAPs from all closed walks of length  $L$ , we must consider the multiples of SAPs  $p$  of length up to  $\ell(p) = L - 1$ . Given the exponential growth in the number of SAPs, this means that *most* of our estimates are affected by large, uncontrolled errors, and it is impossible to exploit Eq. (6.3.1) using solely  $S(L)$ .

This problem has two potential solutions. The first idea is to take into account some error terms  $\text{Err}_p(L)$  in the asymptotic expansion of  $R_p(z)[L]/R(z)[L]$  so as to determine this quantity more precisely. Since all the error terms are exactly available<sup>7</sup>, it seems possible that an extension to Kenyon's arguments would allow us to

<sup>5</sup>The correction term is  $L^{-1/2}$  here because we count simple cycles rather than SAPs. This is responsible for a factor of  $L$  in front of the  $L^{-5/2}$ . Since in addition,  $R(z)[L] \sim \lambda^L/(\pi L)$  for  $L \gg 1$ , this accounts for another factor of  $L$  and finally we get  $L \times L \times L^{-5/2} = L^{-1/2}$ .

<sup>6</sup>These errors have the same origin as those affecting the Eratosthenes-Legendre sieve in number theory!

<sup>7</sup>In fact  $R_p(z)[L]$  itself is in principle exactly available from the extension of Viennot's Lemma to infinite graphs. In this situation however, it is a precise estimate for the sum over SAPs of  $R_p(z)[L]$  which is utterly lacking.

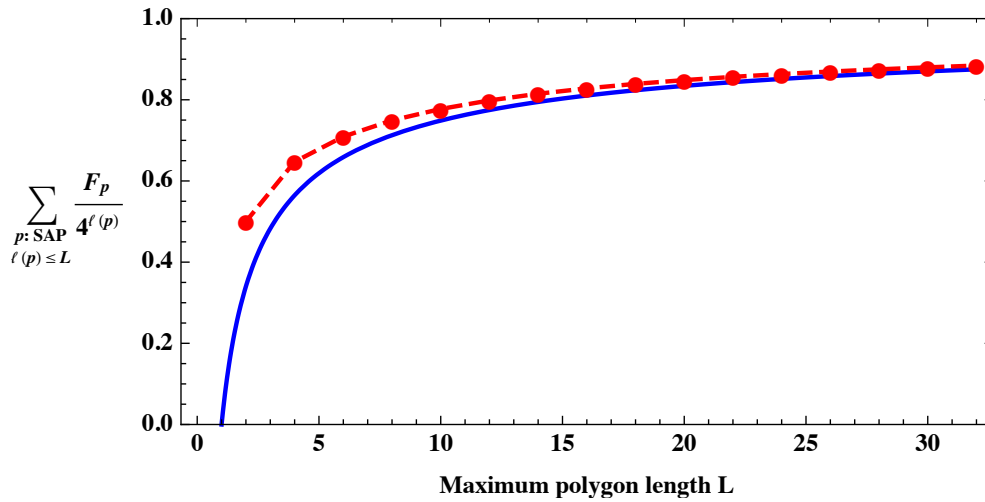


Figure 6.2: In red points and dashed red line: sum over all self-avoiding polygons  $p$  of length at most  $L$  of the fraction  $F_p/4^{\ell(p)}$ , as a function of  $L$ . Solid blue line: dominant term of the asymptotic expansion for this quantity, that is  $1 - L^{-3/5}$ . The discrepancy between exponents  $-3/5$  and the  $-1/2$  expected from SAP counting is due to an accumulation of error terms when summing over SAPs in the infinite sieve theorem.

estimate sums of such error terms generically. This idea suffers from a major drawback: error terms actually *grow* with  $L$  if we consider classes of SAPs for which  $L - \ell(p)$  is fixed. Since most SAPs of length up to  $L - 1$  are close in length to  $L$ , this means that the overall error term affecting Eq. (6.3.1) grows uncontrollably with  $L$ . Thus, an increasingly (and unrealistically) detailed knowledge of the errors is needed as  $L \rightarrow \infty$ , so that this strategy collapses completely with respect to rigorous arguments.

The second approach relies on a crucial foundational work by M. Bousquet-Mélou regarding the enumeration of heaps of pieces satisfying both left and right constraints [28, 27]. This work opens the way for two-sided sieves in the same manner as Viennot’s Lemma relates to the finite and infinite sieve theorems: they give control over both the left and right prime divisors of a walk. Consequently, the maximum length of the primes to be considered in Eq. (6.3.1) is reduced to only  $L/2$ . The “sieving gap” between  $L$  and  $L/2$  dramatically reduces the importance of the error terms to the extent that we expect them all to vanish under the limit  $L \rightarrow \infty$ . Seeing heaps of pieces as an extension of number theory in the vein of Chapter 5, shows that this  $L/2$  is the extension of the  $\sqrt{x}$  gap present in all standard number-theoretic sieves. We can similarly show that the fraction  $F_p \lambda^{-\ell(p)}$  extends the quantity  $\log(x)/\log(p)$  and all identities given here extend (and hence reduce to) valid number-theoretic identities. Non-trivial (novel) results on partial sums of the Möbius function also follow heuristically.

# Chapter 7

## Exact enumeration formulas for simple cycles and simple paths

Counting simple paths, that is trajectories on a graph that do not visit any vertex more than once, is a problem of fundamental importance in enumerative combinatorics [128] with numerous applications, e.g. in sociology [172, 33]. In view of the existing research, this problem should be divided into two main subquestions. One concerns the exact enumeration of "short" simple cycles with direct applications in the analysis of real-world networks. The other, more related to enumerative combinatorics (see e.g. [55, 128]), concerns the asymptotic growth of the number of simple cycles of length  $\ell$  on regular lattices as  $\ell$  tends to infinity.

As these two problems have been recognised for a long time, the strategies implemented so far to solve them have been qualitatively different. The practical enumeration of short simple cycles has been tackled via diverse algorithmic and analytic methods, e.g. the inclusion-exclusion principle [11, 22, 103], recursive expressions of the adjacency matrix [105], sieves [13] or immanantal equations [35]. In contrast, the asymptotic growth in the number of long simple cycles on regular lattices has been mostly studied using probability theory [118, 128, 46].

### 7.1 Counting from weakly connected subgraphs

Expressions for counting simple cycles of small lengths on undirected graphs from traces of the adjacency matrix have been discovered by various authors since the 1950's [172, 91, 3]. In 1972, two Ukrainian mathematicians, Khomenko and Golovko, published an exact formula for counting simple cycles of arbitrary length on any graph [105]. The formula results from an elaborate use of the inclusion-exclusion principle and involves a function defined through a complicated recursion. Possibly owing to its inherent difficulty and lengthy proof, Khomenko and Golovko's result has remained largely unnoticed. In 2009, the Russian mathematicians Sergey Perepechko and Anton Voropaev managed to greatly simplify the formula of Khomenko-Golovko [159], likely by solving the difficult recursion equation involved in it. The formula obtained by Perepechko and Voropaev, one of the most elegant results of enumerative combinatorics, was only announced in a conference talk and, to the best of our knowledge, never published. While the result only applies to simple cycles, we extend it to count simple paths with any specified end points. This leads to a unification of several known formulas for counting simple paths into a single matrix equation. The generalization of Perepechko and Voropaev's result leads to an important simplification that makes use of the additivity of adjacency matrices of disjoint graphs. Thanks to this property, the generalised formula can be reduced to a summation over connected induced subgraphs. A remarkable consequence is an expression that links the Hamiltonian paths of a graph to its connected dominating sets. From a computational point of view, the formulas obtained are particularly effective for sparse graphs, leading to the best general purpose algorithm for this task, see below and [66].

Perepechko and Voropaev's result can be stated as follows.

**Theorem 7.1.1** (Perepechko-Voropaev, 2009). *Let  $G = (E, V)$  be an undirected graph on  $N$  vertices with adjacency matrix  $A$ . The number  $\pi_\ell$  of simple (unoriented) cycles of length  $\ell$  is given by*

$$\pi_\ell = \frac{1}{2\ell} \sum_{i=2}^{\ell} (-1)^{\ell-i} \binom{N-i}{N-\ell} \sum_{S:|S|=i} \text{Tr}(A_S^\ell), \quad 3 \leq \ell \leq N \quad (7.1.1)$$

where the inner sum runs over all non-empty subsets  $S \subseteq V$  of size  $i$  and  $A_S$  is the adjacency matrix of the induced subgraph of  $G$  with vertex set  $S$ .

Equation (7.1.1) seems to have had little more impact than Khomenko-Golovko's result so far in spite of its deep elegance. This is possibly because it involves a sum over subgraphs, thus producing  $\pi_\ell$  in  $O(N^\ell \log N)$

operations [159]. Since the formula was devised primarily within and for a numerical computing community, its value may have been gauged from its sole computational cost.

The alternating signs in the Perepechko-Voropaev formula bears similarities with Bax's approach for counting Hamiltonian paths [11], based on the inclusion-exclusion principle. In fact, applying the trace operator to the matrix  $H_n$  defined in [11] recovers exactly the Perepechko-Voropaev formula for  $\ell = N$ . In this section we show how these two results, among others, can be summarised into a single matrix equation. Consider the matrix  $P(z)$  whose  $(i, j)$ -entry is defined to be the ordinary generating function of simple paths from  $i$  to  $j$ , i.e.

$$P_{ij}(z) = \sum_{\substack{p: i \rightarrow j \\ p \text{ simple}}} p z^{\ell(p)},$$

for  $z$  a formal variable. The information relative to simple paths and simple cycles on the digraph is entirely summarised in  $P(z)$ , making it a natural object of interest. Our first result gives an expression of  $P(z)$  in function of the labeled adjacency matrices of the induced subgraphs of  $G$ . For clarity, we distinguish between open and closed paths, by writing  $P(z) = P_{\text{cl}}(z) + P_{\text{op}}(z)$ , where

- $P_{\text{cl}}(z)$  is the matrix generating series of simple cycles. Its  $i$ -th diagonal entry is the generating function of the simple cycles visiting  $i$ , while the entries outside the diagonal are zero.
- $P_{\text{op}}(z)$  is the generating matrix of open simple paths. For  $i \neq j$ , its  $(i, j)$ -entry is the generating function of simple paths from  $i$  to  $j$ , and its diagonal is zero.

For a square matrix  $M$ , we denote by  $\text{Diag}(M)$  the diagonal matrix obtained by setting to zero all non-diagonal entries in  $M$ . We are now in position to state our first result.

**Theorem 7.1.2.** *It holds*

$$\begin{aligned} i) \quad P_{\text{op}}(z) &= \sum_{S \in \mathcal{S}} (zW_S)^{|S|-1} (\text{Id} - zW_S)^{N-|S|}, \\ ii) \quad P_{\text{cl}}(z) &= \sum_{S \in \mathcal{S}} \text{Diag} \left( (zW_S)^{|S|} (\text{Id} - zW_S)^{N-|S|} \right), \end{aligned}$$

where  $|S|$  denotes the cardinality of  $S$ .

**Remark.** We recover Perepechko-Voropaev's formula by attributing the value  $\omega_{ij} = 1$  to all directed edges, thus replacing  $W$  by  $A$ , and taking the trace of  $P(z)$  in Theorem 7.1.2.

## Counting simple paths from weakly connected sets

A digraph is said to be weakly connected if replacing all its directed edges by undirected edges produces a connected undirected graph. The expression of  $P(z)$  can be reduced to a sum over weakly connected subgraphs of  $G$  owing to the simple property that the adjacency matrix of a digraph with more than one weakly connected component is block diagonal. In particular, letting  $G(S) = G(C_1) \cup \dots \cup G(C_k)$  be the decomposition of  $G(S)$  into weakly connected components, we have for all  $n \geq 1$ ,  $W_S^n = W_{C_1}^n + \dots + W_{C_k}^n$ . This simple observation leads to a profound reduction in the summation over induced subgraphs in Perepechko-Voropaev's formula which we first obtained in [72].

Let  $\mathcal{C} \subseteq \mathcal{S}$  denote the non-empty subsets of  $V$  for which the resulting induced subgraph is weakly connected. For  $C \in \mathcal{C}$ , the weak neighborhood  $N(C)$  of  $C$  in  $G$  is the set of vertices in  $V \setminus C$  that can reach and/or be reached from  $C$  in one step. Formally,

$$N(C) = \{i \in V \setminus C : \exists j \in C, (i, j) \in E \text{ and/or } (j, i) \in E\}.$$

Of course, this definition recovers the classical definition of neighborhood in undirected graphs.

**Theorem 7.1.3.** *The matrix generating series of open and closed simple paths verify:*

$$\begin{aligned} i) \quad P_{\text{op}}(z) &= \sum_{C \in \mathcal{C}} (zW_C)^{|C|-1} (\text{Id} - zW_C)^{|N(C)|} \\ ii) \quad P_{\text{cl}}(z) &= \sum_{C \in \mathcal{C}} \text{Diag} \left( (zW_C)^{|C|} (\text{Id} - zW_C)^{|N(C)|} \right) \end{aligned}$$



**Remark.** On an infinite regular lattice  $G$  such as the square lattice, Theorem 7.1.3 relates the ordinary generating function of the Self-Avoiding Polygons (SAPs) with respect to their length, with a generating function of the polyominoes involving both their perimeters and their areas. Remarkably, the asymptotic behaviours of both sides of the formula are the subjects of famous open conjectures.

$$\sum_{\gamma \in \text{SAP}(G)} \ell(\gamma) z^{\ell(\gamma)} = \sum_p \text{Tr} \left( (zA_p)^{A(p)} (\text{Id} - zA_p)^{P(p)} \right).$$

Here  $z$  is a formal variable,  $A_p$  is the adjacency matrix of the subgraph of  $G$  covered by the polyomino  $p$ ,  $A(p)$  is the area of  $p$  and  $P(p)$  its perimeter.

Another direct application of theorem 7.1.3 concerns Hamiltonian paths, i.e. simple paths of maximal length, which appear in the terms of maximal degrees in the expressions of  $P_{\text{op}}(z)$  and  $P_{\text{cl}}(z)$ . From the formulas in Theorem 7.1.3, the terms of maximal degrees correspond to connected subsets  $C$  such that  $C \cup N(C) = V$ , i.e. dominating sets. This leads to an expression of the number of Hamiltonian paths that only involves the connected dominating sets of  $G$ . For the next result, we denote by  $H$  the Hamiltonian path counting matrix, whose  $(i, j)$ -entry gives the number of Hamiltonian paths from  $i$  to  $j$ .

**Proposition 7.1.1.** *Let  $\mathcal{D}$  be the set of weakly connected dominating sets in  $G$ ,*

$$H = \sum_{D \in \mathcal{D}} (-1)^{N-|D|} \left( A_D^{N-1} + \frac{\text{Tr}(A_D^N)}{N} \text{Id} \right).$$

The number of (oriented) Hamiltonian cycles appears in any diagonal entry of  $H$ ,

$$\pi_N := \frac{1}{N} \sum_{D \in \mathcal{D}} (-1)^{N-|D|} \text{Tr}(A_D^N),$$

where  $N - |D|$  can be replaced by  $|N(D)|$  due to the dominating property. This expression improves on Bax's and Khomenko and Golovko's (Theorem 4 in [105]) results for Hamiltonian cycles in that the sum is restricted to connected dominating sets. Similarly, the total number of open Hamiltonian paths follows by summing all non-diagonal entries of  $H$ .

Open and closed Hamiltonian paths can be dealt with separately yielding a slightly stronger version of the result, namely

$$H_{\text{op}} = \sum_{D \in \mathcal{D}} (-1)^{N-|D|} A_D^{N-1} \quad \text{and} \quad H_{\text{cl}} = \frac{1}{N} \sum_{D \in \mathcal{D}} (-1)^{N-|D|} \text{Tr}(A_D^N) \text{Id}.$$

From a computational point of view, the restriction to weakly connected subgraphs and weakly connected dominating sets provides a clear improvement for counting simple cycles, simple paths and Hamiltonian paths, especially for sparse graphs for which connected induced subgraphs are relatively rare. This observation is made rigorous by the analysis presented in the next section.

## 7.2 Algorithmic analysis of the counting formulae

Counting Hamiltonian cycles and, more generally, all simple cycles passing through a given vertex is a #P-complete problem [194, 31]. The same classification holds for the problem of counting simple paths with fixed endpoints. Unsurprisingly, the best existing algorithms for counting such cycles have time complexities  $O(2^N \text{poly}(N))$ , which scales exponentially with the number  $N$  of vertices on the graph. Under the exponential time hypothesis [98], this exponential scaling is, in principle, the best possible.

Although evaluating the asymptotic running time of an algorithm in the worst case scenario is necessary for the classification of algorithmic performance, it is of little relevance to applications which differ significantly from this scenario. This is precisely the case when counting or enumerating simple cycles or simple paths. Real-world networks, be they from sociology, biology or chemistry, are typically very sparse. At the opposite, the worst case scenarios for this task—the complete graphs—are dense and counting or finding cycles and paths of any kind on them presents no interest. An algorithmic implementation of the results of Theorem 7.1.3 especially tailored for sparse graphs is therefore highly desirable.

In applications it is typically sufficient to count only those simple cycles whose length does not exceed some maximum value  $\ell$ , usually much smaller than the graph size  $N$ . Yet, even with these restrictions, the problem of counting these objects is known to be difficult:

**Theorem 7.2.1** (Flum and Grohe [56]). *Counting simple cycles and simple paths of length  $\ell$  on both directed and undirected graphs, parameterised by  $\ell$ , is #W[1]-complete.*

The complexity classes  $\#W[t]$ ,  $t \geq 1$ , introduced by Flum and Grohe, are relevant for parameterised counting problems corresponding to the classes of the W-hierarchy [44] which, in turn, qualify the difficulty of parametrised decision problems according to the type of circuits needed to determine them. Importantly, the class  $\#W[1]$  is believed to *strictly* contain the class  $\#W[0]$  of all fixed-parameter tractable (FPT) counting problems. We recall that a counting problem  $P$  with input  $x$  is said to be *fixed-parameter tractable* if there is a computable function  $f$  of the parameter  $k$ , a constant  $c$  and an algorithm solving  $P$  in  $f(k) \text{poly}(|x|)$  steps. In this expression,  $|x|$  designates the size of the input [56, 85]. For the sake of simplicity, an algorithm achieving a  $f(k) \text{poly}(|x|)$  asymptotic running time will be said to be FPT.

An algorithm for counting simple cycles and simple paths stems from implementing the formulas of Theorem 7.1.3. Concretely, this was done in MATLAB [65] and PYTHON [144]. The computational complexity of these algorithms is as follows:

**Theorem 7.2.2.** *Let  $G = (V, E)$  be a graph, possibly directed, on  $N$  vertices and  $M$  edges. Let  $|S_\ell|$  be the number of connected induced subgraphs of  $G$  on at most  $\ell$  vertices. Let  $\Delta$  be the maximum degree of any vertex on  $G$  or, if  $G$  is directed, let  $\Delta$  be the maximum degree of any vertex on the undirected version of  $G$ . Then all the simple cycles of length up to  $\ell$  on  $G$  can be counted in time*

$$O(N + M + (\ell^\omega + \ell\Delta)|S_\ell|),$$

and  $O(N + M)$  space. In this expression,  $\omega$  is the exponent of matrix multiplication. The same complexity is achieved when counting the simple paths of length up to  $\ell$  or the simple cycles/paths with fixed endpoints of length up to  $\ell$ .

The important result of Theorem 7.2.2 is that the asymptotic running time of the general purpose algorithm presented here scales as  $\text{poly}(\ell)|S_\ell|$ . In comparison, we show in Section 7.2 that the running times of all other general purpose algorithms scale either with  $N^\ell$ , and  $N^\ell > |S_\ell|$ , or with the number  $|\text{Cycle}_\ell|$  of simple cycles of length at most  $\ell$  on the graph.<sup>1</sup> From these observations, we expect the algorithm presented here to be the best available for graphs with less connected induced subgraphs than simple cycles, something since then confirmed by experiments and theoretical investigations [66].

## Asymptotic running time

In the worst case scenario, that is the complete graphs  $K_N$ , Theorem 7.2.2 implies that the time complexity for counting *all* the simple cycles using the algorithm proposed here is  $O(2^N N^\omega)$  since all induced subgraphs are connected, i.e.  $|S_N| = 2^N$ . This is marginally better than the complexities reported in [103, 13, 12, 179]. However, it is the performance of our algorithm on non-complete graphs that we want to highlight. To this end, it is helpful to recast the time complexity of the algorithm in terms of simple graph parameters.

We can do so by using an upper bound on the number  $|S_k|$  of connected induced subgraphs on  $k$  vertices that involves the maximum degree of any vertex. This result is due to Uehara:

**Lemma 7.2.1** (Uehara [192]). *Let  $\Delta$  be the maximum degree of the undirected version  $G_{undir.}$  of  $G$ . Then the number of connected induced subgraphs on exactly  $k$  vertices in  $G_{undir.}$  is bounded by*

$$|S_{=k}| \leq N \frac{(e\Delta)^k}{(\Delta - 1)k^2},$$

with  $e$  the base of the natural logarithm. It follows that  $|S_\ell| = \sum_{k \leq \ell} |S_{=k}| = O\left(N \frac{\Delta^\ell}{(\Delta - 1)\ell^2}\right)$ .

Furthermore, on a graph with maximum degree  $\Delta$ , there are at most  $M \leq N\Delta$  edges, so that, by Theorem 7.2.2, the time-complexity of counting all the simple cycles of length  $k \leq \ell$  is upper bounded by

$$O\left(N(\Delta + 1) + (\ell^\omega + \ell\Delta)N \frac{\Delta^\ell}{(\Delta - 1)\ell^2}\right) = O(N\Delta + N(\ell^{-1}\Delta + \ell^{\omega-2})\Delta^{\ell-1}), \quad (7.2.1a)$$

$$\sim O(N\ell^{-1}\Delta^\ell), \quad (7.2.1b)$$

where we used that  $\Delta/(\Delta - 1) \leq 2$  as soon as the graph has a connected component with at least 3 vertices.

The bound on  $|S_\ell|$  obtained from Uehara's work is typically *very far from tight*, especially on graphs that are far from regular, such as scale-free networks. Consequently, the running time predicted by Eq. (7.2.1b) is typically much larger than that observed in numerical experiments. However, Eq. (7.2.1b) simplifies the analysis of the running time of the algorithm, which will help us compare it with other algorithms for the same task. We now easily verify that the algorithm is FPT on bounded degree graphs. In fact, on such graphs  $\Delta = O(1)$ , consequently the asymptotic running time scales as  $N$ , that is the algorithm is fixed parameter *linear*.

<sup>1</sup>There is one exception to this observation: by extending an approach of Merris to count Hamiltonian cycles [141], we show in Section 7.2 that all simple cycles can be counted with an asymptotic running time scaling as  $\ell t_{\text{imm}}(\ell)|S_\ell|$ , where  $t_{\text{imm}}(\ell)$  is *exponential* in  $\ell$ . Hence, this extension is still not competitive with the algorithm presented here.

## Detailed comparisons with existing algorithms

### Sieve methods

Bax and Bax and Franklin authored two articles detailing the use of combinatorial sieves to count simple cycles [13, 12], which extend previous results by Karp [103] for counting Hamiltonian cycles. Similar techniques had previously been expounded by Khomenko and Golovko [105, 106] and more recently by Perepechko and Voropaev [159, 160]. All these combinatorial sieves produce the simple cycles via sums over all the induced subgraphs of a graph, i.e. including the non-connected ones. There are  $\binom{N}{\ell}$  such subgraphs of size  $\ell$  on a graph on  $N$  vertices. Assuming  $\ell$  is fixed and much smaller than  $N$ , the number of subgraphs is  $\Omega(N^\ell/\ell!)$ . Consequently, counting all simple cycles of length up to  $\ell$  using these sieves takes at least  $\Omega(N^\ell/\ell!)$  time. If  $\Delta$  is sub-linear in  $N$ , this time complexity is much larger than the asymptotic running time achieved by the algorithm presented here, which is at most  $O(N\Delta^\ell/\ell)$ .

### Zeon algebras

An algorithm for counting simple cycles based on zeon algebras has been proposed by Schott and Staples in [179]. The algorithm relies on the observation that if one attaches a formal variable  $\xi_e$  to each edge  $e$  of the graph, such that any two such variable commute and  $\xi_e^2 = 0$ , then the corresponding labeled adjacency matrix  $(A_\xi)_{ij} := \xi_{ij}A_{ij}$  generates only simple cycles. In other words,  $\text{Tr}(A_\xi^\ell)$  is the number of simple cycles of length  $\ell$  on  $G$ . Unfortunately, this method requires formal matrix multiplications and cannot be implemented fully numerically.

Schott and Staples proved that the average time taken by this algorithm to count simple cycles of length  $\ell$  is  $O(N^4(1+q)^N)$  where  $q \geq \ell N\Delta/(N^2 - \ell)$  [179]. In the typical situation where  $\Delta, \ell \ll N$ , this cost is therefore at least  $O(N^4e^{\ell\Delta})$ . This is exponential in both  $\ell$  and  $\Delta$  and scales as the fourth power of  $N$ , in particular any function  $f(N) = O(N\Delta^\ell/\ell)$ , such as the asymptotic running time of the algorithm proposed here, obeys  $f(N) = o(N^4e^{\ell\Delta})$ .

### Counting using immanants

In 1983, R. Merris discovered an exact formula for counting the Hamiltonian cycles of a graph from a sum over at most  $N$  of its immanants [141, 142]. On noting that any simple cycle is Hamiltonian on a unique connected induced subgraph of the graph, Merris' formula is easily extended to count all simple cycles of length up to  $\ell$  via a sum over the  $|S_\ell|$  connected induced subgraphs of size at most  $\ell$ . In this sum, each term is itself a sum over at most  $\ell$  immanants. Therefore, evaluating the formula takes  $O(t(|S_\ell|) + t_{\text{imm}}(\ell)\ell|S_\ell|)$  time, with  $t(|S_\ell|)$  and  $t_{\text{imm}}(\ell)$  the times taken to find the connected induced subgraphs on at most  $\ell$  vertices and to calculate the required immanants of  $\ell \times \ell$  matrices, respectively.

In the same spirit, G. Cash described in 2007 an approach for counting simple cycles by solving a system of equations involving selected immanantal polynomials of the graph [35]. For length  $\ell$  simple cycles, Cash's approach stems from the solution of a system involving  $p(\ell) - p(\ell - 1)$  equations, where  $p(\ell)$  is the number of integer partitions of  $\ell$ . This number grows as  $\Theta(e^{x\sqrt{\ell}}\ell^{-3/2})$  with  $x = \pi\sqrt{2/3} \sim 2.6$  and consequently solving the system takes  $O(e^{7.7\sqrt{\ell}}\ell^{-9/2})$  time. Since the immanantal polynomials of the graph take  $O(t_{\text{imm}}(N))$  time to calculate, the cost of Cash's approach is  $O(t_{\text{imm}}(N)e^{7.7\sqrt{\ell}}\ell^{-9/2})$ .

The time complexities of both methods are primarily influenced by the time taken to calculate the required immanants. Unfortunately, these are difficult to obtain. First, as recognised by Cash, they require computing the matrix of irreducible representations of the symmetric group  $\mathcal{S}_x$ , a very costly task for large  $x$ . Second, while the determinant of an  $x \times x$  matrix requires only  $O(x^3)$  time, the second immanant  $d_2$  already costs  $O(x^c)$  with  $3 < c \leq 4$  and computing the last immanant, the permanent, is itself a #P-complete problem [193]. The permanent is required by both Merris' and Cash's approaches, meaning that, assuming the exponential time hypothesis,  $t_{\text{imm}}(x)$  grows exponentially in  $x$ . Comparing with Theorem 7.2.2, we observe that neither approach can compete with the algorithm proposed here. The results we present in the next section are in the same vein, as they involve combinations of permanents and determinants summed over the set of induced subgraphs of a graph, of which there are  $\Theta(N^\ell)$ .

### Counting short simple cycles on undirected graphs

When only short simple cycles on *undirected graphs* are of interest, these may be counted via a set of special identities involving the adjacency matrix. This approach was pioneered by Harary and Manvel in the 1970s and has remained popular ever since [91, 3, 37, 149]. The principle of this approach is to distillate the number of simple cycles of length  $k$  from the number of walks of length  $k$ , by removing all closed walks which are not simple from the count. For example, if one wishes to count all the squares, one must count all closed walks of length four, that is  $\text{Tr}(A^4)/4$ , and remove from those all closed walks of the forms  $1 \rightarrow 2 \rightarrow 1 \rightarrow 2 \rightarrow 1$  or  $1 \rightarrow 2 \rightarrow 1 \rightarrow 3 \rightarrow 1$  and  $1 \rightarrow 2 \rightarrow 3 \rightarrow 2 \rightarrow 1$ . The former type of walks traverses a single edge twice, thus is counted by  $|E|/2$ . The two latter types of walks traverse adjacent edges, of which there are  $\sum_{i \in G} \binom{\deg(i)}{2}$  with

$\deg(i)$  the degree of vertex  $i$ . Taken together, these results indicate that the number of squares is

$$n_{\text{squares}} = \frac{1}{4} \text{Tr}(\mathbf{A}^4) - \sum_{i \in G} \binom{\deg(i)}{2} - \frac{1}{2} |E|.$$

Similar identities exist for longer simple cycles but the number of terms they involve grows exponentially with the length of the simple cycles being counted. Alon, Yuster and Zwick presented an algorithm for evaluating these identities up to  $\ell = 7$  in  $O(N^\omega)$  time and  $O(N^2)$  space [3]. This cost grows for longer cycles, being  $O(N^{\omega+1})$  when  $\ell = 8$ , and then  $O(N^{\lfloor \ell/2 \rfloor} \log N)$  when  $\ell = 9, 10$ . To the best of our knowledge, no special identity for counting  $\ell > 17$  cycles has been found. Although such identities must exist, we note that that for  $\ell = 17$  comprises over  $10^5$  terms and is already far beyond what is concretely usable on large real-world networks.

Finally, we note that the space required for running AYZ scales as  $O(N^2)$  rather than  $O(N + M)$ , the former being much larger than the latter on sparse graphs. We found this to be AYZ main limitation in practice,<sup>2</sup> barring us from making computations on networks with over 12,000 nodes. This memory cost is unavoidable since AYZ necessitates the computation of powers of the adjacency matrix  $\mathbf{A}$  of the graph (not just their traces), which quickly become dense even on large sparse graphs. Recall in particular, that  $\mathbf{A}^x$  is full for  $x$  larger than the graph diameter.

### Counting simple cycles via enumeration

Enumerating the simple cycles or simple paths of a graph, that is producing their vertex sequences, is much more time consuming than simply counting them. The best general purpose algorithm for this task is still Johnson's 1975 landmark algorithm [101, 137], which achieves an asymptotic running time of  $O((N + M)(|\text{Cycle}_N| + 1)) \sim O(N\Delta|\text{Cycle}_N|)$ . In this expression,  $|\text{Cycle}_N|$  is the total number of simple cycles (or of simple paths) on  $G$ , including backtracks, that is simple cycles of length 2. This result was recently improved on undirected graphs to  $O(N(|\text{Cycle}_N| + 1) + M)$ , a scaling which is optimal for this task [21].

In the worst case scenario, i.e. on the complete graph  $K_N$ ,  $|\text{Cycle}_N| = O(N!)$ , that is enumerating all simple cycles takes factorial time. For this reason, counting simple cycles via enumeration has often been deemed greatly inefficient, in particular in comparison with the "only" exponential cost  $O(2^N \text{poly}(N))$  achieved by the algorithm presented here as well as other approaches [12]. This conclusion follows from a peculiarity of dense graphs however and for sparse graphs it is not so. Indeed, using the results of Theorem 7.1.3 to count all the simple cycles on a graph costs  $O(N^\omega |S_N|)$ . It follows that if  $N^\omega |S_N| \geq N\Delta|\text{Cycle}_N|$ , then Johnson's algorithm and its variants can count all the simple cycles of a graph via enumeration faster than any combinatorial sieve, including the one presented here. When counting simple cycles of fixed maximum length  $\ell$ , Johnson's algorithm takes  $O(N + M + (\ell + \ell\Delta)|\text{Cycle}_\ell|)$  time,  $|\text{Cycle}_\ell|$  being the total number of simple cycles of length up to  $\ell$ . This means in order for the algorithm presented here to be faster than Johnson's the following must hold  $(1 + \ell^{\omega-1}/\Delta)|S_\ell| \leq |\text{Cycle}_\ell|$ .

## 7.3 Counting via convolutions over induced subgraphs

Let  $\mathcal{G}$  be the set of finite digraphs. For  $G = (V(G), E(G)) \in \mathcal{G}$ , we say that  $H = (V(H), E(H)) \in \mathcal{G}$  is an induced subgraph of  $G$  if  $V(H) \subseteq V(G)$  and  $E(H) = E(G) \cap V(H)^2$ . If  $H \prec G$ , then  $G - H$  designates the subgraph of  $G$  induced by  $V(G) \setminus V(H)$ . Let  $(\mathcal{A}, \cdot, +)$  be an algebra, for two functions  $\phi, \psi : \mathcal{G} \rightarrow \mathcal{A}$ , the induced subgraph convolution between  $\phi$  and  $\psi$  is defined by

$$(\phi * \psi)[G] = \sum_{H \prec G} \phi[H] \psi[G - H], \quad G \in \mathcal{G},$$

where the sum runs over all induced subgraphs of  $G$  including the empty graph  $\emptyset$  and  $G$  itself. In this section, we investigate the induced subgraph convolution between function with values in the algebra  $\mathbb{R}\langle \mathcal{H} \rangle$  of formal series on hikes with real coefficients. Examples of such functions arising from usual expressions of the labeled adjacency matrix  $\mathbf{W}_H$  of a digraph  $H$  have been discussed in Section 5.3.

Our first result is a Mbius inversion relation involving the subgraph convolution:

**Lemma 7.3.1.** *For all  $G \in \mathcal{G}$ ,*

$$\sum_{H \prec G} \det(-\mathbf{W}_H) \text{perm}(\mathbf{W}_{G-H}) = \delta[G] := \begin{cases} 1 & \text{if } G = \emptyset \\ 0 & \text{otherwise,} \end{cases}$$

where we use the convention  $\text{perm}(\mathbf{W}_\emptyset) = \det(-\mathbf{W}_\emptyset) = 1$ .

<sup>2</sup>That is, beyond the fact that AYZ is limited to  $\ell = 7$  on undirected graphs.

The function  $\delta$  is the identity function for the induced subgraph convolution  $*$ , in view of  $\phi * \delta = \phi$  for all  $\phi : \mathcal{G} \rightarrow \mathbb{R}\langle \mathcal{H} \rangle$ . Thus, the lemma establishes that the functions  $G \mapsto \text{perm}(W_G)$  and  $G \mapsto \det(-W_G)$  are mutual inverse through  $*$ . The proof of the Lemma relies on the expression of the permanent and determinant from formal series on self-avoiding hikes, that is on the number-theoretic structure underlying the combinatorics of hike monoids.

**Corollary 7.3.1.** *For all  $G \in \mathcal{G}$ ,*

$$\sum_{H \prec G} \text{perm}(W_H) \det(\text{Id} - W_{G-H}) = \sum_{H \prec G} \text{perm}(\text{Id} + W_H) \det(-W_{G-H}) = 1.$$

Seeing these sums as convolutions makes the proof almost trivial. Letting  $\phi[H] = \det(-W_H)$  and  $\psi[H] = \text{perm}(W_H)$ , the equations of Corollary 7.3.1 read

$$\psi * (\phi * 1) = 1 \quad \text{and} \quad \phi * (\psi * 1) = 1.$$

The result follows directly from Lemma 7.3.1, using the distributivity and commutativity of the convolution. We now derive an expression of the formal series of Hamiltonian cycles. In the spirit of [139], we introduce the derivation operator  $D$  defined by

$$D \sum_{h \in \mathcal{H}} f(h)h = \sum_{h \in \mathcal{H}} \ell(h)f(h)h.$$

This leads to the following theorem for counting the Hamiltonian cycles on  $G$ .

**Theorem 7.3.1.** *Let  $\Gamma_{=G}$  denote the set of primes with support exactly  $V$ , that is the set of Hamiltonian cycles on  $G$ . Let  $\pi[G] := \sum_{\gamma \in \Gamma_{=G}} \gamma$ . Then*

$$D\pi[G] = \sum_{H \prec G} \det(-W_H) D \text{perm}(W_{G-H}) = - \sum_{H \prec G} \text{perm}(W_H) D \det(W_{G-H}).$$

The theorem is proven on expressing the determinants and permanents above as series over the self-avoiding hikes and using the properties of the walk von Mangoldt function.

**Remark.** Because  $\phi$  is the inverse of  $\psi$ , the relation  $D\{\pi\} = \phi * D\{\psi\}$  suggests an expression for  $\pi$  as a logarithm of  $\psi$ . This is indeed the case. Observe that the  $k$ -times convolution

$$\pi^{*k}[G] := \underbrace{\pi * \dots * \pi}_{k \text{ times}}[G] = \sum_{(H_1, \dots, H_k)} \pi[H_1] \cdots \pi[H_k],$$

writes as the sum over all  $k$ -partitions  $H_1, \dots, H_k$  of  $G$  (here, the order is important meaning that there are  $k!$  partitions involving the subgraphs  $H_1, \dots, H_k$ ). Thus, every spanning self-avoiding hike  $h$  is counted exactly once in the exponentiation

$$\exp_*(\pi[G]) = \sum_{k \geq 0} \frac{1}{k!} \pi^{*k}[G] = \psi[G].$$

This aspect originates from an Hopf algebraic structure, which we describe in the next section.

The formal series of simple cycles (of any length) follows from the convolution of  $\pi$  with the constant 1,

$$\Gamma[G] := (\pi * 1)[G] = \sum_{H \prec G} \pi[H] = \sum_{\gamma \in \Gamma_{=G}} \gamma,$$

Because derivation and convolution with the constant are commuting operators, we recover

$$D\Gamma = D\{\pi * 1\} = D\{\pi\} * 1 = (\phi * D\psi) * 1 = \phi * D\{\psi * 1\} = \phi * D\Psi,$$

where  $\Psi[G] = (\psi * 1)[G] = \sum_{H \prec G} \text{perm}(A_H) = \text{perm}(\text{Id} + A_G)$ . This gives the following corollary to Theorem 7.3.1

**Corollary 7.3.2.** *Let  $\Gamma_G$  be the set of all primes, i.e. simple cycles, on  $G$ , then*

$$D \sum_{\gamma \in \Gamma_G} \gamma = \sum_{H \prec G} \det(-W_H) D \text{perm}(\text{Id} + W_{G-H}).$$

We give an alternative approach to this result in the next section. Practical versions of this formula involving the generating function of simple cycles on  $G$  as well as the ordinary adjacency matrix of the graph will also be given.

## 7.4 An Hopf algebra structure for the hikes

Since any hike on a graph can be seen as a disjoint ensemble of connected components, it is natural that an algebraic structure should exist describing the generation of arbitrary hikes from connected ones. In particular, when it comes to the self-avoiding hikes, their connected components are their prime factors. Therefore, if this algebraic structure provides a mean of projecting the set of hikes back onto the set of connected hikes, it might send the self-avoiding ones onto the primes. In this section, we establish these heuristic arguments rigorously by showing that a cocommutative Hopf algebra describes the generation of arbitrary hikes from connected ones. This algebra provides several exact formulas for the formal series of connected hikes and of primes, stemming from projectors onto the irreducible elements of the algebra. We also show that the subgraph convolution operation introduced previously is a necessary and unavoidable feature resulting from this algebra.

We denote  $K$  an algebraically closed field of characteristic zero, and  $K\langle\mathcal{H}\rangle$  is the monoid algebra of  $\mathcal{H}$  over  $K$ , that is essentially the algebra of formal series on hikes. Note that given the isomorphism between such series and linear functions on hikes  $f \in \text{Hom}(\mathcal{H}, K)$ , from now on we shall not distinguish the two and will conveniently write any series  $f \in K\langle\mathcal{H}\rangle$  as  $f = \sum_{h \in \mathcal{H}} f(h)h$ . We designate  $\mathcal{C}$  the ensemble of connected hikes.<sup>3</sup>

We endow  $K\langle\mathcal{H}\rangle$  with an Hopf algebra structure following Schmitt's construction for general trace monoids [178]. We define the comultiplication  $\Delta : K\langle\mathcal{H}\rangle \rightarrow K\langle\mathcal{H}\rangle \otimes K\langle\mathcal{H}\rangle$  and counit  $\epsilon : K\langle\mathcal{H}\rangle \rightarrow K$  by

$$\epsilon = \begin{cases} 1, & \text{if } h = 1, \\ 0, & \text{otherwise,} \end{cases} \quad \text{and} \quad \Delta(h) = \sum_{d|h: V(d) \cap V(h/d) = \emptyset} d \otimes \frac{h}{d}. \quad (7.4.1)$$

In particular, the comultiplication introduced above decomposes any hike into its disjoint divisors and recovers that defined by Schmitt on general trace monoids in [178].

Equipped with these operations,  $K\langle\mathcal{H}\rangle$  forms a cocommutative coalgebra [178]. Its irreducible elements are immediately seen from Eq. (7.4.1) to be the connected hikes since these have no non-empty disjoint divisors. This further confirms that  $\Delta$  pertains to the generation of arbitrary hikes from connected ones. The multiplicative operation between elements of  $K\langle\mathcal{H}\rangle$ , that is the operation that gives it an algebra structure, is identified by the following Lemma [74]:

**Lemma 7.4.1.**  *$K\langle\mathcal{H}\rangle$  is isomorphic as an algebra to the commutative algebra formed by functions on graphs equipped with the induced subgraph convolution.*

We may now invoke standard general results of [178] to observe that the algebraic and coalgebraic structures of  $K\langle\mathcal{H}\rangle$  are compatible, that is  $\Delta$  and  $\epsilon$  are algebra maps and  $K\langle\mathcal{H}\rangle$  is a bialgebra. These results are subsumed in the following theorem, which in addition to the bialgebra structure, provides an antipode for  $K\langle\mathcal{H}\rangle$ , turning it into a Hopf algebra.

**Theorem 7.4.1.**  *$K\langle\mathcal{H}\rangle$  is a cocommutative Hopf algebra, with comultiplication and counit defined above and antipode  $S$  given  $S(h) := (-1)^{c(h)}h$ , where  $c(h)$  is the number of disjoint connected components of  $h$ .*

The generation of arbitrary hikes from connected ones thus gives rise to an Hopf algebra which, we will see, provides means of doing the opposite, that is to obtain the connected hikes from the set of all hikes. Before we proceed to these results, we note that the same algebraic structure relates the self-avoiding hikes with the primes.

**Corollary 7.4.1.**  *$K\langle\mathcal{S}\rangle$  is a cocommutative sub-Hopf algebra of  $K\langle\mathcal{H}\rangle$ .*

The irreducible elements of  $\mathcal{S}$  are now easy to discern: they are the irreducible elements of  $\mathcal{H}$ —the connected hikes—which are also self-avoiding, that is the primes. This observation in conjunction with Corollary 7.4.1 above, implies that any projector from the hikes onto the connected hikes will send the self-avoiding hikes onto the primes. Using standard formula from Hopf algebras we get:

**Theorem 7.4.2.** *For any coalgebra map  $f \in K\langle\mathcal{H}\rangle$ , then  $\log_* f : K\langle\mathcal{H}\rangle \rightarrow K\langle\mathcal{C}\rangle$ , in particular the  $*$ -logarithm of the identity on  $\mathcal{H}$  is the identity on  $\mathcal{C}$ ,*

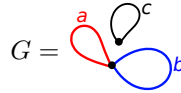
$$\log_* \left( \frac{1}{\det(\text{Id} - W)} \right) = \sum_{h \in \mathcal{C}} h.$$

*For any coalgebra map  $f \in K\langle\mathcal{S}\rangle$ , then  $\log_* f : K\langle\mathcal{S}\rangle \rightarrow K\langle\Gamma_G\rangle$ , in particular the  $*$ -logarithm of the identity on  $\mathcal{S}$  is the identity on  $\Gamma_G$ ,*

$$\log_* \left( \text{perm}(\text{Id} + W) \right) = -\log_* \left( \det(\text{Id} - W) \right) = \sum_{h \in \Gamma_G} h.$$

<sup>3</sup>The notion of connected hike is clear intuitively but a rigorous definition can also be given for it. A hike  $h$  is connected iff for any non-empty divisor  $d$  of  $h$ , we have  $V(d) \cap V(h/d) \neq \emptyset$ .

**Example 7.4.1** (Simple cycles from the logarithm of the determinant). Let us illustrate how the logarithm with respect to induced subgraph convolution distillates the simple cycles from a determinant or a permanent. Consider the following graph with three simple cycles  $a$ ,  $b$  and  $c$  of arbitrary lengths:



for which  $\det(\text{Id} - W) = 1 - a - b - c + ac + bc$ . Expanding the logarithm of this determinant as a series and focusing on the first and second orders to begin with, we have

$$-\log_* \left( \det(\text{Id} - W) \right) = -(-a - b - c + ac + bc) + \frac{1}{2}(-a - b - c + ac + bc)^2 - \dots \quad (7.4.2)$$

Since  $V(a) \cap V(c) = V(b) \cap V(c) = \emptyset$  and  $V(a) \cap V(b) \neq \emptyset$ , terms such as  $a * a$ ,  $a * b$  and  $b * ac$  all vanish and only  $a * c$  and  $b * c$  are non-zero. Thus, expanding the second order leaves  $ac + ca + bc + cb$ . For the same reasons all higher orders of the logarithm are exactly zero. In addition, since  $a$  and  $c$  and  $b$  and  $c$  are vertex-disjoint, they commute, and the second order further simplifies to  $2ac + 2bc$ . Thanks to these observations, Eq. (7.4.2) becomes

$$-\log_* \left( \det(\text{Id} - W) \right) = a + b + c - ac - bc + \frac{1}{2}(2ac + 2bc) = a + b + c,$$

which is indeed the formal series of the primes on  $G$ .

Admittedly, a  $*$ -logarithm is not very convenient to implement. Instead, we turn to its derivative for more practical results

**Corollary 7.4.2.** *Let  $G$  be a non-empty graph, and  $\Gamma := \sum_{h \in \Gamma_G} h$  be the characteristic series of the primes. Then*

$$D\Gamma = D \text{perm}(\text{Id} + W) * \det(\text{Id} - W) = -\text{perm}(\text{Id} + W) * D \det(\text{Id} - W).$$

In practice, prime counting is achieved upon replacing all labeled adjacency matrices with ordinary adjacency matrices  $W \mapsto zA$ , with  $z$  a formal variable. In this situation, formal series on hikes become ordinary generating functions and the derivative operator  $D$  is implemented as a derivative with respect to  $z$ . Then, because of the commutativity of the induced subgraph convolution, Corollary 7.4.2 yields the following variant formulas for the derivative of the ordinary generating function of the primes  $\Gamma(z) := \sum_{\gamma \in \Gamma_G} z^{\ell(\gamma)}$ ,

$$\begin{aligned} \frac{d\Gamma(z)}{dz} &= \sum_{H \prec G} \frac{d}{dz} \text{perm}(\text{Id} + zA_H) \det(-zA_{G-H}) = \sum_{H \prec G} \frac{d}{dz} \text{perm}(zA_H) \det(\text{Id} - zA_{G-H}), \\ \frac{d\Gamma(z)}{dz} &= - \sum_{H \prec G} \text{perm}(\text{Id} + zA_H) \frac{d}{dz} \det(-zA_{G-H}) = - \sum_{H \prec G} \text{perm}(zA_H) \frac{d}{dz} \det(\text{Id} - zA_{G-H}). \end{aligned}$$

## Existence of further counting formula from Lie idempotents

The celebrated Milnor-Moore theorem [145] provides an explicit relation between connected graded cocommutative Hopf algebras and Lie algebras. In this section we exploit this relation to assert the existence of many more formulas for counting simple cycles on graphs. We illustrate this with two examples.

The cocommutative Hopf algebra  $K\langle \mathcal{H} \rangle$  introduced earlier is both graded, with gradation  $c(h)$ , and connected since  $c(h) = 0 \iff h = 1$  so that  $K\langle \mathcal{H} \rangle_{[c(h)=0]}$  is just  $K$  itself as required [148]. Hence, we can use the theorem of Milnor and Moore to obtain that  $K\langle \mathcal{H} \rangle$  is isomorphic to the universal enveloping algebra of the graded Lie algebra formed by the series on connected hikes on the graph, i.e.  $K\langle \mathcal{H} \rangle \simeq U(K\langle \mathcal{C} \rangle)$  which, for simplicity, we shall write  $\mathcal{H} \simeq U(\mathcal{C})$ . By the same arguments, we also have  $\mathcal{S} \simeq U(\Gamma)$ . These results provide new tools to pass from  $\mathcal{H}$  to the free Lie algebra formed by  $\mathcal{C}$  and from  $\mathcal{S}$  to  $\Gamma$ : the Lie idempotents.

Lie idempotents are symmetrisers projecting the tensor algebra  $T(A)$  of a Lie algebra  $A$  onto the free Lie algebra. Now recall that the universal enveloping algebra of the Lie algebra  $A$  is  $U(A) = T(A)/I$ , with  $I$  the two-sided ideal generated by elements of the form  $a \otimes b - b \otimes a - [a, b]$ . In particular, if  $A$  is free, then a Lie idempotent project  $U(A)$  onto  $A$  itself. Since both  $\mathcal{C}$  and  $\Gamma$  are free, this reasoning leads to:

**Theorem 7.4.3.** *Let  $\iota$  be a Lie idempotent. Then*

$$\begin{aligned} \iota : K\langle \mathcal{H} \rangle &\longrightarrow K\langle \mathcal{C} \rangle, \\ &K\langle \mathcal{S} \rangle \longrightarrow K\langle \Gamma \rangle. \end{aligned}$$

We now give two examples of Lie idempotents to illustrate this result.

**Example 7.4.2** (Eulerian idempotent). Let  $A$  be a cocommutative connected graded  $K$ -bialgebra with product  $*$  and let  $\text{id}_A$  be the identity map on  $A$ . Then the endomorphism  $\epsilon : \log_*(\text{id}_A)$  projects  $A$  onto the  $K$ -submodule of primitive elements and is called the Eulerian idempotent of  $A$  [83]. Theorem 7.4.2 thus appears to state the Eulerian idempotents on  $\mathcal{H}$  and  $\mathcal{S}$ .

**Example 7.4.3** (Dynkin idempotent). Let  $K$  a commutative  $\mathbb{Q}$ -algebra and  $A$  be a cocommutative connected graded  $K$ -Hopf algebra with product  $*$ . Let  $S$  be antipode of  $A$  and for any  $a \in A$  define  $E(a) := \text{deg}(a)a$ , with  $\text{deg}(a)$  the grade of  $a$ . Then the endomorphism of  $A$  denoted  $\mathfrak{d} := S * E$  projects  $A$  onto the  $K$ -submodule of primitive elements and is called the Dynkin idempotent of  $A$  [198, 157, 83]. In the context of the self-avoiding hikes,  $\text{deg}(h) = c(h) = \Omega(h) = \omega(h)$ , with  $\omega$  the number of distinct prime factors of  $h$ . Thus the Dynkin idempotent on  $\mathcal{S}$  reads<sup>4</sup>

$$\Gamma = \sum_{h \in \mathcal{S}} (-1)^{\Omega(h)} h \sum_{h \in \mathcal{S}} \omega(h) h.$$

In fact, this result is recovered from a straightforward argument in the reduced incidence algebra of  $\mathcal{S}$ . Indeed, a direct multiplication of  $\Gamma$  with the zeta function of  $\mathcal{S}$  (i.e. the identity on  $\mathcal{S}$ ) gives

$$\Gamma \zeta_{\mathcal{S}} = \sum_{h \in \mathcal{S}} \left( \sum_{\gamma \in \Gamma, \gamma|h} 1 \right) h = \sum_{h \in \mathcal{S}} \omega(h) h,$$

and the Dynkin idempotent follows after a Möbius inversion of the above relation.

Many more Lie idempotents have been discovered and can be found in the relevant literature, see e.g. [156, 157, 190, 83] and references therein. By Theorem 7.4.3, each one of them provides a formula for counting the primes, that is the simple cycles, on arbitrary weighted directed graphs.

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<sup>4</sup>A similar, though less interesting, relation holds on  $\mathcal{H}$  with both  $\Omega(h)$  and  $\omega(h)$  replaced by  $c(h)$ . It yields the identity on  $\mathcal{C}$ .



## Chapter 8

# On the *tenuous* relation between walks and their graphs

With the help of dependency graphs, hike monoids provide a mean of discussing the properties of sets of walks and hikes without explicitly referring to the graph on which these exist. Indeed, the dependency graph  $H$  of a hike monoid  $\mathcal{H}$  encodes the “cycle skeleton” of a digraph  $G$ , as vertices of  $H$  are simple cycles on  $G$  and edges in  $H$  exist whenever two simple cycles of  $G$  share at least one vertex. In particular, sets of closed walks and more generally of hikes on two digraphs  $G$  and  $G'$  sharing the *same* hike dependency graph  $H$  are related through a bijection. This bijection stems from the isomorphism between their hike monoids  $\mathcal{H}_G$  and  $\mathcal{H}_{G'}$ . Indeed, these monoids have the same presentation because they have the same number of generators (this being the number of nodes in the hike dependency graph  $H$ ) as well as the same commutation relations between these generators (the edges in the complement  $H^c$  of  $H$ ). Then  $\mathcal{H}_G$  and  $\mathcal{H}_{G'}$  are isomorphic and there is a bijection between their sets of words, that is the sets of hikes (and thus of walks) on  $G$  and  $G'$ . Conversely, the existence of an isomorphism between hike monoids  $\mathcal{H}_G$  and  $\mathcal{H}_{G'}$  implies that  $G$  and  $G'$  share the same hike dependency graph. Relating graph properties and walk properties is thus equivalent to understanding which hike dependency graphs do exist and what properties of a digraph can we ascertain from its sole hike dependency graph.

Let  $\phi$  be the map which to any digraph  $G$  associates  $\phi(G)$ , the dependency graph of the hike monoid of  $G$ . We say that two digraphs  $G_1$  and  $G_2$  are  $\phi$ -equivalent if  $\phi(G_1) = \phi(G_2)$  and we denote this by  $G_1 \sim_\phi G_2$ . Any digraph transformation passing between two  $\phi$ -equivalent digraphs implements an isomorphism between their hike monoids since these two digraphs share the same hike dependency graph. The problem of understanding the relation between graph properties and walk properties can therefore be formulated as two questions on  $\phi$ :

1.  $\phi$ -Surjectivity: Given a graph  $H$ , is there a digraph  $G$  such that  $\phi(G) = H$ ?

If this is the case we say that  $H$  is *realizable* and that  $G$  *realises*  $H$ . Question 1. is equivalent to asking which trace monoid are hike monoids since any graph  $H$  is necessarily the dependency graph of a trace monoid.

2.  $\phi$ -Injectivity: Given a graph  $H$  determine  $\phi^{-1}(H)$ . Equivalently, what are all digraph transformations that induce isomorphisms of hike monoids?

From the examples presented earlier in the introduction we know already that  $\phi$  is not injective. A good question is thus to characterise the class  $\phi^{-1}(H)$  of all digraphs with hike dependency graph  $H$ . This, in turn, is equivalent to determining all digraphs transformations that induce isomorphisms of hike monoids since any two digraphs in  $\phi^{-1}(H)$  are related by such a transformation.

Observe that hike monoids, map  $\phi$  and questions 1. and 2. naturally extend to multidigraphs. In fact the set of all graphs realizable by multidigraphs is exactly the set of graphs realizable by digraphs since every digraph is a multidigraph and, for any directed multigraph, we can construct a digraph with identical hike monoid by adding transient vertices in the middle of each directed multi-edge. As a consequence, from now on we work equally with multidigraphs and digraphs referring to both as ‘digraphs’.

### 8.1 Realizable cycle structures in digraphs

Before we address the surjectivity and injectivity questions, we begin with three properties of the map  $\phi$  that reduce considerations to connected dependency graphs  $H$  and strongly connected multidigraphs  $G$ :

**Proposition 8.1.1.** *Let  $G$  be a digraph. We have*

1. If  $G$  is strongly connected, then its hike dependency graph  $\phi(G)$  is a connected graph.
2. Let  $G_1, \dots, G_n$  be the strongly connected components of  $G$ . Then  $\phi(G) = \bigsqcup_{i \in [n]} \phi(G_i)$ .
3. Let  $H$  be a connected realizable graph. Then  $H$  is realizable by a strongly connected digraph.

We now present some preliminary examples and observations to give the reader a better idea concerning the two questions and the difficulties they present.

First of all, not all graphs are realizable or equivalently, not all trace monoids are hike monoids. The smallest example of a graph that is unrealizable is the square

$$H = \begin{array}{cc} (a) & (b) \\ | & | \\ (d) & (c) \end{array} \quad (8.1.1)$$

Let us give an intuitive proof of this statement while we defer a more general formal proof of it to Proposition 8.1.2. By trying to build a digraph  $G$  such that  $\phi(G) = H$ , we will necessarily construct additional simple cycles. We begin with a simple cycle of arbitrary length corresponding to vertex  $a$  (1. of Figure 8.1). We then add the simple cycles corresponding to  $b$  and  $d$ . They must both share at least one vertex with simple cycle  $a$  but not with one another (2. of Figure 8.1). We finish by adding simple cycle  $c$ , which must share a vertex with  $b$  and  $d$  but not with  $a$  (3. of Figure 8.1). By doing so we created two new simple cycles, the internal black one and the external gray one (3. of Figure 8.1).

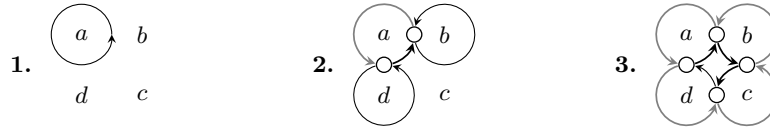


Figure 8.1: The square graph of (8.1.1) is unrealizable: **1.** First consider simple cycle  $a$ . **2.** Cycles  $b$  and  $d$  must intersect  $a$ . **3.** Concluding with the construction of  $d$ , we obtain 6 simple cycles:  $a, b, c$  and  $d$  plus the internal black simple cycle and the external gray one.

A natural approach could be to propose that a graph comprising a unrealizable graph as induced subgraph may itself be unrealizable. This cannot be so: consider for example the following graph  $H$  comprising the unrealizable square (highlighted with gray edges) as induced subgraph. It turns out that  $H$  is realised by the bidirected graph shown on the right,

$$H = \begin{array}{c} \circ \\ \diagup \quad \diagdown \\ \circ \quad \quad \circ \\ \diagdown \quad \diagup \\ \circ \end{array} \quad \begin{array}{c} \circ \\ \leftarrow \quad \rightarrow \\ \circ \quad \quad \circ \\ \leftarrow \quad \rightarrow \\ \circ \end{array} \in \phi^{-1}(H) \quad (8.1.2)$$

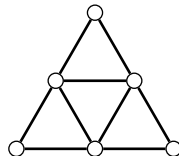
This suggests that the problem with realizability lies in part with cycles made of simple cycles, which must themselves be represented as vertices in  $H$ . We formalise this intuition and elaborate on it with the following proposition.

**Proposition 8.1.2.** *Let  $H = (V_H, E_H)$  be a realizable graph. Then for any induced simple cycle  $C = (c_1, \dots, c_n)$  of length at least 4 in  $H$ , there exist two vertices  $w_1, w_2 \in V_H$  such that:*

- for all vertices  $c_i$  in  $C$ , edges  $\{w_1, c_i\}$  and  $\{w_2, c_i\}$  are both in  $E_H$ .
- the neighbourhoods of  $w_1$  and  $w_2$  are included in the neighbourhood of  $C$ . That is to say if  $\{v, w_1\} \in E_H$  or  $\{v, w_2\} \in E_H$  then either  $v$  is in  $C$  or there exists  $c_i$  in  $C$  such that  $\{v, c_i\} \in E_H$ .

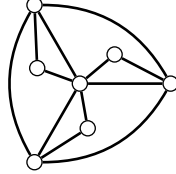
Furthermore, if edge  $\{w_1, w_2\}$  is not in  $H$  then for any  $i \in [n]$  there exists a vertex  $c'_i$  of  $H$  such that edges  $\{c_i, c'_i\}$  and  $\{c_{i+1}, c'_i\}$  are in  $E_H$ , under the convention  $c_{n+1} = c_1$ .

Triangles themselves are no obstacle to realizability as any triangle is realizable by a bouquet of three self-loops on the same vertex. This does not entail that any chordal graph is realizable however. For example, the triforme graph:



is unrealizable for the same reasons barring the square from being realised. In fact, this graph can be seen as the particular case of Proposition 8.1.2 for cycles of length 3. Indeed, the reader may attempt to build a digraph with a trifold dependency graph to see that because of the 3 external vertices, the cycles composing the central triangle necessarily imply the existence of two further cycles sharing vertices with every other cycle hence a pair of vertices connected to all vertices of the trifold, contradicting its structure.

All observations made so far point to realizability as depending solely on the induced cycles of  $H$  and their neighborhood, with the need to distinguish long (length  $\ell \geq 4$ ) from short ones (exception of the trifold graph). This is in fact not true; for example the following graph is unrealizable yet possesses neither an induced cycle of length  $\ell \geq 4$  nor a trifold of triangles:



**Surjectivity: which dependency graphs are realizable?**

As suggested by our observations so far, understanding the image of  $\phi$  is more complicated than it may first appear. Ideally, one would like to have a criterion for deciding if a graph is realizable, i.e. if it is in the image of  $\phi$ . Such a criterion remains elusive and if it exists, it must be highly non-trivial as we will demonstrate. Nonetheless we here establish that realizability is *decidable* by providing an algebraic condition that is equivalent to it. While this algebraization does not in itself shed additional light on realizability it leads to an algorithm for systematically checking for it.

Given a digraph  $G = (V, E)$  and  $H = \phi(G)$  its hike dependency graph we have, by definition, that the vertices of  $H$  correspond to the simple cycles of  $G$ . Conversely we may ask under what form do the vertices of  $G$  manifest themselves in  $H$ ? Given  $v$  a vertex of  $G$ , all simple cycles of  $G$  visiting  $v$  share at least this vertex hence do not commute in  $\mathcal{H}_G$ . This implies that they are all mutually connected by edges in  $H$ , i.e. they form a clique  $\kappa_v$ . The fact that vertices of  $G$  yield cliques in  $H$  leads to the following observations:

- i) The set  $\{\kappa_v\}_{v \in V}$  is a *clique cover* of  $H$ , that is each clique  $\kappa_v$  is a subgraph of  $H$  and every edge and vertex of  $H$  appears in at least one  $\kappa_v$ .
- ii) For  $W \subseteq V$ , the set  $\bigcap_{v \in W} \kappa_v \setminus \bigcup_{v \in V \setminus W} \kappa_v$  corresponds to the simple cycles of  $G$  with exactly  $W$  as vertex set.

Let us now give a criterion equivalent to realizability, discovered by T. Karaboghossian. For  $S$  a set, we denote by  $\mathfrak{C}_S$  the set of permutations over  $S$  with cycle decomposition of length 1.

**Theorem 8.1.1.** *Let  $H$  be a graph. Then  $H$  is realizable if and only if there exists a clique cover  $\{\kappa_1, \dots, \kappa_n\}$  of  $H$  such that the following polynomial system in variables  $(m_{ij})_{i,j \in [n]}$  admits an integer solution:*

$$\forall W \subseteq [n], \quad \sum_{\sigma \in \mathfrak{C}_W} \prod_{v \in W} m_{v, \sigma(v)} = |\mathcal{K}_W|, \tag{8.1.3}$$

where  $\mathcal{K}_W := \bigcap_{v \in W} \kappa_v \setminus \bigcup_{v \in [n] \setminus W} \kappa_v$ . In this case,  $H$  is realised by the digraph  $G$  with vertex set  $[n]$  and adjacency matrix  $A$  defined by  $A_{i,j} := m_{i,j}$  for  $1 \leq i, j \leq n$ .

**Corollary 8.1.1.** *Realizability is decidable.*

We can ignore clique covers such that  $\kappa_i \subseteq \kappa_j$  for some  $i \neq j$ . Indeed, if for such a clique cover the system (8.1.3) admits an integer solution, then no cycles would pass by the vertex  $i$  in the associated digraph, since we have  $|\mathcal{K}_W| = 0$  for any  $W$  containing  $i$ . Hence the digraph obtained by removing vertex  $i$  still realises  $H$  and corresponds to the clique cover obtained by removing the clique  $\kappa_i$ . In the sequel, we call trivial any clique  $\kappa_i$  such that  $\kappa_i \subseteq \kappa_j$  for some  $j \neq i$ .

We can deduce the following corollary from Theorem 8.1.1.

**Corollary 8.1.2.** *All trees are realizable.*

As mentioned in Corollary 8.1.1, realizability is decidable: an algorithm checking for it can work through all possible cliques covers of a graph  $H$ , verifying for each such cover if the accompanying system (8.1.3) admits an integer solution.

Using Proposition 8.1.2 (p. 73) to test for non-realizability and with ad-hoc arguments in remaining undecided cases, we computed the number of unlabelled connected realizable graphs with up to 7 vertices as (OEIS

A348365, computations based on the list of unlabelled connected graphs available at <http://users.cecs.anu.edu.au/~bdm/data/graphs.html> and [138].)

1, 1, 2, 5, 15, 58, 265.

In comparison, the number of unlabelled connected graphs on up to 7 vertices is known to be (OEIS A001349)

1, 1, 2, 6, 21, 112, 853.

Whilst most graphs are realizable for small number of vertices this changes when more vertices are considered. We conjecture that the proportion of realizable graphs on  $n$  vertices with respect to all unlabelled connected graphs on  $n$  vertices decreases as  $n$  increases.

We conclude this section by an observation about those graphs that are unrealizable. Since they are not, we might think that the elements of the corresponding trace monoids  $\mathcal{T}$  cannot be drawn as cycles on a digraph and are therefore essentially different from walks and hikes. This however is incorrect:

**Proposition 8.1.3.** *Let  $H$  be a graph that is unrealizable. Then there exist at least one realizable graph  $H'$  such that  $H$  is an induced subgraph of  $H'$ . Equivalently, let  $\mathcal{T}$  be a trace monoid that is not a hike monoid. Then  $\mathcal{T}$  is a submonoid of a hike monoid  $\mathcal{H}'$ .*

This indicates that elements of  $\mathcal{T}$  are walks and walk-like objects after all, yet these are not drawable as such by themselves. Perhaps more strikingly, since  $\mathcal{T}$  is a monoid in its own right it is *algebraically closed*. Elements of  $\mathcal{H}' \setminus \mathcal{T}$  are, in this sense, algebraically unrelated to those of  $\mathcal{T}$ . Yet allowing these additional elements turns the undrawable members of  $\mathcal{T}$  into drawable objects. As a corollary there cannot be a forbidden induced-subgraph criterion for realizability.

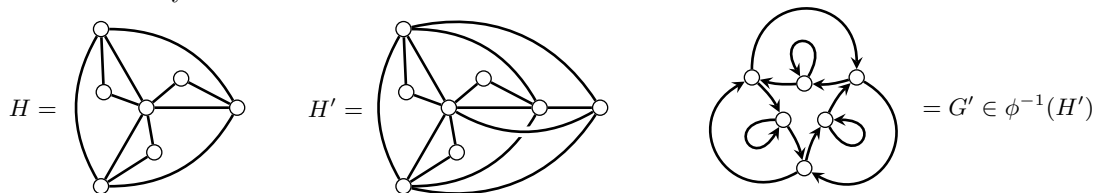


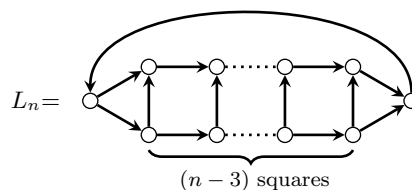
Figure 8.2: An example of Proposition 8.1.3, graph  $H$  is unrealizable yet appears as an induced subgraph of  $H'$  which is realised by the digraph  $G'$  shown on the right.

### Injectivity: graphs with isomorphic hike monoids

We now turn to question 2 pertaining to  $\phi$ -injectivity, that is we seek to find a description of  $\phi$ -equivalence. In [58] we present two sufficient conditions for two digraphs to be  $\phi$ -equivalent, but also show that these fail to be necessary. Relying on the sufficiency of these conditions we obtain sets of transformations that reduce the number of vertices and edges in digraphs while preserving their hike dependency graphs. For example, we obtain that the problem of realizability is reducible to cubic graphs, that is digraphs where all vertices have total degree 3:

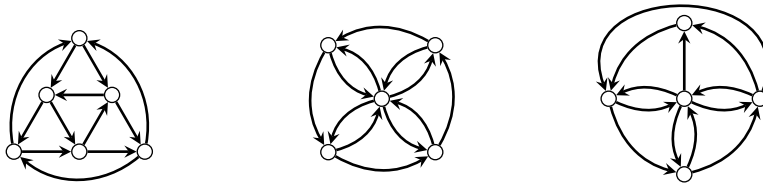
**Proposition 8.1.4.** *A graph is realizable if and only if it is realizable by a cubic graph.*

This and the other transformations found give us a potential characterisations of  $\phi$ -equivalence:  $G_1 \sim_\phi G_2$  if and only if  $G_1$  and  $G_2$  reduce to the same cubic graph after recursively applying transformations preserving the hike monoidal structure. The cubic graph so obtained would then be a canonical representative of the  $\phi$ -equivalent class  $\phi^{-1}(H)$  to which  $G_1$  and  $G_2$  belong. For example, all complete graphs on  $n$  vertices  $H = K_n$  are realizable, being realised by the cubic ladder digraph  $L_n$ ,

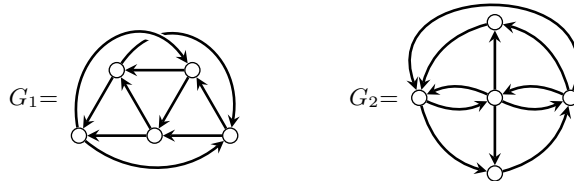


which satisfies  $\phi(L_n) = K_n$  for  $n \geq 3$ . The graph  $K_n$  is also realised by the bouquet graph  $B_n$  on  $n$  self-loops attached to the same vertices, as predicted by other transformations.

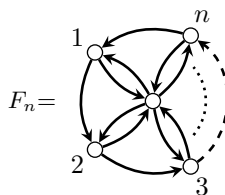
Unfortunately while it is true that two digraphs reducing to the same digraph are necessarily  $\phi$ -equivalent, the converse proposition does not hold. For example the following three digraphs are realizations of the complete graph on 17 vertices  $K_{17}$ , yet do not reduce to the same digraph,



More generally we found that for most graph theoretic properties, we could construct a realization of  $K_n$  that has the property and another that does not have it. For example both of the following digraphs realise  $K_{12}$



yet  $G_1$  is vertex-transitive while  $G_2$  is not,  $G_2$  is planar and  $G_1$  is not; or consider the flower graph  $F_n$  on  $n$  petals



for which  $\phi(F_n) = K_{n^2+1}$ . Flower  $F_n$  has a highly skewed degree distribution while that of the ladder  $L_{n^2+1}$  is uniform; etc. This means that even considering the purportedly simpler case of the complete graphs  $H = K_n$ , we still find a profusion of  $\phi$ -equivalent graphs which do not seem to be related to one another in any obvious way. These observations show that to pursue a full characterisation of  $\phi$ -equivalence we need an exhaustive description of the hike dependency graphs of all graphs with in- and out-degrees at least 2. We could not find such a description—and a plethora of cases make this task clearly daunting.

## 8.2 Simple graphs do not relate well with their simple cycles

We recall that  $P_G = (\mathcal{H}, \leq)$  denotes the poset of hikes  $\mathcal{H}$  partially ordered by left division:  $h \leq h' \iff h|h'$ . Observe that the minimal elements of  $P_G$  are the simple cycles and two simple cycles  $c, c'$  commute if and only if there exists  $h$  such that  $c \leq h$  and  $c' \leq h$ . Thus, knowing the poset  $P_G$  reduces exactly to knowing the simple cycles and their commutativity relations (i.e. the pairs of intersecting cycles). We now aim to characterise the precise information on a digraph  $G$  that is contained in its hike poset  $P_G$ .

Let  $A$  denote the adjacency matrix of  $G$ . Replacing  $W$  by  $zA$ , for  $z$  a formal variable, in Eq. (5.2.4) yields a slight modification of the characteristic polynomial of  $G$  by  $\det(\text{Id} - zA) = \sum_{h \in \mathcal{H}} \mu(h)z^{\ell(h)}$ . This expression indicates that knowing the poset  $P_G$ , along with the length function  $\ell : P_G \rightarrow \mathbb{N}$ , suffices to recover the spectrum of a digraph  $G$  of known size  $N$ . On the other hand, the information given by the hike structure  $(P_G, \ell)$  is not sufficient to reconstruct  $G$  exactly. For instance, all acyclic digraphs on  $N$  vertices have their hike posets reduced to  $\{1\}$  and are therefore indistinguishable from their hike structure. Things are somewhat different for undirected graphs which are in fact characterised by their hike structure, provided they contain no isolated vertex and all information about their backtracks is retained. Since the connected components of  $G$  are apparent in  $P_G$ , we shall assume that  $G$  is connected without loss of generality.

**Proposition 8.2.1.** *Let  $G$  be a connected simple graph. Then, the hike structure  $(P_G, \ell)$  determines  $G$  uniquely up to isomorphism.*

Of course, the length function provides a significant amount of information and the question remains to know whether an undirected graphs  $G$  with no isolated vertex can be reconstructed from the poset  $P_G$  only. This turns out to be the case for all undirected graphs but two exceptions:  $K_3$ , the complete graph on 3 vertices and  $K_{1,5}$ , the complete bipartite graph on 1 and 5 vertices.

**Theorem 8.2.1.** *Let  $G$  be a connected bi-directed digraph with no self-loop. The hike poset  $P_G$  determines  $G$  uniquely up to isomorphism, unless  $G \in \{K_3, K_{1,5}\}$ .*

The proof of the theorem relies exclusively on simple cycles of length 2 (called backtracks) sustained by every undirected edge  $\{i, j\}$  on  $G$ . Vertices of the hike dependency graph  $H$  of  $G$  corresponding to backtracks in  $G$  can always be identified even though the lengths of the simple cycles corresponding to the vertices of  $H$  are not

known (with the single exception  $H = K_5$  leading to the  $\{K_3, K_{1,5}\}$  special case). Now the induced subgraph of  $H$  formed by the backtracks is the line graph  $L(G)$  of  $G$ , which is well known to determine  $G$  uniquely. In this context, the condition that the graph contains no self-loop is crucial. Indeed, when the length is unknown, a self-loop is indistinguishable from a pendent edge, i.e. an edge with an endpoint of degree one in  $G$ .

While this result seems to be quite powerful at first glance, the seemingly harmless assumption that the graph is bidirected (i.e. effectively undirected, that is simple) is essential. Should even a single edge be directed the theorem would completely fail to hold. In other terms, the theorem makes no use of longer simple cycles, so much so that if the information regarding the backtracks is discarded from  $H$ , that is we only have access to  $\phi(G) \setminus L(G)$ , then graphs suffer from exactly the same shortfalls as directed graphs when it comes to relating them to their closed walks. That is,

- There are graphs  $G$  and  $G'$  with  $\phi(G)/L(G) = \phi(G')/L(G')$  and  $G$  and  $G'$  do not share fundamental graph theoretic properties. See Figure 8.3 below.

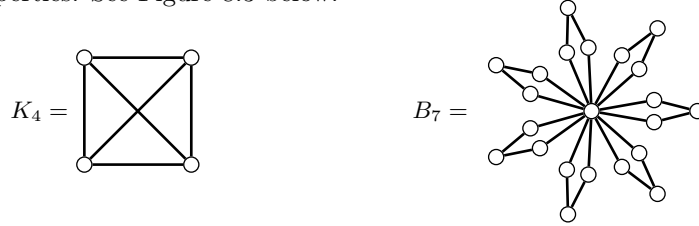


Figure 8.3: A pair of graphs with  $\phi(K_4)/L(K_4) = \phi(B_7)/L(B_7)$ , graph  $K_4$  on the left is Hamiltonian and vertex-transitive but not bipartite unlike the bouquet graph  $B_7$  on the right, which is bipartite and neither Hamiltonian nor vertex-transitive.

- Given a graph  $H$ , deciding whether there exists a graph  $G$  such that  $H = \phi(G)/L(G)$  is widely open.

These issues are pressing since many tools of modern network analysis and algebraic graph theory explicitly disregard or forbid backtracks. This includes backtrackless walks methods [10], Ihara zeta function and primitive orbits [188] and open problems about graphs and cycles, foremost among which is the cycle double cover conjecture [100].

### 8.3 Invariants of hike monoids

Recall that for a digraph  $G$ ,  $H = \phi(G)$  is the dependency graph of its hike monoid, which is the trace monoid generated by its simple cycles under the partial commutation rule that two cycles commute if and only if they share no vertex.

Given that isomorphisms of hike monoids implement profound changes on digraphs, it is worth investigating quantities left invariant by these isomorphisms. The first type of such invariants are algebraic quantities based on the adjacency matrix.

**Proposition 8.3.1.** *Let  $G$  and  $G'$  be two  $\phi$ -equivalent digraphs and let  $A$  and  $A'$  be their adjacency matrices, respectively. Then:*

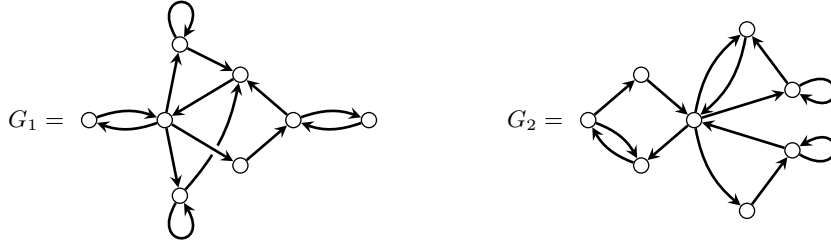
- 1)  $\det(\text{Id} - A) = \det(\text{Id}' - A')$ ,
- 2)  $\text{perm}(\text{Id} + A) = \text{perm}(\text{Id}' + A')$ ,

where  $\text{Id}$  and  $\text{Id}'$  are identity matrices of appropriate sizes.

The proposition is proven on expliciting the above invariants as hike series over self-avoiding hikes, which are completely and solely determined by the hike dependency graph. The list of algebraic invariants provided above is *not* exhaustive, many more invariants can for example be inferred from the Hopf structure described in §7.4. To see this consider two algebraic invariants of hike monoids  $a(G)$  and  $b(G)$  defined on a digraph  $G$  and all its induced subgraphs  $g \prec G$ . Then the induced subgraph convolution  $(a * b)(G) = \sum_{g \prec G} a(g)b(G \setminus g)$  is also an algebraic invariant of hike monoids. In other terms if  $G$  and  $G'$  are two  $\phi$ -equivalent digraphs, then  $a(G) = a(G')$ ,  $b(G) = b(G')$  and  $(a * b)(G) = (a * b)(G')$ . As an instance of this we unify and generalise assertions 1) and 2) with  $\text{perm}(\text{Id} + A)^{*k}$ , the  $k$ th-induced subgraph convolution of the permanent with itself, which is therefore an invariant of hike monoids for all  $k \in \mathbb{Z}$ .

If the isomorphism of hike monoids between  $\mathcal{H}_G$  and  $\mathcal{H}_{G'}$  is length preserving, then all algebraic quantities computable from their adjacency matrices are identical (e.g. degree sequence, graph spectra, permanental polynomial  $\text{perm}(\text{Id} - zA)$  etc). Allowing for the addition of transient vertices it is always possible to construct a pair of digraphs related by a length-preserving isomorphism of hike monoids from a pair of digraphs related

by an isomorphism that does not preserve the length. This gives a systematic mean of generating cospectral pairs, although the digraphs so generated are much more similar than just cospectral (remark also that there are pairs of cospectral graphs do not share the same hike dependency graph). Below is an example of digraphs related by such a morphism:



The second type of invariant are combinatorial invariants sensitive to how walks and hikes are composed of cycles:

**Proposition 8.3.2.** *Let  $G = (V_G, E_G)$  be a digraph,  $\mathcal{H}_G$  its hike monoid and  $\mathcal{W}_G \subset \mathcal{H}_G$  be the set of walks in  $\mathcal{H}_G$ , that is the set of hikes  $h = c_1 \cdots c_k \in \mathcal{H}_G$  with a unique right simple cycle  $c_k$ . Let  $\Omega(h)$  be the number of simple cycles in a hike  $h$ . Let  $f_{\mathcal{H}_G}^\Omega(z) := \sum_{h \in \mathcal{H}_G} z^{\Omega(h)}$ ,  $f_{\mathcal{W}_G}^\Omega(z) := \sum_{h \in \mathcal{W}_G} z^{\Omega(h)}$ , be the associated ordinary generating functions on hikes and walks, respectively.*

*Then  $G \sim_{\Phi} G'$  implies*

1.  $f_{\mathcal{H}_G}^\Omega(z) = f_{\mathcal{H}_{G'}}^\Omega(z)$ ;
2.  $f_{\mathcal{W}_G}^\Omega(z) = f_{\mathcal{W}_{G'}}^\Omega(z)$ .

*Now consider the set  $\mathcal{W}_{G:i \rightarrow j}$  of rooted walks  $w$  from vertex  $i$  to vertex  $j$  in  $G$ . Let  $\Omega(w)$  designate the number of loops erased from  $w$  following Lawler's loop erasing procedure [122]. Let  $\sigma(\cdot)$  be an additive function on hikes. Then  $G \sim_{\Phi} G'$  implies that for all  $i, j \in V_G$  there exists  $i', j' \in V_{G'}$  with*

3.  $f_{\mathcal{W}_{G:i \rightarrow j}}^\Omega(z) = f_{\mathcal{W}_{G':i' \rightarrow j'}}^\Omega(z)$ ;
4. *The shape of the branched continued fraction representation of the generating series associated with an additive function  $\sigma$  defined on rooted walks from  $i$  to  $j$  on  $G$  is the same as that representing the generating function of  $\sigma$  on rooted walks from  $i'$  to  $j'$  on  $G'$ .*

Invariant 4. exploits both the number-theoretic properties of hike monoids and the bialgebraic structure obeyed by graph walks implying the path-sum theorem for the ordinary generating function associated with  $\sigma$ .

**Example 8.3.1.** Consider the following two graphs with identical hike dependency graph:

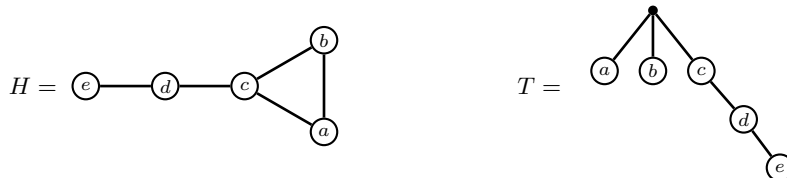


Let  $\sigma$  be the length function  $\ell$ , which is additive as necessary. Then the path-sum continued fraction representation of the ordinary generating function of all rooted closed walks from vertex  $\circ$  to itself on  $G$  and  $G'$  associated with the length function is

$$\sum_{w \in \mathcal{W}_{G:\circ \rightarrow \circ}} z^{\ell(w)} = \frac{1}{1 - z - z^2 - \frac{z^3}{1 - \frac{z^2}{1 - z}}} = (\text{Id} - zA_G)_{\circ\circ}^{-1},$$

$$\sum_{w \in \mathcal{W}_{G':\circ \rightarrow \circ}} z^{\ell(w)} = \frac{1}{1 - z - z - \frac{z^2}{1 - \frac{z^4}{1 - z^2}}} = (\text{Id}' - zA_{G'})_{\circ\circ}^{-1},$$

where  $A_G$  and  $A_{G'}$  are the adjacency matrices of  $G$  and  $G'$ , respectively. The common structure  $T$  of both fractions is readily apparent and stems from the hike dependency graph  $H = \phi(G) = \phi(G')$  as explained in the proof of Proposition 8.3.2:



In  $G$ ,  $a$  and  $e$  are self-loops,  $b$  and  $d$  are backtracks and  $c$  is a triangle. In  $G'$ ,  $a$  and  $b$  are self-loops,  $c$  and  $e$  are backtracks and  $d$  is a square. Since  $\Omega$  is additive the same structure  $T$  appears in  $f_{\mathcal{W}_{G:1 \rightarrow 1}}^\Omega(z) = f_{\mathcal{W}_{G':1 \rightarrow 1}}^\Omega(z)$ ,

$$f_{\mathcal{W}_{G:1 \rightarrow 1}}^\Omega(z) = f_{\mathcal{W}_{G':1 \rightarrow 1}}^\Omega(z) = \frac{1}{1 - z - z - \frac{z}{1 - \frac{z}{1 - z}}}.$$

The picture painted by these investigations is that the relation between digraphs and their hikes is in fact rather weak: no graph theoretic property seems to be directly related to the arrangement of simple cycles on a digraph. Among the graph properties we found may be lost whilst leaving the hike monoidal structure of cycles invariant are vertex-transitivity, regularity, planarity, bipartiteness, (bi)directedness, Hamiltonicity, being Eulerian, being chordal, being triangle-free, chromatic number, graph spectra, in- and out-degree distributions and a majority of algebraic quantities computable from adjacency matrices. This list is undoubtedly non-exhaustive. As a corollary, there is a great variety of digraphs with isomorphic hike monoids and characterizing all transformations relating such digraphs remains completely open.

Conversely, deciding which arrangements of simple cycles exist at all is highly non-trivial, even allowing for multidigraphs to realise them as was done here. We have shown that realizability is equivalent to the existence of integer solutions to polynomial systems of equations, making realizability decidable but no less obscure. The characterization and existence questions concern simple undirected graphs too as soon as information about their line graph is removed. That is, simple graphs do not relate to their simple cycles of length  $\ell \neq 2$  any better than multidigraphs do to their simple cycles of any length.

All of this demonstrates that walks are in fact much less dependent on the digraphs on which they take place than might have first been thought; and that a “*theory of walks*” distinct from graph theory needs to be developed. Here we proceeded by relying on hike monoids, which provide a representation for walks and walk-like objects that is markedly detached from graphs sustaining those walks. As monoids, hike monoids are plain trace monoids. Unfortunately, while the latter are well understood, there is no simple way to know which trace monoids are hike monoids. Although we have formulated most of our results in terms of dependency graphs, expressing them directly as statements on trace monoids makes this fact even more clear. Consider for example the following family of trace monoids with identical independence relations but differing number of generators:

$$\begin{aligned} \mathcal{T}_0 &= \{a, b, c, d \mid ac = ca, bd = db\}, \\ \mathcal{T}_n &= \{a, b, c, d, x_1, \dots, x_n \mid ac = ca, bd = db\}. \end{aligned}$$

Among these very similar trace monoids, we know that  $\mathcal{T}_0, \mathcal{T}_1, \mathcal{T}_3, \mathcal{T}_5, \mathcal{T}_9, \mathcal{T}_{17}$  and  $\mathcal{T}_{29}$  are not hike monoids, while all others are. Trace theory does not seem to be any better equipped than graph theory to address the questions raised here.



# Chapter 9

## Further applications of hike monoids

Hike monoids have found applications in network analysis, through the novel formulas for cycle counting and the finite sieve theorem. In this chapter, we briefly summarise these applications.

### 9.1 Cycle counting in social analysis and computer science

The algorithm for counting simple cycles and simple paths presented and analysed in §7.2 based on the formulas of §7.1 is sufficiently performant to enable its concrete use in the analysis of large real-world networks, in particular in sociology, econometry and computer science.

#### Evaluating balance on social networks

In the social sciences, complex systems may conveniently be represented by graphs whose nodes represent social entities (people, tribes, companies etc.) and whose edges represent interactions between these entities (e.g. acquaintance, war, financial exchanges etc.). Relations of amity and enmity between entities are well encoded by signed networks, where an edge is assigned a positive value if two entities are acquainted and in good terms, and a negative one if there are instead enemies [90, 151, 52]. Such networks provide a natural setting to study inter-personal relationships and their correlations.

For example, one could expect that people are friendly towards the friends of their friends, a situation that is said to be “balanced”. More generally, on signed networks, a group of individuals who are cyclically connected—i.e. forming a triangle, a square, a pentagon etc.—are said to be balanced if the number of negative edges in the cycle is even. Otherwise the cycle is said to be unbalanced. Starting with Heider’s work in the 1940s, sociologists have conjectured that such negative cycles are the cause of tension and thus, that social networks should evolve into a state where balanced cycles are largely predominant [95, 33, 5], the so-called “Heider’s conjecture”. The question of whether the conjecture is satisfied by real-social networks and if not, by how much it fails to be true, has been discussed since Heider’s formulation in 1946 [95].

Mathematically speaking, this sociological question translates into the following problem: on a signed network  $G$ , determine for all  $\ell$  the percentage of negatively-signed simple cycles of length  $\ell$ . This problem remained largely unsolved owing to its natural formulation in terms of simple cycles, making it formally NP-hard to verify (see §7.2) and practically beyond the reach of current algorithms when it comes to large, real, social networks. This changed thanks to the algorithm we introduced in §7.2 whose improved performances were sufficient to tackle the question for cycles of length up to 15. More precisely the algorithm was tasked with evaluating the ratio  $R_\ell$  of the number of negatively signed simple cycles of length  $\ell$  to the total number of simple cycles of length  $\ell$ , i.e.

$$R_\ell := \frac{N_\ell^-}{N_\ell^- + N_\ell^+}.$$

Here  $N_\ell^-$  (resp.  $N_\ell^+$ ) is the number of unbalanced (resp. balanced) simple cycles of length  $\ell$ . In particular,  $R_\ell = 0$  when the network is perfectly balanced for a length  $\ell$ , while  $R_\ell = 1$  indicates a totally unbalanced situation. In order to ascertain the significance of the results,  $R_\ell$  is compared with that obtained on a graph with the same proportion  $p$  of negative directed edges than the real network under study, but where the sign of any directed edge is negative with probability  $p$ . In particular, in the null-hypothesis model, the signs of any two directed edges are *independent* random variables. Then the probability that a simple cycle  $c$  of length  $\ell$  be negative (i.e. unbalanced) is

$$\text{Prob}(c \text{ negative}) = \sum_{i=0}^{\lceil \ell/2 \rceil - 1} \binom{\ell}{i} p^{2i+1} (1-p)^{\ell-2i-1}. \quad (9.1.1)$$

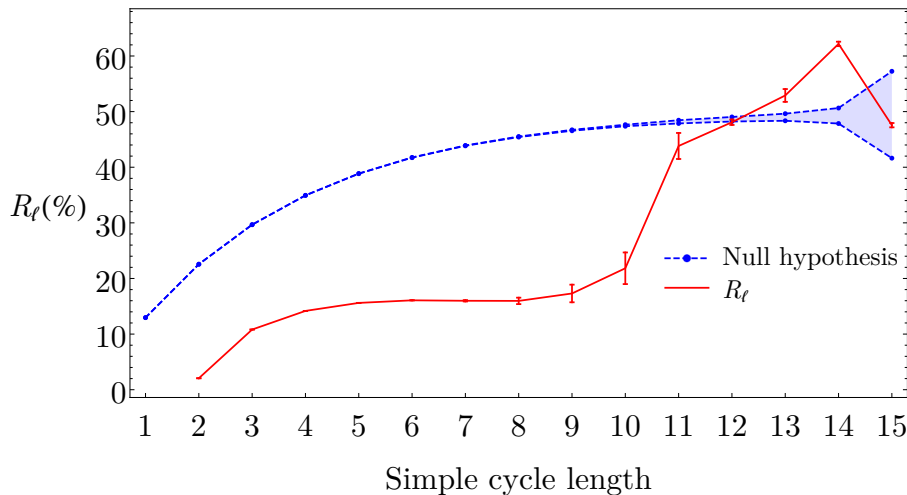


Figure 9.1: Computed percentage of negatively signed simple cycles on the Epinions network for cycle length up to 15 (red line and error bars). The blue shaded region bordered by dashed blue lines shows the values of  $R_\ell$  compatible with the null-hypothesis, as determined by Eq. (9.1.1) with the  $2\sigma$  interval.

Supposing for simplicity that the signs of any two simple cycles are independent random variables then the probability distribution for  $N_\ell^- / (N_\ell^- + N_\ell^+)$  in the null-hypothesis is a binomial law with expectation value  $R_\ell^{\text{null}}$  given by Eq. (9.1.1). Consequently, in this simple model the null-hypothesis is compatible up to a near 95% confidence level with any value of  $R_\ell$  within the  $2\sigma$  interval  $R_\ell^{\text{null}} \pm 2\sqrt{R_\ell^{\text{null}}(1 - R_\ell^{\text{null}}) / \sqrt{N_\ell^- + N_\ell^+}}$ . The assumption that the signs of any two simple cycles are independent random variables is not true on real social networks. Calculating the null-hypothesis without this assumption is very difficult in practice however. Indeed, a more accurate null model is given by evaluating the average balance ratios of all lengths over all random shufflings of the edges-signs from the social network under study. We also implemented this more accurate model and found only minor modifications that did not affect the overall conclusions of our study.

Concretely, we studied one small (Gahuku-Gama tribe network) and three large real-world networks (Wiki-elections, Slashdot and Epinions). The observations we made are broadly similar on the three large networks and so, for brevity, we here report the results only in the case of Epinions. This is a directed graph with 131,828 vertices and 841,372 edges [48], representing positive/negative relations between the users of the now-defunct consumer review website Epinions.com. We find the balance ratio  $R_\ell$  to transition from small to high values at around  $\ell \sim 10$ . Strikingly, for  $4 \leq \ell \leq 9$ ,  $R_\ell$  is almost constant around 15% witnessing a very strong, almost length-independent, inter-edge correlation. This example and the other analysed in our study show that social networks are indeed strongly balanced. More precisely, the percentage of negatively signed simple cycles is greatly depressed as compared to an independent sampling scenario (the null hypothesis), typically up to lengths of circa  $\ell \sim 10$ . As explained in [73], this is a signature of strong inter-edges correlations with correlation length  $\xi \simeq 10/2 = 5$  since most edges are bidirected. The correlation depth, which quantifies the degree up to which individuals are correlated with their neighbours, is thus close to 5. A rebound of the balance ratio to over 50%, above and beyond the null-hypothesis, following the transition is also clearly detectable in the data, indicating that much of the imbalance is shifted to long simple cycles. Sociologically this seems to indicate that conflict is strongly suppressed in close communities of up to 5 people and rather shifted to larger communities of over  $\sim 12$  people, where its dilution seems to allow for its management. In terms of modeling, our results suggest that the simplest model for the balance ratio  $R_\ell$  on large (sparse) social networks is a step function, with the step located circa  $\xi \sim 5$ , that is  $\ell \sim 10$ . Consequently, Heider's conjecture is verified only for short simple cycles and fails for longer ones.

## The all-paths and cycles graph kernel

With the recent rise in the amount of structured data available, there has been considerable interest in methods for machine learning with graphs. Many of these approaches have been kernel methods, which focus on measuring the similarity between graphs. Kernel methods are very popular methods for pattern recognition in machine vision and machine learning because they allow the use of a wide variety of classification and clustering tools through the definition of a suitable kernel function for the type of data at hand. A kernel function is a function  $K(A, B)$  between two objects,  $A$  and  $B$ , which in effect measures their similarity. Most graph kernels are of the convolution type [94], which decompose the structural object into parts and measure the similarity between those parts. Particular examples include the intersection kernel, the optimal-assignment kernel [112] and the cross-product kernel. In the cross-product kernel, the objects are decomposed into sets of parts  $X_A$  and  $X_B$

which are then compared individually

$$K(A, B) = \sum_{x_i \in X_A} \sum_{x_j \in X_B} K_B(x_i, x_j)$$

where  $K_B(\cdot, \cdot)$  is a base kernel measuring the similarity of parts. Many types of parts have been proposed for such a decomposition, including walks, cycles and paths. In [26], Borgwardt and Kriegel proposed the “all-paths kernel”, decomposing the graphs into the set of all paths between any pair of vertices. They noted that this was an NP-hard decomposition, and very difficult to compute in practice. Instead, they computed the shortest-path kernel, an approximation which considers a single path between each pair with the shortest geodesic length.

Relying on the novel algorithm of §7.2 in [78] we managed to compute an “all-paths and cycles kernel”, an extension of the all-paths kernel, further enriched by including the simple cycles as well. Extensive evaluations on a variety of graph datasets demonstrate that the all-paths and cycles kernel has superior performance to the shortest-path kernel and state-of-the-art performance overall.

## 9.2 Sieves on hikes as a cycle centrality measure

### Theory & motivations

Networks, that is collections of nodes together with sets of edges linking some of these nodes, naturally encode relations (the edges) between entities (the nodes). The trajectories on the network, i.e. the walks, represent the dynamical processes of the system of entities. Networks and walks play a ubiquitous role across many domains, from economy to defence through biology and physics, where graphical models are essential tools to master the interactions and dynamics of complex systems.

Network analysis has slowly progressed from questions concerning individual entities to questions regarding the dynamics of the system, from the local to the global scale. Already over the course of the development of vertex-centralities, i.e. measures of the importance of individual nodes, it became clear that vertex-neighborhoods, subgraphs and motifs were of paramount importance to understand the evolution of real networks [146, 205]. For example, in a biological context Estrada and Rodríguez-Velázquez showed that protein-lethality in *Saccharomyces cerevisiae* was better accounted for by an analysis of the subgraphs to which a protein belongs in the protein-protein interaction network (PPI) rather than by its degree [51]. In another study, Mukthar *et al.* showed that while a number of the proteins of the plant *Arabidopsis thaliana* under attack by pathogens were high degree nodes (hubs) in the plant PPI, dozens of these proteins were “targeted significantly more often [...] than expected given their respective degrees”. They concluded that protein-targeting by pathogens “cannot be explained merely by the high connectivity of those target [proteins]” [150]. In addition, it is also well known that in PPIs, certain small subgraphs of protein interactions, called motifs, are over-represented as compared to what one might expect from random networks [152]. These motifs are believed to perform crucial roles in emergent biological functions [202], such as the formation of protein complexes, functions which are not readily apparent at the level of single proteins [93, 152].

In spite of all of these observations, much attention is still devoted to individual nodes when exploring the dynamics and properties of complex networks. This is possibly because the versatility, ease of implementation and easy to grasp definition of many vertex centralities is lacking an equivalent at the cycle or subgraph level. It is a central goal of the mathematical tools we presented in [80] to remediate to this situation.

We propose a centrality measure for individual cycles based on the premise that a cycle is central if it intersects an important proportion of all the information flows on the network. In concrete applications, these flows represent actual dynamical processes, that is sequences of interactions between discrete entities, such as wealth exchanges between economic actors or successions of protein reactions in a living organism. This premise provides a clear meaning for the centrality as well as a contextual framework within which to appraise its results. To translate these ideas into mathematical tools, we propose to count all walks  $\omega$  which have the same *last* erased loop per Lawler’s procedure. This unambiguously attributes every walk to a single cycle since the last erased loop is unique. In addition, by the results of §5.3 this loop presents the only vertices from which the walk can be started without changing its equivalence class in the Cartier-Foata monoid. This entails that all walks which are structurally similar are attributed to the same cycle. Finally, instead of naively counting infinitely many walks, we shall calculate the fraction of walks with a cycle  $\gamma$  as last erased loop among all the closed walks on the graph. This fraction is a well-defined quantity given exactly by the finite sieve theorem of §6.2:

**Definition 9.2.1** (Cycle centrality). Let  $G$  be a possibly weighted (di)graph, and let  $\lambda$  be its maximum eigenvalue. Let  $A$  be the adjacency matrix of  $G$ , including weights if any. For any cycle  $\gamma$  of length  $\ell(\gamma)$ , let  $A_{G \setminus \gamma}$  be the adjacency matrix of the graph  $G$  where all vertices visited by  $\gamma$  and the edges adjacent to them have been removed. We define the centrality  $c(\gamma)$  of the cycle  $\gamma$  as

$$c(\gamma) := \lambda^{-\ell(\gamma)} \det \left( \text{Id} - \frac{1}{\lambda} A_{G \setminus \gamma} \right).$$

As outlined in the introduction to this section, the centrality  $c(\gamma)$  has a precise combinatorial meaning underpinning its role as a measure of cycle importance. Rigorously we have:

**Proposition 9.2.1.** *Let  $G$  be a (di)graph with adjacency matrix  $\mathbf{A}$  and let  $\gamma$  be a cycle on  $G$ . Then the total number  $n_\gamma(k)$  of cycles of length  $k$  on  $G$  intersecting the cycle  $\gamma$  is asymptotically given by  $n_\gamma(k) \sim c(\gamma)(\det(\text{Id} - z\mathbf{A})^{-1})[z^k]$  as  $k \rightarrow \infty$ .*

**Proposition 9.2.2.** *Let  $G$  be a (weighted di)graph with non-negative edge weights and let  $\Gamma(G)$  be the set of all simple cycles on  $G$ . Then for  $\gamma \in \Gamma(G)$ ,  $0 < c(\gamma) \leq 1$ . Furthermore  $0 < \sum_{\gamma \in \Gamma(G)} c(\gamma) = \alpha \leq 1$  is the (weighted) fraction of all hikes on  $G$  which are walks.*

The fact that  $\sum_{\gamma \in \Gamma(G)} \alpha^{-1}c(\gamma) = 1$  confirms that there is a probabilistic interpretation for the centralities  $c(\gamma)$ . Remarkably this interpretation continues to hold on infinite vertex-transitive graphs, provided  $\alpha^{-1}c(\gamma)$  is understood as  $F(\gamma)/\lambda^\ell(\gamma)$  in the sense of Chapter 6.

**Proposition 9.2.3.** *Let  $G$  be a finite graph or an infinite vertex-transitive graph,  $\lambda$  the largest eigenvalue of  $G$  and let  $\gamma$  be a simple cycle on it. Let  $w$  be a random walk with uniform edge-transition probability  $1/\lambda$ . Run the walk until it comes back to its starting point. Then the probability  $\mathbb{P}(w \mapsto \gamma)$  that the last erased loop of  $w$  be  $\gamma$  is equal to the fraction of all closed walks (including those passing an arbitrary number of times through the origin) which are right-multiples of  $\gamma$  in the hike monoid  $\mathcal{H}_G$ ,  $\mathbb{P}(w \mapsto \gamma) = c(\gamma)$ .*

The logarithm of  $c(\gamma)$  also has a probabilistic interpretation based on results by Espinasse and Rochet [49]:

**Proposition 9.2.4.** *Let  $G$  be a finite graph or an infinite vertex-transitive graph and let  $\gamma$  be a simple cycle on it. Let  $\mathbb{E}_w(\cdot)$  designate the expectation value of a random variable with respect to the closed random walks (defined up to translation if  $G$  is infinite) and weighted with probability  $\lambda^{-\ell(w)}$ . Then*

$$\log(c(\gamma)) = \sum_{w: \text{walk}} \frac{\Lambda_\gamma(w)}{\ell_\gamma(w)} \lambda^{-\ell(w)} = \mathbb{E}_w \left( \frac{\Lambda_\gamma(w)}{\ell_\gamma(w)} \right).$$

Here  $\Lambda_\gamma(w)$  counts the vertices that are both in  $\gamma$  and the unique right divisor of  $w$  and  $\ell_\gamma(w)$  is the number of vertices of  $\gamma$  visited by  $w$ , counted with multiplicity.

Function  $\Lambda_\gamma(w)$  is a kind of  $\gamma$ -overlap von Mangoldt function: defining  $\Lambda_\gamma(h)$  to be 0 when the hike  $h$  is not a walk and otherwise  $\Lambda_\gamma(h)$  is as in the Proposition above, we have  $\Lambda_\gamma(h) = \Lambda(h)$  when  $\gamma$  is the unique right prime divisor of  $h$ . The combination of two preceding Propositions implies *the rather uncommon result* that the entropy of the distribution of  $c(\gamma)$  values is a double expectation value: it is the expectation value over the SAPs of an expectation value over walks. This entropy has not yet been properly studied.

**Remark.** If  $\gamma$  is taken to be the empty walk on some vertex  $i$ , then  $c(i)$  is the asymptotic proportion of closed walks passing through  $i$  on  $G$  and a measure of the importance of this vertex. This centrality is essentially the same as the eigenvector centrality. Indeed take  $G$  a (weighted) graph with adjacency matrix  $\mathbf{A}$  and largest eigenvalue  $\lambda$ . Let  $\text{eig}(i)$  be the  $i$ th entry of the eigenvector corresponding to eigenvalue  $\lambda$ . Then there exists a constant  $\eta$  such that for all vertices,  $c(i) = \eta \text{eig}(i)^2$ . In fact  $\eta = \lim_{z \rightarrow 1/\lambda} (1 - \lambda z)^{-1} \det(\text{Id} - z\mathbf{A})$ .

## Predicting protein targeting in plants

We first consider the protein-protein interaction network (PPI) obtained by Mukhtar *et al.* in a landmark study of plant-pathogens interactions between the plant *Arabidopsis thaliana*, the bacterium *Pseudomonas syringae* and the oomycete *Hyaloperonospora arabidopsidis*. The network, comprises 3,148 interactions between 926 proteins, of which 170 are known to participate in plant immunity and 137 are targeted by effectors from one or both pathogens [150].

The state-of-the-art model posits a positive correlation between protein-targeting and the degree-centrality of the proteins. Mukhtar *et al.* confirmed such a correlation, showing it to be statistically significant, yet also observed shortfalls of the model, such as numerous low-degree targets and hubs targeted by few pathogen-effectors, if at all. Nonetheless, the degree-based model is the best available vertex-based model, see Table (9.1). Mukhtar *et al.* also showed that highly connected proteins tend to be involved in immune interactions [150]. Furthermore, subsequent biological studies, notably into oomycetes, have shown that pathogen effectors are potent stimulants of immune activity in *Arabidopsis thaliana*. Consequently, we might expect the PPI to comprise small protein motifs involving not only a pathogen target, but also one or more interactions with an immune protein, interactions which may be stimulated by the activity of the pathogen on the target, and an accompanying central protein. If we now hypothesise that pathogens primarily aim at disrupting a sizeable proportion of sequences of protein reactions in the host, then the motifs mentioned above should have high cycle-centrality. This is because in the context of PPIs the cycle-centrality of a motif measures the fraction of

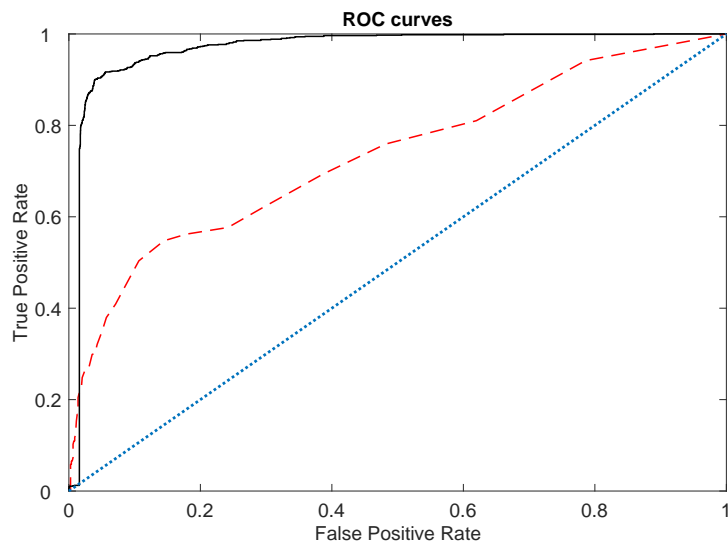


Figure 9.2: Solid black line: ROC curve of the dominant-triad model in the plant-pathogen PPI of *A. thaliana*, *P. syringae* and *H. arabidopsidis*. In this model, all triads involving AT5G08080 and/or AT5G22290 are ranked in descending order according to cycle-centrality. A true positive is a triad involving at least one more target and at least one immune reaction, while a false positive is a triad which does not meet both of these criteria. Red dashed line: ROC curve of the degree-based model proposed in [150], where proteins are ranked in descending order according to their degree in the PPI. A true positive is a protein targeted by at least one pathogen effector. Dotted line: null-hypothesis model with random protein-targeting.

sequences of protein interactions intercepted by the motif. In other words, pathogen-targets should primarily be found in triads with dominant cycle-centrality involving at least one target, one or more central proteins, and one or more immune interactions.

To test this model, we calculated the cycle-centrality of all 113,398 triads of proteins in the PPI. We then selected those triads involving a protein involved in plant resistance against bacteria or one with a role in stress responses. Among the selected triads, we classified as true positive those which involve at least one target and at least one protein related to immunity. Finally, in order to compare the performances of the dominant-triad and degree-based models, we obtained the ROC curves for both. The results, presented on Fig. (9.2), clearly show the dominant-triad model out-performing the degree-based one of [150]. The performances of models based on summing vertex-centralities in cycles are reported in Table (9.1) for comparison. These results suggest that the hypothesis where pathogens select their targets to maximise the fraction of disrupted sequences of protein reactions better fits the observations than the hypothesis where they target high-degree nodes of the PPI. In particular, the model explains why hubs are not the only targets nor necessarily the most targeted proteins, as interactions with peripheral proteins in the immediate vicinity of a central protein are seemingly equally disruptive to the ensemble of sequences of reactions on the PPI. The performance of the dominant-triad model also underscores the remarkable efficiency of the plant immune response: nearly all triads with the highest cycle-centrality involving a pathogen target also involve an immune interaction. Taken together, these observations paint the picture of a PPI where two central proteins are immediately surrounded by numerous pathogen targets and a flurry of immune interactions.

Performances of protein-targeting models			
	Model	ROC AUC	Discrimination
Cycle-based	1. Dominant-triad $c(\gamma)$	<b>0.97</b>	<b>0.47</b>
	2. $\Sigma_R$ ( $\alpha = 0.85/\lambda$ )	0.89	0.39
	3. $\Sigma_{CS}$	0.88	0.38
	4. $\Sigma_{eig}$	0.87	0.37
	5. $\Sigma_R$ ( $\alpha = 0.5/\lambda$ )	0.85	0.35
Vertex-based	6. Degree centrality [150]	0.73	0.23
	7. Resolvent centrality ( $\alpha = 0.5/\lambda$ )	0.28	0.22
	8. Resolvent centrality ( $\alpha = 0.85/\lambda$ )	0.28	0.22
	9. Exponential centrality	0.60	0.10
	10. Eigenvector centrality	0.41	0.09

Table 9.1: The ROC AUC is the area under the ROC curve. A perfect model making only correct predictions would have ROC AUC=1, while the null-hypothesis yields ROC AUC=0.5. The discrimination is the (absolute) area between the ROC curve and the null-hypothesis line. The crucial difference between vertex-based and cycle-based models is that the former attempt at directly identifying individual protein-targets, while the latter aim at identifying targeted triads.

### Finding biological protein complexes

The PPI network of the yeast *Saccharomyces cerevisiae* has been mapped by [92], which provides a network comprising 5303 interactions between 1689 individual proteins. These proteins are known to belong to complexes, a curated list of which is provided by the Munich Information center on Protein Sequences (MIPS) [87]. These complexes are not readily apparent from the PPI alone, which comprises no information on complexes. Yet using the cycle centrality  $c(\gamma)$  we can detect them directly from the topology of the PPI. To do so we analysed the PPI in three steps. Firstly, we found all edges (that is connected pairs of vertices) connected triplets (triangles and paths on 3 vertices) and connected quadruplets of proteins on the network. Secondly, we calculated the centralities  $c(\cdot)$  of these objects. To present the third step of our analysis, we invite the reader to observe the distribution of centrality values, which we show at the top of Fig. (9.3) in the case of triplets. Triplet centralities fall into separate plateau-like ensembles. Therefore, the third and final step of our analysis is to gather the list of all proteins appearing in all the triplets whose centrality values placed them in the same plateau. We then compare these lists of proteins with the biological complexes found in curated databases [168]. Remarkably, these lists of proteins correspond to actual biological complexes. Mathematically, the fact that biological complexes lead to clustered plateau-like centrality values for triplets means that the frequency with which proteins belonging to these complexes are involved in successions of proteins reactions depends first and foremost on the complexes themselves. In other terms, the frequency of protein activation is determined at the complex level. For a full discussion of the biological activity of the identified complexes, see [79].

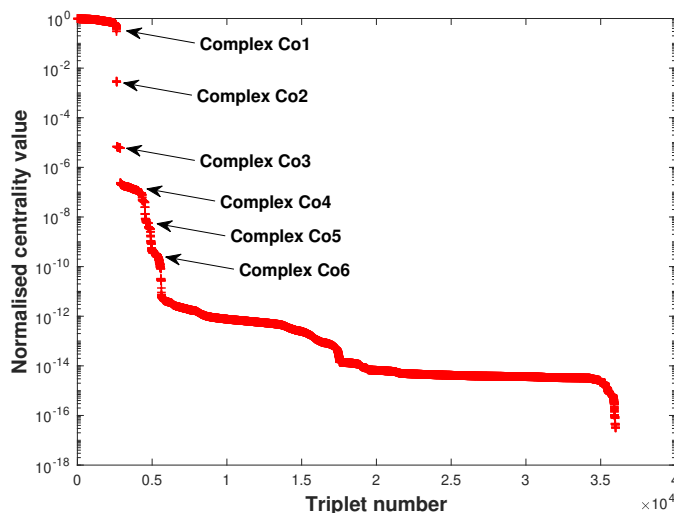


Figure 9.3: Distributions of triplet centralities on the PPI of the yeast.

# Chapter 10

## And from there...

The two branches of ‘walk theory’ presented in this report offer different perspectives of further development:

In the first branch, the operadic context of the CAP-co-preLie bialgebra ought to be explored to better connect it to Feynman categories in particular. This might help in extending some of the tools presented here, in particular the path-sum theorem, to renormalization procedures and seek a continuum version of it, with walks made of continuous steps. This is necessary to tackle resummation of non-Abelian Feynman diagrams for physical systems with continuous degrees of freedom for example. That this is possible might already be indicated by an alternative interpretation of the  $\star$ -algebras, seeing  $\star$ -products as simply summing up continuous walks on a graph that is both spatially discrete and continuous along the time-dimension. Mathematically, this description is equivalent to that presented here, where the discrete graph and the time-dependence of its edge weights are treated separately. Re-summations of continuous walks may be arduous however as it generally leads to incurable divergences. In the case of time mentioned above, such divergences are concretely avoided by the impossibility of backward time-travel, leading to unconditional convergence of  $\star$ -Neumann series.<sup>1</sup>

The main area of current development—to the point of taking much of my research time at the expense of all other venues of research—is that of tackling fractional and non-linear ODEs as well as PDEs within extended  $\star$ -algebras. The underlying ideas, given in more details below, are strongly unifying, lending the path-sum theorem a quasi-universal applicability. This *will work*, e.g. the solution of fractional and non-linear systems of ODEs have already been given a path-sum formulation although the general theory is still under construction.

For the second branch, at the moment a bit starved of research-time, I view sieves on hikes as uniquely powerful tools to tackle counting problems. The asymptotic behaviour of the fraction  $F(p)$  and the control of errors are the two main areas of development as explained in details below. Another interesting problem raised in Chapter 8 is that of characterizing hike monoids, i.e. those arrangements of cycles that exist on graphs. The fact that this problem is profoundly non-trivial is a signature of its importance. Every single aspect of the question turned out to be unexpectedly difficult. For every intuition we found an abundance of seemingly unrelated and always surprising counter-examples. This is the only problem of my career that led to a publication with essentially no positive results and at this point I sincerely have no idea how to even conceive what a possible solution would look like. That is, it feels like we do not have the right mathematical framework for it. As I discussed with collaborators, I have the vague intuition that the characterization of hike monoids is related to the cycle double cover conjecture, but my intuitions on the matter have been systematically wrong so far!

### 10.1 Exotic umbral calculi for path-sum solutions to non-linear ODEs and PDEs

The solution of non-autonomous systems of linear ODEs as path-sums in  $\star$ -algebras necessarily invites the question of whether a similar approach might work for other types of equations?

Consider firstly the non-linear ODEs. An insurmountable issue seems to obstruct any hope for these: the path-sum theorem is inherently limited to linear problems. Indeed, take for example the graph  $G$  with a single vertex and one self-loop  $c$  on it. Then the series of all closed walks on  $G$  is  $\Sigma_G := 1 + c + c^2 + \dots \equiv 1/(1 - c)$ . Now if we add a weight function  $w(\cdot)$  to the loop  $c$  and since the weight of a walk is the product of the weights of the edges it traverses,  $\forall n \in \mathbb{N}$ ,  $w(c^n) = w(c)^n$  leading formally to  $w(\Sigma_G) = 1/(1 - w(c))$ . In particular  $w(\Sigma_G)$  solves a linear equation, namely

$$w(c)w(\Sigma_G) = w(\Sigma_G) - 1.$$

---

<sup>1</sup>Interpreting  $\star$ -products as walks along the time-dimension is the way non-autonomous ODEs were solved in [67]. In this context the fact that  $\Theta(t' - t) = 0$  when  $t' < t$  is a signature of causality.

Now let us impose different weights to turn this into a non-linear equation, e.g. weights that depends on the length of a walk  $\omega$  as  $W(\omega) := f(\ell(\omega))w(\omega)$  with  $f : \mathbb{N} \rightarrow \mathbb{C}$ . One verifies easily that if the path-sum theorem hold for these weights then one should still have  $W(\Sigma_G) = 1/(1 - W(\Sigma_G))$ , which imposes that  $f(n) = \prod_i f(n_i)$  for any weak composition  $\{n_i\}$  of  $n$ , i.e.  $\sum_i n_i = n$ . In other terms, the path-sum resummation which exploits the bialgebraic structure on walks necessitates purely geometric weights and these are found only in solutions to linear problems.

To use the path-sum theorem one must therefore map a non-linear problem of interest to a linear one *exactly*, or else forfeit any hope of interesting applications. For weights depending on the length and the ordinary product, this means seeking operators  $O$  mapping the weights  $f(\ell)$  to geometric ones  $f(\ell) = O[\prod_i f(n_i)]$ ,  $\sum_i n_i = n$ . Oddly, this ad-hoc strategy works in all cases where it was given a chance, enabling e.g. weights  $f(n) = 1/n!$ ,  $f(n) = 1/n$  or  $f_q(n) = \binom{q}{n}$  to be used in conjunction with path-sums [77]. We mention the true underlying cause of success of this approach below, but first we turn to a related question about ODEs.

In the context of differential equations, and since the time-ordered exponential is a  $\star$ -resolvent, seeking a linear formulation for a non-linear problem is equivalent to seeking a solution of such a problem in terms of time-ordered exponentials. This idea was first explored by A. A. Agrachev and R. V. Gamkrelidze [1, 2] and later by Y. Kosovtsov in a series of powerful but completely overlooked contributions [107, 108, 109]. The key take-away message is that it is indeed formally possible to do so. Take for example the non-linear ODE,

$$\dot{u} = u^2, \quad u(0) = u_0$$

Kosovtsov made the following observational trick: introduce  $S(\omega, t) = e^{\omega u(t)}$  so that  $\partial_\omega S(\omega, t)|_{\omega=0}$  recovers  $u$ . Then observe that  $\partial_t S(\omega, t) = \omega \dot{u}(t) S(\omega, t)$  while for all  $n \in \mathbb{N}$  we get  $\partial_\omega^n S(\omega, t) = u(t)^n S(\omega, t)$ . Then the original equation reads, for  $S$ ,

$$\partial_t S(\omega, t) = \omega \partial_\omega^2 S(\omega, t)$$

This is now a linear ODE in  $S(\omega, t)$  that we solve as we did so far: introduce the (time-wise) Green's function  $G_S := \delta' \star S\Theta$ . This yields  $G_S = \omega \partial_\omega \Theta \star G_S$  where  $\delta'$ ,  $\Theta$  and the  $\star$ -products are all with respect to time. It follows that

$$G_S = (1_\star - \omega \partial_\omega^2 \Theta)^\star^{-1},$$

is a  $\star$ -resolvent. Remark crucially that this resolvent involves an operator  $\partial_\omega^2$ . This is perfectly fine because this operator is  $\partial_\omega^2 \equiv \delta''$  an element of  $\mathcal{D}$  just as those elements of  $\text{Sm}_\Theta$  encountered so far in ordinary linear ODEs. The  $\star$ -resolvent formal solution guarantees the applicability of the path-sum theorem to systems of non-linear ODEs and their amenability to  $\star$ -linear algebra methods, including a Lanczos procedure for tridiagonalization. Since  $\text{Inv}(\mathcal{D})$  is a Fréchet Lie-group to which  $\delta'$  belongs, non-integers  $\star$ -powers of  $\delta'$  are meaningfully accessible as functions of  $\delta'$ . This observation justifies the calculus of fractional derivatives with the  $\star$ -algebra framework and allows it to tackle fractional differential equations, yielding  $\star$ -resolvent formal solutions for them as well.<sup>2</sup>

In the context of recurrence equations, exact linearization is an indirect consequence of umbral methods. Classical umbral calculus concerns itself with the combinatorial study of polynomial sequences. The central tool is the umbral algebra formed by power series seen as both automorphisms and as linear functionals of the vector space  $\mathcal{P}$  of polynomials [171]. An umbral operator  $U_f$  associated with a series  $f(t)$  is an automorphism of  $\mathcal{P}$  that allows for global treatments of all polynomials of a sequence related to  $f$  at once. Products of umbral operators correspond to the composition of the associated series  $U_f.U_g = U_{f \circ g}$ . This effectively allows one to perform exact linearization because if one disposes of a formal derivation operator  $D$ , then it must hold that for any function  $\Phi$  and umbral operator  $U_f$ ,

$$\Phi(D).U_f = U_f.\Phi(f(D)),$$

In other terms, multiplying  $\Phi(f(D))$ —which may be non-linear in  $f$ —by the umbral operator associated with  $f$  turns it into  $\Phi(D).U_f$ , which is purely linear in  $f$ . This gives the proper explanation for Kosovtsov's trick and for the “operator-mapping weights to geometric ones” strategy. More precisely, umbral calculi on ‘exotic’ vector spaces explain both observations:  $S(\omega, t)$  is one of the representations of the umbral operator associated with  $u$  in an umbral calculus where  $\mathcal{P}$  is replaced by  $\mathcal{C}^\infty[I]$ ; and so are the operators  $O$  in an umbral calculus on the vector space  $\mathcal{F}$  of functions  $\mathbb{N} \rightarrow \mathbb{C}$ . We may now understand the  $\star$ -product as implementing the umbral composition on  $\mathcal{C}^\infty[I]$  via multiplication of operators on  $\mathcal{C}^\infty(I^2)$ . The Fréchet Lie-group  $\text{Inv}(\mathcal{D})$  plays for this umbral calculus the same role as the Riordan group [184, 38] does for the classical umbral construction on  $\mathcal{P}$ . This line of research points to an ‘universality’ theorem for graph walks and path-sums, something along the lines of the following conjecture (to which assumptions may yet be missing or need altering):

<sup>2</sup>Applicability of the path-sum theorem to such equations is known since my thesis. These unpublished results rely on an explicit representation of the derivative operator on a basis. A basis independent modern outlook using the  $\star$ -product is under development by S. Pozza and F. Durastante



**Conjecture 10.1.1.** *Let  $V$  be a (possibly infinite dimensional) vector space. Let  $S := \{s_1, \dots, s_n\} \in \text{Seq}(V)^{\otimes n}$  be a set of  $n \in \mathbb{N}$  (discrete or continuously indexed) sequences of elements of  $V$ . Let  $\mathcal{E}(S) = 0$  be a possibly non-linear, non autonomous system of, ordinary, partial or fractional equations to be solved in  $S$  and let  $A \in V^{n \times n}$  represent the sparsity structure of that system. Then there exists  $\mathbf{a}, \mathbf{b} \in V^{n \times n}$  and a product  $\bullet$  such that the solution is  $S = \mathbf{a} \bullet R_A \bullet \mathbf{b}$  where  $R_A$  is the  $\bullet$ -resolvent of  $A$ .*

Sequences of objects over vector spaces naturally come with a product  $\bullet$  (umbral composition) because these sequences are in bijection with endomorphisms of  $V$  (the umbral operators associated to the sequences), which form a natural algebra under composition. Combined with the path-sum expression for  $R_A$  in terms of the internal structure of  $A$  (seen as some sort of adjacency matrix,  $A$  gives rise to a graph  $G$  on which the path-sum makes sense), this provides an almost universal mean of tackling structured problems by providing formal solutions to such problems.

## 10.2 Sieves on hikes

Both the finite and the infinite sieve theorems have not been exploited to their full potential yet. In the finite case, the cycle centrality §9.2 deserves a closer look, in particular the associated entropy which has the curious property of also being an expectation value over SAPs of an expectation value over walks. But the main area of development should be the SAP-counting problem itself as detailed in §6.3:

### Asymptotic behaviour of one-sided sieves

A one-sided sieve on hikes suffers from an accumulation of errors hindering its direct use for SAP-counting. This is in line with the blight affecting the Eratosthenes-Legendre sieve from number theory. While the origin of these errors is sufficiently well understood, it is the main term itself that lacks understanding. For example it is still necessary to rely on R. Kenyon’s results [104] to obtain the  $1 - L^{-3/5}$  asymptotics for the series  $S(L)$  (see Fig. 6.2). That should not be: clearly a truly developed command of the sieve would produce this asymptotic by itself, a necessary step for further progress. The fundamental issue is that in spite of now having exactly access to the fraction  $F(\gamma)$  for any SAP  $\gamma$ , there lacks estimations for sums of fractions  $F(\gamma)$  over *infinite families* of SAPs. This may only be accessed via a better control of the asymptotic behaviour of determinants of infinite graphs with finite holes, something that may now be tackled with the tools of [54, 81]. For example, we obtain:

**Proposition 10.2.1** (Unpublished). *Let  $\gamma_{4L}$  with the square SAP on the infinite square lattice with side length  $L$ . Then the fraction of closed walks whose last erased loop is  $\gamma_{4L}$  behaves asymptotically, when  $L \rightarrow +\infty$ , as*

$$\frac{(4\sqrt{2} - 4)^{4L}}{4^{4L}}.$$

As a corollary, the connective constant of the square lattice obeys  $\mu > \sqrt{2} + 1$ .

While not revolutionary the above bound stems from purely theoretical arguments with no explicit counting of anything involved and exemplifies the connection with the SAP counting problem. Refinements of the above bound can be made on studying other families of SAPs such as rectangles, but as explained in §6.3, to determine  $\mu$  exactly likely necessitates two-sided sieves.

### Two-sided sieves

For such sieves one aims at controlling both the right and left divisors of hikes. Let  $\mathcal{M}_1, \mathcal{M}_2$  be sets of hikes such that one desires counting only those hikes whose left divisors are in  $\mathcal{M}_2$  and whose right divisors are in  $\mathcal{M}_1$ . Then, translating Bousquet-Mélou and Viennot’s results on heaps of pieces to the language of hikes, one obtains for finite graphs the following extension of Viennot’s lemma:

$$\sum_{\substack{h = p_2 h' p_1 \\ p_1 \in \mathcal{M}_1, p_2 \in \mathcal{M}_2}} z^{\ell(h)} = \sum_{h' \in \mathcal{P}_{G \setminus \{\mathcal{M}_1, \mathcal{M}_2\}}^{\text{s.a.}}} z^{\ell(h')} \frac{\det(\mathbb{I} - zA_{G \setminus \{h', \mathcal{M}_1\}}) \det(\mathbb{I} - zA_{G \setminus \{h', \mathcal{M}_2\}})}{\det(\mathbb{I} - zA_{G \setminus \{h'\}})}.$$

Here  $\mathcal{P}_{G \setminus \{\mathcal{M}_1, \mathcal{M}_2\}}^{\text{s.a.}}$  is the set of self-avoiding hikes on the subgraph of  $G$  obtained on deleting all vertices visited by at least one element  $\mathcal{M}_1 \cup \mathcal{M}_2$  and all edges adjacent to them. Similarly,  $G \setminus \{h', \mathcal{M}_1\}$  Exploiting this result concretely is difficult because of the sum over the set  $\mathcal{P}_{G \setminus \{\mathcal{M}_1, \mathcal{M}_2\}}^{\text{s.a.}}$ , on which little is known in general. Choosing  $\mathcal{M}_1$  and  $\mathcal{M}_2$  to control this set precisely is possible but necessitates a good control of the asymptotic behaviours of the above determinants as  $G$  becomes infinite. This is now feasible thanks to [54, 81]. For example we obtain:

**Theorem 10.2.1** (Unpublished). *Let  $G$  be the infinite regular lattice with degree  $\lambda$  and fix a vertex on it. Let  $W_{SAP_r}(2\ell)$  be the number of closed walks on  $G$  of length  $2\ell \gg 1$  and which begin by a self-avoiding section that moves at least a distance of  $r$  from the starting point. Then*

$$W_{SAP_r}(2\ell) \sim \frac{\lambda^{2\ell}}{\pi\ell} \alpha^{2r^2}, \quad \text{as } \ell \rightarrow +\infty$$

Here  $\alpha$  is the constant relating hike and walk densities defined in Lemma 6.2.1.

Remarkably, on the square lattice this implies that  $W_{SAP_r}(2\ell)$  grows exponentially with  $\ell$  only if  $r = \sqrt{2q\ell}$  with  $q < \frac{\pi \log(2)}{\pi \log(4) - 4C} \simeq \pi$  and  $C$  being Catalan's constant. Given that all SAP of length  $2\ell$  begin with a self-avoiding section of length  $2\ell$ , and given that the number of such SAPs is known to grow exponentially with  $\ell$ , we deduce that the fraction of those SAPs that are fully contained in the ball of radius  $\sqrt{2q\ell}$  centered on the origin goes to 1 as  $\ell$  goes to infinity. This is non-trivial since it relates to the dimension of the SAPs curves on the square lattice. Two-sided sieves necessitate much more studies to be fully understood, in particular naive approaches to the associated error terms yield permanents of infinite graphs with finite holes, quantities which are wholly unexplored.

# List of Symbols

$(\alpha)'_G$	Vertex $\alpha$ dressed by all closed walks rooted in $\alpha$ on $G$	p. 17
$\mathcal{C}^\infty(I^2)$	Set of functions that are smooth on an open neighborhood of compact $I^2$	p. 20
$A_G$	Adjacency matrix of graph $G$	p. 18
$c(\gamma)$	Cycle centrality of simple cycle $\gamma$	p. 82
$\mathcal{D}$	Set of distributions	p. 20
$\delta$	Dirac delta distribution	p. 20
$\Delta_{\text{CP}}$	Co-preLie coproduct on walks	p. 14
$E$	Edge set of a graph	p. 44
$\tilde{f}$	A function that is smooth on a compact $I$ of interest	p. 20
$\mathcal{F}$	Reduced incidence algebra of a hike poset	p. 47
$F_p \lambda^{-\ell(p)}$	Fraction of all closed-walk multiples of a SAP $p$	p. 52
$\phi(\cdot)$	Map sending a graph to its hike dependency graph	p. 72
$G$	Graph, digraph, multi-(di)graph	p. 44
$\mathbf{G}$	Green's matrix of a system of linear non-autonomous ODEs	p. 26
$\mathfrak{G}$	Semi continuous graph with discrete (space-like) and continuous (time-like) edges	p. 20
$\mathcal{G}$	Set of finite digraphs	p. 67
$\gamma$	Simple cycle	p. 17
$\Gamma(G)_\alpha$	Set of simple cycles from $\alpha$ to itself on $G$	p. 17
$\mathbf{H}$	Hamiltonian matrix	p. 33
$\Theta$	Heaviside Theta distribution	p. 20
$\mathcal{H}$	Hike monoid	p. 46
$H$	Hike dependency graph	p. 46
$H^c$	Hike independency graph	p. 46
$h$	Hike	p. 46
$\prec$	Induced subgraph relation	p. 57
$1_\star$	Identity element for the $\star$ -product	p. 21
$\text{Id}_\star$	Identity matrix times the identity element for the $\star$ -product	p. 26
$K_n$	Complete graph on $n$ vertices	p. 75
$K$	Algebraically closed field of characteristic 0	p. 12
$\lambda$	Hike Liouville function	p. 50
	Dominant eigenvalue of a graph	p. 55
$\Lambda$	Hike von Mangoldt function	p. 48
$\mu$	Mbius function on hikes	p. 47
$\odot$	Nesting product	p. 16
$P_G$	Poset of hikes on graph $G$ ordered per left-divisibility	p. 47
$\mathcal{P}^{\text{s.a.}}$	Set of self-avoiding hike constructible from the primes of set $\mathcal{P}$	p. 56
$\pi_\ell$	Number of of simple cycles of length $\ell$	p. 62
$\Pi(G)_{\alpha\omega}$	Set of simple paths from $\alpha$ to $\omega$ on $G$	p. 17
$\omega(\cdot)$	Number of prime factors of a hike	p. 48
$\Omega(\cdot)$	Number of distinct prime factors of a hike	p. 50
$\omega^{k,k'}$	Closed walk $w_k \cdots w_{k'}$ cut out of $\omega = w_0 \cdots w_\ell$	p. 12
$\omega_{k,k'}$	Remainder $w_0 \cdots w_k \cdots w_{k'+1} \cdots w_\ell$ after removal of $\omega^{k,k'}$ from $\omega$	p. 12
$\mathcal{S}f(s)$	Series associated with the function on hikes $f$	p. 48
$\Sigma_{G;\alpha\omega}$	Formal series of all walks from $\alpha$ to $\omega$ on $G$	p. 17
$\star, \star_I, \star_{\mathbb{R}}$	Star-product	p. 21
$*$	Subgraph convolution	p. 67
$\mathcal{T}$	Trace monoid	p. 45
$\mathcal{T}_{\text{CF}}$	Trace monoid of Cartier-Foata	p. 45
$T_n$	Tridiagonal matrix output of $\star$ -Lanczos	p. 29

$\mathfrak{T}$	Time-ordering operator	p. 19
$U$	Evolution operator, time-ordered exponential	p. 19
$V$	Vertex set of a graph	p. 44
$w, \omega$	Walk	p. 12
$W$	Labelled adjacency matrix of a graph	p. 18
$\mathcal{W}(G)$	Set of all walks on $G$	p. 12
	$K$ -vector space of rooted walks on $G$	p. 12
$\mathcal{W}(G)_{\alpha\omega}$	Set of all rooted walks on $G$ from $\alpha$ to $\omega$	p. 17
$z$	Formal variable	Throughout
$\zeta$	Zeta function on hikes	p. 48

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