The discrete magnetic Laplacian: geometric and spectral preorders with applications

by

John Stewart Fabila Carrasco

A dissertation submitted by in partial fulfilment of the requirements for the degree of Doctor of Philosophy in

Mathematical Engineering

UNIVERSIDAD CARLOS III DE MADRID

Advisor:
Fernando Lledó

Madrid, June 2020.

Published and submitted content

The main results of this thesis are based on the next list of papers.

- J. S. Fabila-Carrasco, F. Lledó, and O. Post. Spectral gaps and discrete magnetic Laplacians. *Linear Algebra and its Applications* **547** (2018): 183-216.
  https://doi.org/10.1016/j.laa.2018.02.006

  I am an author of this work, and it is included in Chapter 2, 3 and 4. The material from this source included in this thesis is not singled out with typographic means and references.

- J. S. Fabila-Carrasco and F. Lledó. Covering graphs, magnetic spectral gaps and applications to polymers and nanoribbons. *Symmetry* **11**(9) (2019): 1163.
  https://doi.org/10.3390/sym11091163

  I am an author of this work, and it is included in Chapter 2, 3 and 4. The material from this source included in this thesis is not singled out with typographic means and references.

- J. S. Fabila-Carrasco, F. Lledó, and O. Post. Spectral order of discrete weighted graphs. *In preparation.*

- J. S. Fabila-Carrasco, F. Lledó, and O. Post. A construction of isospectral graphs. *In preparation.*

The previous papers were presented by the author of this dissertation in the next following talks:

- Q-Math Seminar at Universidad Carlos III de Madrid. *Spectral gaps and the magnetic Laplacian on graphs*. March 2017.

  https://aplicaciones.uc3m.es/publicacion/agenda/show?id=30895

- 11^{th} Workshop of Young Researches in Mathematics at Universidad Complutense de Madrid. *Spectral gaps and discrete magnetic Laplacians*. September 2017.

  http://www.mat.ucm.es/imi/YoungResearchers17/Abstracts/Abstract_JSFabilaCarrasco.pdf

- Q-Math Seminar at Universidad Carlos III de Madrid. *Comparing graphs using the spectrum of the magnetic Laplacian*. January 2018.

  http://www.q-math.es/Other.php?year=2017/2018

- Analysis Seminar at the University of Trier. *Spectral ordering of discrete weighted graphs*. September 2018.

- Analysis Seminar at the University of Trier. *Construction of families of isospectral graphs*. November 2018.

- Discrete Mathematics Seminar at Universidad de Valladolid. *Construction of cospectral graphs*. June 2019.

  http://smd2019.blogs.inf.uva.es/programa/

- 13^{th} Workshop of Young Researches in Mathematics at Universidad Complutense de Madrid. *Construction of cospectral graphs*. September 2019.

  http://blogs.mat.ucm.es/mmatavan/wp-content/uploads/sites/12/2019/09/cartel-WorkshopJovenes2019F.pdf

Also, a simple code for the software *Wolfram Mathematica* was written to compute the eigenvalues for any finite magnetic weighted graph. The code is presented in Appendix B and it is available in the git repository:

https://github.com/JohnFabila/Magnetic-Laplacian.

Agradecimientos

Quiero agradecer a mi tutor Fernando Lledó por haber hecho posible esta tesis. Me refiero no solo al trabajo en conjunto para desarrollar las matemáticas presentadas en este trabajo, sino también al apoyo personal a lo largo de estos años, para conmigo y para con mi familia. Gracias.

Un agradecimiento muy especial al Dr. Olaf Post por involucrarse tan activamente en este trabajo, por recibirme en la Universidad de Trier y hacer mi estancia junto con la de mi familia lo más placentera posible en esta bella ciudad. Gracias a su esposa Linda y a su hijo Felix por todas esas comidas y paseos. Esos tres meses en Alemania han sido de lo más maravillosos. *Danke Olaf*.

Gracias a la Universidad Carlos III de Madrid y a todo el personal del Departamento de Matemáticas por el apoyo que me brindaron en estos años y a todos mis compañeros de despacho a lo largo de este tiempo.

Un agradecimiento a Carlos Marijuán, por su involucramiento y sus comentarios, que permitieron mejorar notablemente la notación del presente trabajo.

A mi familia por su apoyo, lo sentía tan cercano a pesar de los 9,000 km. de distancia. Gracias a mis padres: Agustina y Efraín. A mis hermanas: Gwendy y Debbie. A mis sobrinas: Daniela, Andrea y a Dieguito bebé.

Finalmente, gracias a Are por ser la mejor compañera de esta vida y a Sofia, por ser el motor de todo. Gracias a ellas por su amor, su comprensión y cariño que me dieron las fuerzas necesarias para llegar hasta aquí.

Mencionar a todas las personas que me han apoyado en mi formación profesional y personal para la culminación de esta tesis doctoral es una tarea imposible.

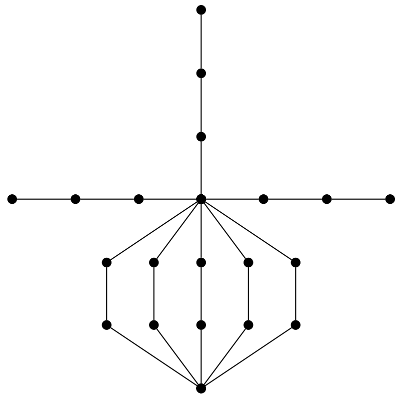
Gracias totales...

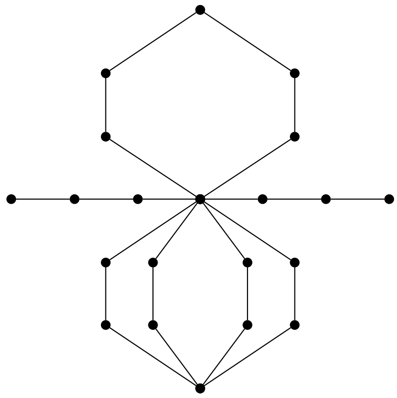
Este trabajo fue apoyado por el Ministerio de Economía y Competitividad mediante los programas DGI MTM2014-54692-P y MTM2017-84098-P. También se recibió la ayuda de

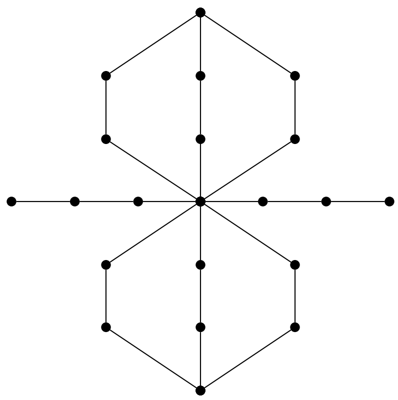
movilidad modalidad B en el 2018 para la realización de una estancia de tres meses en la Universidad de Trier, Alemania.

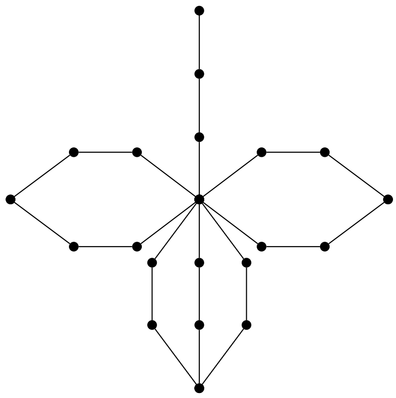
Para el mundo de Sofia

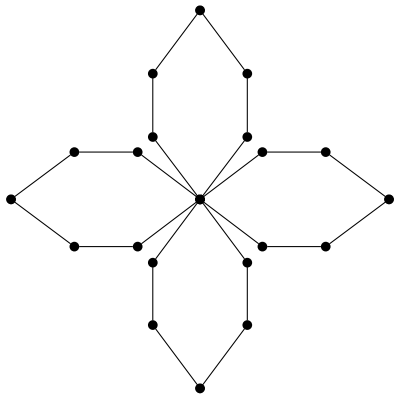
y para todos esos héroes desconocidos. . .











Contents

0 Introduction

Graph Theory is an important part of discrete mathematics with increasingly strong links to other branches. There are important connections with pure mathematics like Algebra [Big93; GR01], Combinatorics [LL00], Geometry [AL95; PR00], Group Theory [DD89; Lub94], Riemannian Manifolds [Maj13] and graph-like spaces [Pos12], to mention only a few. For example, a graph can be seen as a discrete structure resulting from a limit of specific continuous structure like, e.g., a Riemannian Manifold [Sin06]. The graph can have additional structure, for example, *metric graphs* [BC08; LP08a; Pos12] or a metric graph together with a self-adjoint differential operator, known as *quantum graph* [BK13; Kuc04; Kuc05] (see also references therein). However, its interest does not come only from a theoretical, but also from an applied point of view. Many problems in real-life can be modelled by a diagram (*graph*) that consists of a set of points (*vertices*) together with some lines joining pairs of points (*edges*). Some applications of graph theory are, for example, in social-networks [HRH02], chemistry [Jan+07] or computer science [Deo74].

Graphs are also interesting spaces on which one can do analysis. This branch of the mathematics is known as spectral graph theory [Bap10; Chu97; Exn+08; Mer94]. The analysis on graphs is a relatively new and active area of research. In the last years, the subject has experienced significant growth due to its role as an essential modern tool for applied mathematics; for example, the graphs are indispensable tools in communication and social networks [CS11]. The spectral graph theory associates an operators (or matrices) to the graph and compute or give an estimation of its spectrum. Finally, we relate the spectrum to the structural property of the graph. The connection between the topological and combinatorial structure of the graph through the spectrum of the operator is particularly interesting [LL93]. The *Cheeger constant* of a graph gives one these relations, and such constant is the discrete analogue of the Cheeger isoperimetric constant of a compact Riemannian manifold [Che70]. The *Cheeger constant* is a measure of the *bottleneck* of a graph, and it has much interest in many areas [BS97], for example, for the constructions of well-connected computer networks. The graphs related to these networks are sparse graphs which are highly connected; such graphs are known as *expander graphs*. Some explicit constructions of expander graphs are studied, for example, in [LPS88; Mar73; MSS15]. Also, the analysis on graphs is useful in spectral clustering, one of the most used and modern techniques for exploratory data analysis, see, e.g. [Lux07].

On a discrete graph, the most prominent operator is the discrete Laplacian (denoted by Δ). Such operator is the discrete analogue of the Laplacian on Riemannian manifolds [Ros97]. Some standard literature in the topic is [BH12; Chu97; CDS95; Spi12]. The discrete Laplacian can be generalised in a natural way to include a magnetic field which is modelled by a magnetic potential function defined on the edges of the graph. Such operator is called in [Shu94] the Discrete Magnetic Laplacian (*DML* for short) and is denoted by Δ_α. The analysis of the *DML* is interesting for theoretical issues and in applications to mathematical physics, particularly in solid state and condensed matters physic, where the graphs have the free action of a crystallographic group. In [Sun94], Sunada generalises the magnetic Laplacian for graphs with a free action of a finitely generated group. The analysis of the spectrum of the magnetic Laplacian is a particularly rich object of study because the presence of the magnetic potential amplifies the relationship between the operator and the topology of the graph (see [DM06; HS99; GM08] and the references therein).

In the present dissertation, we are interested in the spectral properties of the magnetic Laplacian. We study the spectrum of the Magnetic Laplacian under some geometrical perturbation on the graph. In particular, we are interested in the existence of spectral gaps, i.e., intervals that do not contain spectrum. We begin this dissertation giving a general context and a brief summary of some studies about the *DML* and in relation to the work in this thesis.

The spectrum of the magnetic Laplacian

The motivation for the study of the *DML* comes from mathematical physics, where a Schrödinger operator describes the dynamic of a quantum physical system. Thus, the study of the spectra of such operator is an essential topic in this field. The magnetic Laplacians is the discrete analogue of the Schrödinger operator with a magnetic field (see, e.g. [AHS78]). Moreover, the interest comes from other topics, recently the language of discrete forms and discrete differential operators has been studied in [DKT08] or [GP10]. In particular, a magnetic potential is a discrete form that has been used to study a discrete electromagnetic and the Maxwell's discrete equations restricted to lattices (cf. [Bar08]). The study of the spectrum of the magnetic Laplacian goes one step further and promises to be thrilling for theory and applications (for example, for the visualisation of directed networks [Fan+18]).

An additional motivation for the study of the magnetic Laplacian comes from the fact that it is a natural generalisation of the usual Laplacian Δ. More precisely, any magnetic potential α (where α can be also interpreted as a 1-form acting on the graph) induces a magnetic flux on each cycle of the graph. Two magnetic potentials are cohomologous if and only if they induce the same magnetic flux [LL93]. If the magnetic potential is cohomologous to zero (i.e., α acts trivially on the graph or the magnetic flux is zero on each cycle), then the usual Laplacian Δ is unitarily equivalent to the Δ_α. In particular, the spectrum of the usual Laplacian coincides with the spectrum of the magnetic potential with vector potential cohomologous to zero. The usual Laplacian has been studied for example in [BH12; Chu97; Spi12] (see also the references cited therein) while for the magnetic Laplacian we refer to [HS99; MY99; KS14].

The Laplacian Δ is an operator defined on the set of vertices of the graph and depends only on the vertices adjacent to it. Thus, the Laplacian is a second-order local operator. In the case that the graph is finite, the spectrum of the magnetic Laplacian is simply the set of eigenvalues of finite multiplicity. Some results known for the spectrum of finite graphs can be extended to infinite graphs (see, e.g. [Moh82]). For example, if the graph is finite or infinite, it can be shown that the Laplacian is a bounded, self-adjoint and positive operator [Chu97; Spi12]; hence its spectrum is a compact subset of the real numbers. However, when the graph is infinite, the spectrum of the magnetic Laplacian is a more complex object.

Some natural questions arise from the study of the spectrum of the Laplacian. We are interested in this dissertation in the following questions :

- *Question 1:* What can we say about the spectrum of the Laplacian on infinite graphs? [Moh82]
- *Question 2:* Does the spectrum have gaps? [Sun08]
- *Question 3:* Which graphs are determined by their spectrum? [DH03]

The solution of these questions is an active area of research, and some general overview of results of infinite graphs are, for example [Moh82; MW89]. However, it is almost impossible to give a general answer, and only partial solutions have been given in recent years.

Some answers to Question 1. One possibility to answer *Question 1* is to work with special cases of infinite graphs to address this question. Some few examples are the following:

- The Laplacian on infinite graphs in terms of the exponential growth is studied in [Moh91].
- The Laplacian on infinite periodic graphs, cf., [HS04b; HS99; LP08a; KS14; KS15; Sun08].
- The Laplacian on infinite trees with pendant edges, see, e.g., [Suz13].
- The Laplacian on infinite graphs are studied with Dirichlet and Neumann boundary conditions in [Hae+12].

In general, it is a well-known fact that the spectrum of Laplacians or, more generally, Schrödinger operators with periodic potentials, on Abelian coverings, have band structure. These properties of the Laplacians are discussed, e.g., in [GT84; GT87; Skr85] and the references therein. In the context of periodic manifolds or metric graphs, Dirichlet-Neumann bracketing allows to localise the spectrum of the differential operator in certain closed intervals whose endpoints are specified by the Laplacian on a fundamental domain with Dirichlet or Neumann boundary conditions (see, e.g., [LP07; LP08a; LP08b] and references cited therein). In [KS15] the authors develop a bracketing technique similar to the Dirichlet-Neumann bracketing and proved estimates of the position of the spectral bands for the combinatorial Laplacian in terms of suitable Neumann and

Dirichlet eigenvalue intervals. Moreover, they give an upper estimate of the total band length in terms of these eigenvalues and some geometric data of the graph; this method is extended in [KS17a] to the case of magnetic Laplacians with periodic magnetic vector potentials.

The spectrum of a periodic operator consists of a continuous part (which is the union of intervals or spectral bands separated by gaps) and a set of eigenvalues with infinite multiplicity. The spectrum is described in terms of a so-called Floquet (or Bloch) parameter. This parameter is the dual of the Abelian group acting on the structure. If two consecutive spectral bands of a bounded self-adjoint operator T do not overlap, then we say that the spectrum has a spectral gap, i.e., a maximal non-empty interval $(a, b) \subset [-\|T\|, \|T\|]$ that does not intersect the spectrum of the operator. A method to open gaps in the spectrum — completely independent of the periodicity of the underlying graph — was presented by Aizenman and Schenker in [SA00], decorating each vertex of the original graph with a copy of a given finite graph.

Some answers to Question 2. The study of the spectral bands/gaps from *Question 2* is a quite natural situation in several fields of mathematics and physics. In solid state physics, where—for example in semiconductors or its optical counterparts, photonic crystals—the operators modelling the dynamics of particles have some forbidden energy regions (see, e.g., [Kuc01; KK02]). In band-gap engineering, a process to control de band/gap of some materials, for semiconductors is controlled for example with the composition of alloys [SN10], and for the nanoribbons with temperature [Han+07], etc. Depending on the type of the periodic structure involved, spectral gaps may be produced by deformation of the geometry (cf., [LP07; LP08b; Pos03]) or by a suitable decoration of the periodic metric/discrete graph (see, e.g., [SA00; KS15; LP08a; Suz13] and [Kuc05, Section 4].

The study of energy-gaps has been widely studied. The gaps in nanoribbons as a function of the width can be found in [SCL06]. The gaps in the armchair structure can appear because quantum confinement and for the zigzag structure can appear because of an edge magnetization [ZG11].

Some answers to Question 3. For a graph, we can associate several types of matrices and operators. The spectral graph theory studies the relationship between the structure of the graph and the spectrum of these operators. Some graphs have a different structure but the same spectrum for some Laplacian. These graphs are called isospectral or cospectral with respect to the Laplacian. Some construction of isospectral graphs for the adjacency matrix can be found in [GM82]. In this reference, the construction studied can produce almost all the graphs on 9 vertices that have a isospectral pair for the adjacency matrix, i.e, graphs that are not determined by its spectrum. In [HS04a], it is enumerated all graphs on at most 11 vertices that are determinate by their spectrum. Isospectral graphs for the combinatorial Laplacian are studied in [HS04a; Mer97; CDS95], etc. Some construction for the normalized Laplacian is presented in [But10; BG11; Tan98]. However, little is known for the isospectral graphs with magnetic potential. The magnetic potential related with the signless Laplacian (i.e., if $\alpha_e = \pi$ for each edge of the graph), and its construction of isospectral graphs can be found in [HS04a].

The next table taken from [BG11] (see also [HS04a]) shows the number of graphs with an isospectral mate for different types of Laplacians: for the combinational Laplacian, the signless (combinatorial) Laplacian and for the normalized Laplacian.

No. vertices	No. graphs	Combinatorial	Signless	Normalized
1	1	0	0	0
2	2	0	0	0
3	4	0	0	0
4	11	0	2	2
5	34	0	4	4
6	156	4	16	14
7	1044	130	102	52
8	12346	1767	1201	201
9	274668	42595	19001	1092

Observe that as the order of the graph increases, the number of isospectral graphs for the normalized Laplacian is clearly lower than in the case of Laplacians with other weights. Many of the isospectral mates are found by computer programs that list the number of simple graphs with a fixed (and small) number of vertices and, then, determine the spectra of the corresponding Laplacians by hand. Given the huge complexity of graphs as the order increases it is clear that this strategy is limited. Few constructions are known for determining isospectral graphs for the normalized Laplacian.

Answers to Question 1 in this dissertation. We treat a special kind of infinite graphs, that are known as *periodic graphs* or *covering graph*, and we consider the magnetic Laplacian with periodic potential acting on it. We prove that the spectrum of the Laplacian on the periodic graph can be reduced to the study of the spectrum of the magnetic Laplacian in the finite quotient graph (cf. Chapter 3). Thus, information on the spectrum on the finite quotient can be *lifted* to the periodic graph.

Answers to Question 2 in this dissertation. We study the spectral gaps of the magnetic Laplacian on periodic graphs and give a geometrical criterion to detect spectral gaps (cf. Chapter 4). For the study of the magnetic Laplacian, we develop a discrete bracketing technique that will be useful to localise the spectrum of the periodic graphs.

Answers to Question 3 in this dissertation. In Chapter 5, we present a new geometrical construction leading to an infinite collection of families of graphs, where all the elements in each family are (finite) isospectral (weighted) graphs for the magnetic Laplacian with standard weights. One motivation for the choice of standard weights is given by the previous table. The construction is based on the the preorder of graphs introduced in Chapter 2. Moreover, the parametrization of the isospectral graphs in each family is given by a number theoretic notion: the different partitions of a natural number.

The answers we give to all the previous questions are based on a new and fundamental tool that we developed in Chapter 2 of the thesis on which the results of the remaining chapters are based. Concretely, we present two different preorders (i.e., a reflexive and transitive relation) on the discrete graphs. The first one is based on a geometric perturbation of the graph. The second one is related to the order of the eigenvalues of the Laplacian (which are real and non-negative). We also present some applications of these preorders in other fields like, for example, in chemical graph theory (cf. Chapter 6).

The Laplacian under some graph perturbation has been studied for example in the next papers: the spectral radius of the normalized Laplacian in [Guo07], the last eigenvalue of signless Laplacian in [WF12], for the adjacency matrix in [CR17], for some operation for the normalized Laplacian in [Che+04], and many more. Also, the perturbation that consists on the virtualisation of vertices and edges on discrete graphs studied in this dissertation is motivated by the metric graph case considered in [LP08a]. The perturbation operation on graphs gives us a natural geometric preorder, and we reference [ST93; TM76] for some others preorder and orders in graph theory.

Structure of this thesis.

In this section, we will summarise the essential result and techniques developed in each chapter of the present dissertation. We begin showing in Figure 0.1 the logical dependence of each chapter. As mentioned above, the preorder introduced and developed in Chapter 2, will be the base of the results presented in Chapter 4-6.

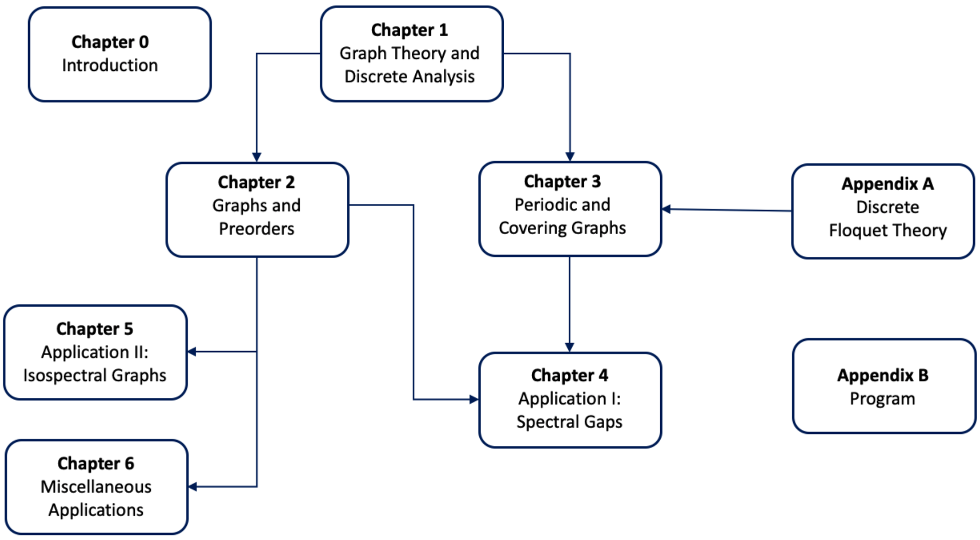


FIGURE 0.1: This first figure shows the interdependences of the chapters and suggests some pathways through the thesis.

Notation

We denote a magnetic weighted graph (*MW*-graph for short) as $\mathbf{G} = (G, \alpha, w)$, where G is a graph, w are the weights on edges and vertices and α a vector potential. Any magnetic weighted graph has canonically associated a *DML* denoted as $\Delta^{\mathbf{G}} = \Delta_\alpha^G$. We will present our analysis for graphs with arbitrary weights w on vertices and on edges. Nevertheless, the standard and combinatorial weights will be a privileged class of examples. In this dissertation, we study the spectrum of discrete magnetic Laplacians on infinite discrete coverings graphs

$$\pi: \widetilde{\boldsymbol{G}} \to \boldsymbol{G} = \widetilde{\boldsymbol{G}}/\Gamma \ ,$$

where Γ is an (Abelian) lattice group acting freely on $\widetilde{G}$ (also the graph $\widetilde{G}$ is called as Γ-periodic graph with finite quotient G). We say that $\widetilde{\boldsymbol{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ is a Γ-periodic magnetic weighted graph if Γ is an Abelian group, $\widetilde{G} \to G = \widetilde{G}/\Gamma$ is a Γ-covering and $\widetilde{w}$ and $\widetilde{\alpha}$ are periodic with respect to the group action. In particular, $\widetilde{\alpha}$ on the edges of the covering graph $\widetilde{G}$ modelling a magnetic field acting on the graph.

This dissertation is organised as follows.

Chapter 1

In this chapter, we provide the necessary notation and fundamental results in graph theory and discrete analysis needed for the subsequent chapters. In Section 1.1, we present an elementary introduction to the Theory of Graphs (some standard references are [BM08; Sun13]). The combinatorial structure of the graph consists of vertices and edges, but often need to add some information (as costs on edges and vertices). Thus, in Section 1.2, we introduce the notion of a weighted graph. The introduction of a magnetic potential acting on the graph appears in many physical applications (see, e.g., [ARZ87]), therefore in Section 1.3, we present some relevant results related to the magnetic potential. This complete the description of the structure needed: a discrete weighted graph with magnetic potential, that allows defining the twisted derivative in Section 1.4. Then, the most important operator in this dissertation, the discrete magnetic Laplacian is defined in Section 1.5, and some important properties of the spectrum of the operator are collected in Section1.6, more results on spectral graph theory of Laplacians can be found, e.g., in [Chu97; Spi12]. The importance of this first chapter is the introduction of the language for working with several Laplacians at the same time (normalized Laplacian, combinatorial Laplacian, signless Laplacian and more).

Chapter 2

In this chapter, we define two preorders in the class of magnetic weighted graphs. A *geometrical* preorder $\sqsubseteq$ for finite and infinite magnetic weighted graphs is defined in Section 2.1, moreover, for the class of magnetic graphs with normalized or combinatorial weights, the relation $\sqsubseteq$ is, in fact, a partial order (Theorem 2.1.6). Also, a *spectral* preorder $\preccurlyeq$ for finite magnetic graphs is defined in Section 2.2. The relation between the *geometrical* preorder and the *spectral* preorder is shown in Section 2.3. Moreover, for finite graphs, we prove in Theorem 2.3.3 that the preorder $\sqsubseteq$ implies the preorder $\preccurlyeq$. We recalled the well-know variational characterisation of the eigenvalues for an operator on a finite dimension (Theorem 2.3.2) which will be fundamental in Chapter 2. Finally, in Section 2.4, we study the behaviour of the spectrum of the magnetic Laplacian under some perturbation or elementary operations, and obtain results for general weights on the graph. For example, if we delete an edge (Theorem 2.4.1), for contracting two vertices (Theorem 2.4.5), virtualising edges (Corollary 2.4.10) and virtualising vertices (Corollary 2.4.15). With all the results, we develop a discrete bracketing technique for finite weighted graphs which is based on the manipulation of the graph. This method is based on a selective virtualisation of specific edges $E_0 \subset E$ and vertices $V_0 \subset V$ of a given weighted graph $\boldsymbol{G} = (G, \alpha, w)$, where α is the magnetic potential and w denotes the weights on V and E, respectively. The process of edge and vertex virtualisation produces two different graphs $\boldsymbol{G}^- = (G^-, \alpha^-, w^-)$ respectively $\boldsymbol{G}^+ = (G^+, \alpha^+, w^+)$ with induced vector potentials and weights, such that the spectra of the corresponding *DML* have the following relation:

$$\lambda_k(\Delta_{\alpha^-}^{\mathbf{G}^-}) \le \lambda_k(\Delta_\alpha^{\boldsymbol{G}}) \le \lambda_k(\Delta_{\alpha^+}^{\mathbf{G}^+}), \quad k = 1, \ldots, n-r,$$

where $n = |V(G)|$ is the order of the graph and r is the number of virtualised vertices. We then say that $\Delta_{\alpha^-}^{\mathbf{G}^-}$ is *spectrally smaller* than $\Delta_\alpha^{\boldsymbol{G}}$ (resp. $\Delta_\alpha^{\boldsymbol{G}}$ is *spectrally smaller* than $\Delta_{\alpha^+}^{\mathbf{G}^+}$) and write

$$\Delta_{\alpha^-}^{\mathbf{G}^-} \preccurlyeq \Delta_\alpha^{\boldsymbol{G}} \preccurlyeq \Delta_{\alpha^+}^{\mathbf{G}^+}.$$

Virtualising the edges E_0 on which the vector potential is supported and a corresponding set of vertices V_0 in the neighbourhood of E_0 (see Chapter 2 for precise definitions) we are able to localise the *DML* on $\boldsymbol{G}^\pm$. This allows to introduced the so-called bracketing intervals

$$J_k := [\lambda_k(\Delta^{\mathbf{G}^-}), \lambda_k(\Delta^{\mathbf{G}^+})]$$

in which we are going to localise later the spectrum of Laplacian on the periodic graph.

Chapter 3

In this chapter, we introduce the notion of a covering graph (Section 3.1) or Γ-periodic graph (Section 3.2) with Γ an Abelian discrete group and denoted as $\widetilde{G}$. Also, we define a Γ-periodic magnetic weighted graph $\widetilde{\boldsymbol{G}} = \widetilde{\boldsymbol{G}}$, where $\widetilde{G}$ is a Γ-periodic graph with $\widetilde{\alpha}$ and $\widetilde{w}$ are Γ-invariant, and finite quotient $\boldsymbol{G} = \widetilde{\boldsymbol{G}}/\Gamma$. In Definition 3.2.5, we introduce the notion of a fundamental domain (denoted as D). In Section 3.3, we introduce a discrete version of Floquet theory. In Section 3.4, we interpret the magnetic potential $\widetilde{\alpha}$ on the periodic graph $\widetilde{G}$ as a Floquet parameter in the finite quotient. We introduce the family of magnetic potentials with the lifting property and denoted as $\mathcal{A}_D$ (see Definition 3.4.1). Such subclass of magnetic potentials is necessary to prove the main result in this chapter: Theorem 3.4.2. In this result, we show the equivalence of the spectrum of the magnetic Laplacian on a periodic weighted graph with the union of the spectrum of the magnetic Laplacian for the family of magnetic potential acting in the finite quotient $\mathcal{A}_D$.

Theorem (3.4.2)**.** Consider a Γ-periodic weighted graph $\widetilde{\boldsymbol{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ with D a fundamental domain. If $\boldsymbol{G} = (G, \alpha, w)$ where $\boldsymbol{G} = \widetilde{\boldsymbol{G}}/\Gamma$, then

$$\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{\boldsymbol{G}}}) = \bigcup_{\alpha \in \mathcal{A}_D} \sigma(\Delta_\alpha^{\boldsymbol{G}}).$$

Chapter 4

In this chapter, we study the Laplacian $\Delta^{\widetilde{G}}$ (with standard, combinatorial or general periodic weights) on the infinite periodic graph $\widetilde{G}$ that has not the maximal possible interval as its spectrum. Such Laplacians are said to have a *spectral gap*. To show the existence of spectral gaps, we use the discrete bracketing technique based on *virtualisation* of edges and vertices on G for the discrete magnetic Laplacian on $\boldsymbol{G}$ (Chapter 2). Given a weighted graph (G, w) and $\mathcal{A}$ a family of magnetic potential acting on the graph G, we introduce the notion of *magnetic spectral gap* (with respect to $\mathcal{A}$), which in the case of standard weights is given by

$$\mathcal{MS}^{\boldsymbol{G}}_{\mathcal{A}} = [0,2] \setminus \bigcup_{\alpha \in \mathcal{A}} \sigma(\Delta^{\boldsymbol{G}}_{\alpha}) \,.$$

In other words, the magnetic spectral gap is the intersection of all resolvent sets of the magnetic Laplacian $\Delta^{\boldsymbol{G}}_{\alpha}$ for all $\alpha \in \mathcal{A}$ with the set $[0,2]$. If $\boldsymbol{G}$ is a tree, then $\mathcal{MS}^{\boldsymbol{G}}_{\mathcal{A}}$ coincides with the spectral gaps $\mathcal{S}^{\boldsymbol{G}}$ of the usual Laplacian $\Delta^{\boldsymbol{G}}$ with $\alpha = 0$ (see Section 4.1 for the details).

Let $\boldsymbol{G} = (G, \alpha, w)$ be a finite magnetic weighted graph, in Theorem 4.1.3 we present a simple geometric conditions on $\boldsymbol{G}$ that implies the existence of magnetic spectral gaps for a family of magnetic potential $\mathcal{A}$ acting on G. In Subsection 4.1.2, we study the spectral gaps in Γ-periodic weighted graph, and in Theorem 4.1.10 we solve the Higuchi-Shirai's conjecture for $\mathbb{Z}$-periodic trees, i.e.,

Theorem (4.1.10)**.** Let $\widetilde{\boldsymbol{G}} = (\widetilde{G}, 0, \widetilde{w})$ be a $\mathbb{Z}$-periodic tree with standard or combinatorial weights and quotient graph $\boldsymbol{G} = (G, 0, w)$. Then the following conditions are equivalent:

(i) $\widetilde{\boldsymbol{G}}$ has the full spectrum property;
(ii) $\mathcal{S}^{\widetilde{\boldsymbol{G}}} = \emptyset$;
(iii) $\widetilde{G}$ is the lattice $\mathbb{Z}$;
(iv) $\mathcal{MS}^{\boldsymbol{G}} = \emptyset$;
(v) G is a cycle graph;
(vi) G has no vertex of degree 1.

We conclude this chapter showing in Section 4.2 how to apply the methods developed to several classes of examples of periodic graphs. The first example gives an alternative and simple proof of the result by Suzuki in [Suz13] on the existence of spectral gaps for $\mathbb{Z}$-periodic graphs with pendants edges.

The other examples are more elaborate and include modelisations of *polypropylene* and *polyacetylene* molecules. We also prove the existence of spectral gaps in these periodic structures. The last model can be understood as an intermediate covering of the graphene, where the quotient has Betti number 2. One of the new aspects of the present dissertation is the generalisation of results in [FLP18] to include a periodic magnetic field $\widetilde{\alpha}$ on the covering graph $\pi \colon \widetilde{\boldsymbol{G}} \to \boldsymbol{G} = \widetilde{\boldsymbol{G}}/\Gamma$. In this sense, $\widetilde{\alpha}$ may be used as a control parameter for the system that serves to modify the size and the regions where the spectral gaps are localised. We apply our techniques to the graphs modelling the polyacetylene polymer as well as to graphene nanoribbons. The *nanoribbons* are

$\mathbb{Z}$-periodic strips of graphene either with an armchair or zig-zag boundaries (see, e.g., Figure 4.10). Figure 0.2 corresponds to an armchair nanoribbon with a width 3. It can be seen how a periodic magnetic potential with constant value $\widetilde{\alpha} \in [0, 2\pi)$ on each cycle (and plotted on the horizontal axis) affects the spectral bands (grey vertical intervals that appear as the intersection of the region with a line $\widetilde{\alpha} = const$) and the spectral gaps (white vertical intervals). We refer to Section 4.2.5 for additional details of the construction.

In the case of the polyacetylene polymer, we find a spectral gap that is stable under perturbation of the (constant) magnetic field. Moreover, if the value of the magnetic potential is π on each edge, i.e., $\alpha_e = \pi$, then the spectrum of the *DML* degenerates to five eigenvalues of infinite multiplicity. This discrete model suggests that a varying uniform magnetic field may drastically change the conductance of a material arranged as a periodic planar graph.

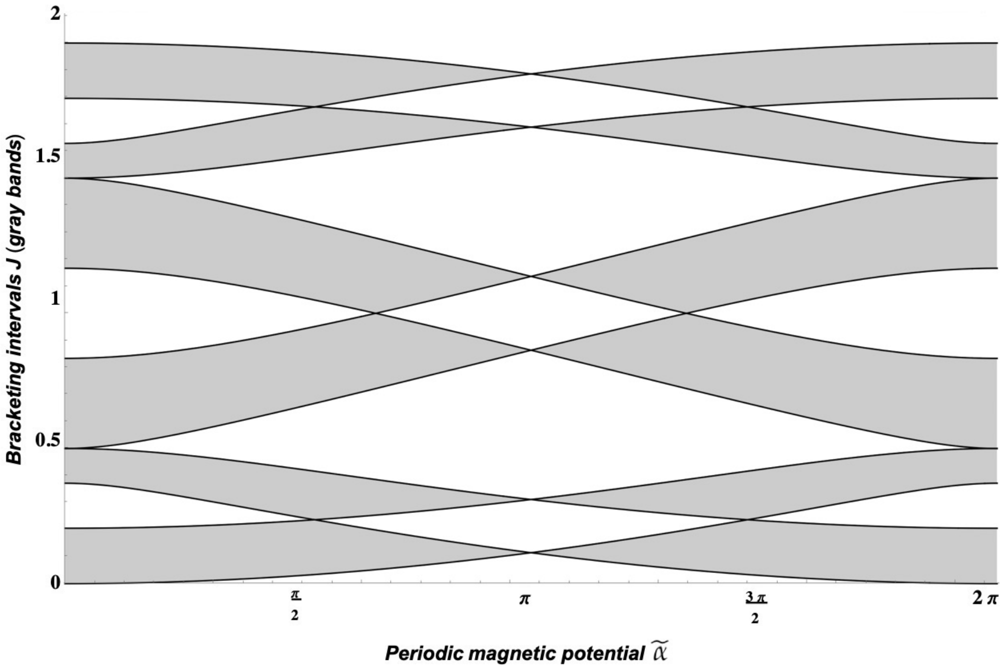


FIGURE 0.2: The structure of the bracketing intervals J is represented with grey bands and the spectral gaps with white bands. Both bands depend on the constant (periodic) magnetic potential $\widetilde{\alpha}$ acting on *3-aGNR*.

Chapter 5

Using the geometric perturbation as elementary operation on the graphs developed in Section 2.1, we present in this chapter a geometrical method of construction of isospectral magnetic weighted graphs. Let $\boldsymbol{G}_1 = (G_1, \alpha_1, w_1)$ and $\boldsymbol{G}_2 = (G_2, \alpha_2, w_2)$ be two magnetic weighted graph. We say that $\boldsymbol{G}_1$ and $\boldsymbol{G}_2$ are *isospectral* if they have the same spectrum, i.e., satisfy

$$\sigma\left(\Delta_{\alpha_1}^{G_1}\right) = \sigma\left(\Delta_{\alpha_2}^{G_2}\right) .$$

In this chapter, we treat the spectrum as a *multiset*. We begin with a motivating class of example in Section 5.1, where we consider $\mathfrak{G}$ as a family of magnetic weighted graphs with the standard weights. By contracting vertices of different elements of the family $\mathfrak{G}$ with respect to a partition of a natural number, give us a new graph. Then, if we take two partitions of the same natural number, with the previous construction, we create two graphs with the same spectrum. In Section 5.2, we generalise the previous example, and two crucial characteristics of the family of graphs $\mathfrak{G}$ are introduced. The *spectral* property is in Definition 5.2.5, and a *geometrical* property is in Definition 5.2.10. These properties give us in Theorem 5.2.12 a general construction for isospectral graphs. We conclude the chapter with Section 5.3, where we show how to apply, in an example, for the construction of isospectral graphs with magnetic potential.

Chapter 6

In this chapter, we present several applications of the results of Chapter 2 and 3. In Section 6.1, we present some composite operation, like contracting edges and deleting vertices. These composite operations are a combination of the two fundamental operations studied in Section 2.4: delete an edge and contracting vertices. In Section 6.2, we show some simple applications to the combinatorics. For example, how to apply the results for the fundamental notion of the graph minor. Also, we apply the preorder in Subsection 6.2.1 to obtain a relation with the *Cheeger constant* or *isoperimetric number* and the *frustration index* denoted as $h_k(\mathbf{G})$ where $\mathbf{G}$ is a magnetic weighted graph. In particular, we show in Theorem 6.2.8 that if $\mathbf{G} \sqsubseteq \mathbf{G}'$ then $h_k(\mathbf{G}) \leq h_k(\mathbf{G}')$. In the final part of the chapter (Section 6.3), we include some application in Chemical graph theory. In particular, we show order relation for the most important chemical indices that model certain properties of the molecule, like the Wiener index, Kirchoff index, and many more.

Chapter 7

This final chapter, present a conclusion of the results of this dissertation, and we propose some lines of investigation for the future.

The thesis also contains an appendix. In Appendix A we describe in detail the Floquet theory for periodic graphs. We apply this theory in Chapters 3 and 4. Moreover, we present in Appendix B the code made for Mathematica 12.0 to compute the many examples on which this thesis is based.

1 Graph Theory and Discrete Analysis

For the convenience of the reader and to do this thesis as self-contained as possible, in this first rychapter, we include some of the most important definitions, examples and results in Spectral Graph Theory needed later.

A graph is an abstract mathematical object that describes a set of objects (vertices) and a relation between them (edges). We present in Section 1.1 an introduction to the Theory of Graphs. We include the formal definition of graphs (we allow multiples edges and loops) which is one of the fundamental objects in this thesis. We will also introduce important concepts needed later like graph homomorphism (that are function between graphs). Also, we include some essential properties of graphs (bipartite, connected and more). We show some standard examples of graphs (complete, path, cycle, along with others) and operation with them (contracting vertices and delete edges). Also we introduce the definition of an open graph. Additional results and motivations can be found in, e.g. [BM08; Die05] and the references therein.

In Section 1.2, we put additional structure to the graphs: we will introduce weights on vertices and edges. In Section 1.3, we introduce an essential ingredient, that is the magnetic potential. The second fundamental object in our analysis in this thesis is the discrete magnetic Laplacian (Section 1.4). It is a natural generalisation of the usual Laplacian and incorporates the presence of a magnetic field on the graph. Typically the magnetic field is introduced in the analysis via a vector potential which is a function of the edges $\alpha\colon E \to \mathbb{R}/2\pi\mathbb{Z}$. Discrete magnetic Laplacians have already been treated, e.g., in [MY02; MY99] and [Sun94]. Magnetic Laplacians on Abelian covering graphs are discussed in [HS99; HS04b]. Korotyaev and Saburova treated discrete Schrödinger operators on discrete graphs in a series of articles (see, e.g., [KS14; KS15; KS16; KS17a; KS17b] and references therein).

In Section 1.5, we present a geometric definition of discrete Laplacians on a weighted graph. The general structures on graphs will allow treating many classes of Laplacian operators (standard, combinatorial, signless or discrete magnetic Laplacians) in a unified way. Our general approach will allow us to compare all these classes of operators from a spectral point of view. We conclude this chapter recalling some crucial results on the spectrum of the discrete magnetic Laplacians (Section 1.6). For completeness, we also include some detailed proofs, even if most of the results are known to experts.

1.1 Graph Theory

The following formal definition of a *graph* is taken from [Sun13].

Definition 1.1.1. A *graph* G is an ordered pair $G = (V, E)$ of disjoint sets V and E with two maps $\partial := \partial_G : E \to V \times V$ (*incidence map*) and $\iota := \iota_G : E \to E$ (*inversion map*) such that

$$\iota^2 = I_E \quad \text{(the identity map on } E\text{)}$$
$$\iota(e) \neq e, \quad \partial(\iota(e)) = \tau(\partial(e)), \quad \text{for all } e \in E,$$

where $\tau : V \times V \to V \times V$ is defined by $\tau(u, v) := (v, u)$. If we put $\partial(e) = (\partial^-(e), \partial^+(e))$, we obtain the maps $\partial^- : E \to V$ and $\partial^+ : E \to V$ with the relation $\partial^+(\iota(e)) = \partial^-(e)$ for all $e \in E$.

In what follows, $V = V(G)$ is the set of the *vertices* of the graph G, and $E = E(G)$ is the set of its *(directed) edges* of G. If it is clear from the context, we will omit the argument G and use simply V, E, ∂, ι (and others) instead of the symbols $V(G), E(G), \partial_G, \iota_G$.

The map $\partial = \partial_G$ is the *incidence map* that associates an ordered pair of (not necessarily distinct) vertices of G for each edge of G, while the map ι is called the *inversion map* and we usually write $\iota(e)$ in form $\bar{e}$. With this notation, the equality $\partial(\iota(e)) = \tau(\partial(e))$ is expressed as $\partial^-(\bar{e}) = \partial^+(e)$ and $\partial^-(e) = \partial^+(\bar{e})$. The *inversion map* gives rise to an action of $\mathbb{Z}_2 = \mathbb{Z}/2\mathbb{Z}$ on E. An *undirected edge* is an element of the orbit space $E/\mathbb{Z}_2$, i.e., a undirected edge is obtained by identifying e and $\bar{e}$. Along this thesis, by an edge we mean e or $\bar{e}$ and by undirected edge we mean the class of e with both directions.

Given an edge $e \in E$, we say that $\partial^-(e)$ is the origin, $\partial^+(e)$ is the end and $\bar{e}$ is the *inversion* of e (*inverse edge* or *opposite edge*).

A *loop* is an edge e such that $\partial^+(e) = \partial^-(e)$. Two edges e_1 and e_2 are *multiple edges* (or *parallel edges*) if $e_1 \neq e_2$ with $\partial^+(e_1) = \partial^+(e_2)$ and $\partial^-(e_1) = \partial^-(e_2)$.

A graph is *simple* if it has no loops or multiple edges.

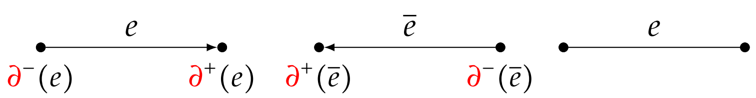


FIGURE 1.1: The representation of one (directed) edge, its inverse (directed) edge and the (undirected) edge, i.e., the class of e with both directions.

In a diagram representation of a graph, we represent each directed edge by an arrow, as is shown in Figure 1.1. Then e and $\bar{e}$ are expressed by the same line having arrows with opposite direction. However, we usually omit arrows when we draw the graph as in Figure 1.2

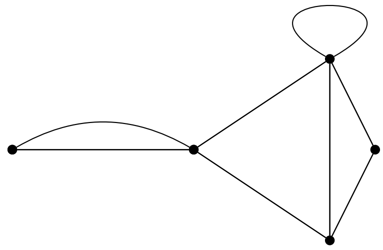


FIGURE 1.2: Example of a graph G with a loop and one multiples edges. Each line represents both directed edges e and $\overline{e}$.

For a vertex $v \in V$, the set of directed edges with origin v (resp. end v) is denoted as E_v^-(resp. E_v^+), i.e.,

$$E_v^{\pm} := \{e \in E \mid \partial^{\pm}(e) = v\} \ .$$

Observe that the loops appear two times on each set $E_v^{\pm}$. Also, define $E_v := E_v^- \cup E_v^+$. Throughout this thesis, we only consider *locally finite graphs*; that is, graphs $G = (V, E)$ such that $|E_v^{\pm}|$ is finite for any $v \in V$.

The *degree of a vertex v* in the graph G, denoted by $\deg_G(v)$, is the number of elements of E_v^+ (that is the same that E_v^-), i.e., $deg_G(v) = |E_v^+| = |E_v^-|$. A vertex v with $\deg_G(v) = 0$ is called an *isolated vertex*.

For two subsets $V_1, V_2 \subset V$, we define

$$E(V_1, V_2) := \{\, e \in E \,|\, \partial^-(e) \in V_1 \text{ and } \partial^+(e) \in V_2 \text{ or } \partial^-(e) \in V_1 \text{ and } \partial^+(e) \in V_2 \,\} \qquad (1.1.1)$$

the set of all edges with one vertex in V_1 and another one in V_2. If $V_1 = V_2$ we write $E(V_1)$ instead of $E(V_1, V_1)$. For $V_1 = \{v_1\}$, we simply write $E(v_1, V_2)$ instead of $E(\{v_1\}, V_2)$ and similarly for $V_2 = \{v_2\}$. The set of loops at v is $E(v) = E(v, v)$.

A set is a *discrete* set if it is either finite or countably infinite set. A graph $G = (V, E)$ considered in this thesis are *discrete graphs*, i.e., the sets V and E are discrete. The graph G is a *finite graph* if the sets V and E are finite sets. The graph G is an *infinite graph* if the sets V or/and E are infinite sets. If the graph is finite, the order of the graph denoted as $|G|$ is the number of vertices, i.e., $|G| = |E(G)|$.

Let $G = (V(G), E(G))$ and $H = (V(H), E(H))$ be two graphs. A *graph homomorphism* $\varphi\colon G \to H$ is a correspondence of vertices and edges that preserve the incidence relation among them. More precisely, it is a pair $\varphi = (\varphi_V, \varphi_E)$ of maps

$$\varphi_V\colon V(G) \to V(H), \quad \varphi_E\colon E(G) \to E(H)$$

such that satisfies for every $e \in E(G)$ the following

$$\begin{aligned} \partial_H^-(\varphi_E(e)) &= \varphi_V(\partial_G^-(e)) \ , \\ \partial_H^+(\varphi_E(e)) &= \varphi_V(\partial_G^+(e)) \ , \\ \overline{\varphi_E(e)} &= \varphi_E(\overline{e}) \ . \end{aligned}$$

For simplicity, we will use the same symbol φ for both φ_V and φ_E.

The mapping φ is a *graph isomorphism* if φ_V and φ_E are bijective, in this case, G and H are *isomorphic graphs*, and we will denote this as $G \cong H$. The map φ is a *graph automorphism* if $G = H$ and φ is an isomorphism.

The *Betti number* $b(G)$ of a finite graph $G = (V, E)$ is defined as

$$b(G) := |E| - |V| + 1 \, . \tag{1.1.2}$$

1.1.1 Families of Graphs

In this part, we show how construct graphs from other graphs. Also, we present certain types and families of graphs. Both play a prominent role in this dissertation.

When we analyse the virtualisation processes of vertices, edges in Chapter 2 and fundamental domains of periodic graphs in Chapter 3, it will be convenient to consider the following substructure of a graph.

Definition 1.1.2. Let $G = (V, E)$ be a discrete graph with incidence function ∂_G. Consider $V_1 \subset V$ and $E_1 \subset E$ that contains both orientation of each edge with $\partial_1 = \partial_G \restriction_{E_1}$. Define $G_1 = (V_1, E_1)$ with incidence function ∂_1, then:

(i) If $E_1 \subset E(V_1)$, then G_1 is a graph (Definition 1.1.1), in this case, we say that the graph G_1 is a *subgraph* of G.

(ii) Moreover, if $E_1 = E(V_1)$, then G_1 is also a graph. We say that the graph G_1 is a say an *induced subgraph* of G by the set V_0 and we denote $G_1 = G[V_0]$.

(iii) If $E_1 \notin E(V_1)$, then G_1 is not a graph. We say that G_1 is an *open subgraph* in G. We call

$$\begin{aligned} E(G_1, G) :=& E(V_1, V \setminus V_1) \cap E_1 \\ =& \{e \in E_1 \mid \partial^- e \in V_1 \text{ and } \partial^+ e \notin V_1 \text{ or } \partial^+ e \in V_1 \text{ and } \partial^- e \notin V_1\} \end{aligned} \tag{1.1.3}$$

the set of *connecting edges* of the open subgraph G_1 to G.

Remark 1.1.3.

(i) Note that a partial subgraph $G_1 = (V_1, E_1)$ is not a graph as in Definition 1.1.1, since we do not exclude edges $e \in E$ with $\partial(e) \notin V_1 \times V_1$. The edges not mapped into $V_1 \times V_1$ under ∂_G are precisely the connecting directed edges of G_1 to G. In other words, we only have $\partial_G \colon E(G_1, G) \to V \times V$, but $\partial_G \colon E_1 \setminus E(G_1, G) \to V_1 \times V_1$.

(ii) In contrast, for a subgraph or an induced subgraph, G_1 is itself a discrete graph as $E_1 \subset E(V_1)$ and hence ∂_G maps E_1 into $V_1 \times V_1$. Moreover, a subgraph (or an induced subgraph), the set of connecting edges from G_1 to G is empty.

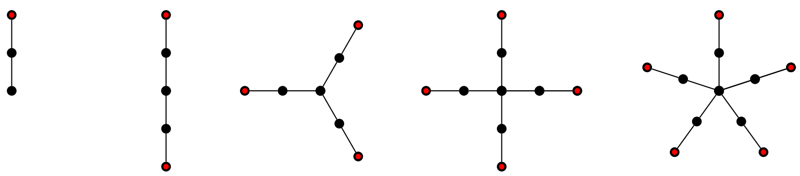
A *complete graph* on n vertices, is a simple graph in which any two vertices u, v are connected by an oriented edge from u to v. A graph is *bipartite* if its vertices V can be partitioned into two subsets V_1 and V_2 so that every edge has one end in V_1 and one end in V_2. A bipartite graph G with bipartition V_1 and V_2 is denoted as $G[V_1, V_2]$. If

$G[V_1, V_2]$ is a simple graph such that every vertex in V_1 is adjacent to every vertex in V_2, then G is called a *completed bipartite graph*. A *star* is a complete bipartite graph with $|V_1| = 1$ or $|V_2| = 1$.

A *path* in the graph G is a sequence of directed edges $c = (e_1, e_2, \dots, e_n)$ with $\partial^+(e_i) = \partial^-(e_{i+1})$ for $1 \le i \le n-1$. A *closed path* in the graph is a path with $\partial^+(e_n) = \partial^-(e_1)$.

A graph G is *connected* if for any two vertices u, v it exists a path from u to v. The graph G is a *tree* if G has no cycles. If G_1 is a tree and G_1 is a subgraph of G with $V(G_1) = V(G)$, we say that G_1 is an *induced tree* of G.

Given two natural numbers n and m, the (n,m)-star is the graph defined by the star graph with n edges S_n and change all the edge of the star with a path on m edges. See Figure 1.3 for an example of $(2,n)$-stars.



$(1,2)$-star $(2,2)$-star $(3,2)$-star $(4,2)$-star $(5,2)$-star

FIGURE 1.3: Examples of (n,m)-stars.

1.1.2 Basic Operations with Graphs

One basic way of combining graphs is with the *union*. Let G_1 and G_2 be two graphs, the *disjoint union* of the graphs denoted as $G_1 \dot\cup G_2$ is the graph with vertex set V making of the disjoint union $V(G_1) \dot\cup V(G_2)$, edge set E is the disjoint union $E(G_1) \dot\cup E(G_2)$ and incidence function $\partial_{G_1 \dot\cup G_2} \restriction_{E(G_i)} = \partial_{G_i}$ for $i = 1, 2$. This operation (which is associative and commutative) can extend to an arbitrary number of graphs. If $G_1 = G_2$, we denote $G_1 \dot\cup G_1 = (G_1)^2$. Every graph may be expressed as a disjoint union of connected graphs, these graphs are called the *connected components* (or simply, *components*) of G, and the number of components is denoted as $c(G)$. The next definition formalise it.

Delete edges

The first operation on graphs is the edge deletion. By this operation, we obtain a new graph, and for this reason, we should delete set of edges E_0 that contains both direction of each edge, i.e., $E_0 = \overline{E}_0$ where $\overline{E}_0 := \{\overline{e} \mid e \in E_0\}$. In particular, by delete an edge, we mean delete the both orientation of the edge in the graph.

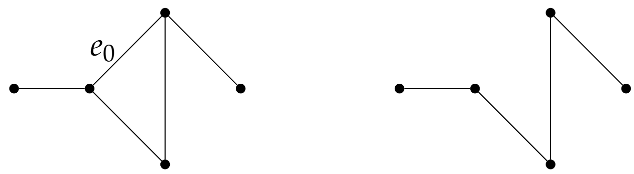
Definition 1.1.4 (Deleting edges). Let $G = (V, E)$ be a graph and $E_0 \subset E$ such that $E_0 = \overline{E}_0$, *delete edges* E_0 of the graph G (denoted by $G - E_0$) is the subgraph defined by $G - E_0 = (V, E \setminus E_0)$ with the same incidence function that G, i.e., $\partial_{G-E_0} = \partial_G \restriction_{E \setminus E_0}$.

If the set E_0 contains only one edge with both directions, i.e., if $E_0 = \{e_0, \overline{e_0}\}$, we will write $G - e_0$ rather than $G - \{e_0, \overline{e_0}\}$. This operation is fundamental in the next sections, c.f. Subsection 2.4.1.

An example of G and $G - \{e_0\}$ is shown in Figure 2.2. The reverse operation is called *adding edges*: We say that G is obtained from a graph G' by *adding the edges* $E_0 \subset G'$ if $G' = G - E_0$; for short we write $G = G' + E_0$ and also $G = G' + e_0$ if $E_0 = \{e_0, \overline{e_0}\}$.

The *inclusion homomorphism* is a graph homomorphism given by $i := i_{E_0} : G - E_0 \to G$ that acts as the identity in $V(G - E_0) = V(G)$ and the inclusion in $E(G - E_0) \subset E(G)$.

Let G be a graph; an edge e_0 is a *cut edge* if the deletion of the edge increases the number of connected components of G, i.e., $c(G - e_0) = c(G) + 1$. Thus a cut edge of a connected graph is one edge such deletion results in a disconnected graph.



(A) The graph G. (B) The graph $G' = G - e_0$.

FIGURE 1.4: If we delete the edge e_0 from graph G in Figure 2.2A, we obtain the graph $G' = G - e_0$ in Figure 2.2B.

Contracting vertices

The second operation is the contraction of vertices, also know as glueing vertices o merging vertices.

Let $G = (V, E)$ be a graph and $\sim$ be an equivalence relation on the set V, i.e., $\sim$ is a relation on V which is reflexive, symmetric and transitive. The equivalence classes of $v \in V$ under the equivalence relation $\sim$ is denoted as $[v]$ and is defined by

$$[v] := \{ v' \in V \,|\, v' \sim v \} .$$

The set of all the equivalence relations of V by the equivalence $\sim$ is denoted by:

$$V/\!\sim\; := \{[v] \,|\, v \in V\}$$

There is a natural map from V to $V/\!\sim$, called the *projection* of the equivalence relation $\sim$, i.e.,

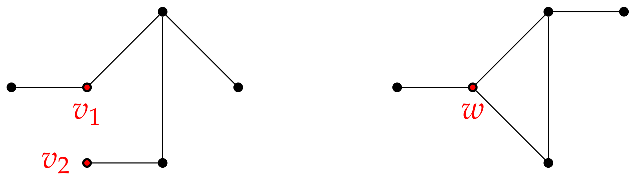
$$\pi : V \to V/\!\sim \quad \text{defined by} \quad \pi(v) = [v] . \tag{1.1.4}$$

Under the previous condition, the next operation on graphs is defined.

Definition 1.1.5 (Contracting vertices). Let $G = (V, E)$ be a graph and $\sim$ denote an equivalence relation on the set V, *contracting the vertices* (respect to $\sim$) of the graph G (denoted by $G/\sim$) is the graph defined by $G/\sim := (V/\sim, E)$ and incidence function $\partial^+_{G/\sim} := \pi \circ \partial^+_G$ and $\partial^-_{G/\sim} := \pi \circ \partial^-_G$.

Let G be a graph and $\sim$ an equivalence relation on $V(G)$. If the relation $\sim$ identifies only the vertices $v_1, \ldots, v_r \in V(G)$ to one vertex in G', we also say that G' is obtained from G by *glueing the vertices* $v_1, \ldots, v_r \in V$. We write $G' = G/\{v_1, \ldots, v_r\}$ for short (see Figure 1.5 for the case $r = 2$). The spectrum of the *DML* under the vertex contraction is studied in Subsection 2.4.2.

The reverse operation is called *splitting*: we say that G' is a *vertex splitting* of G if there is an equivalence relation $\sim$ on $V(G')$ such that $G = G'/\sim$.



(A) The graph G. (B) The graph $G' = G/\{v_1, v_2\}$ where $w = [v_1] = [v_2]$.

FIGURE 1.5: Contracting the vertices v_1 and v_2 of the graph G in 1.5A gives the graph $G' = G/\{v_1, v_2\}$ in Figure 1.5B.

Given the graph G and $G/\sim$, we have a natural graph homomorphism, named *projection map* defined as $\pi: G \to G/\sim$ given by $\pi(v) = [v]$ and $\pi(e) = e$.

Note that if we glue two *adjacent* vertices v_1 and v_2, all edges joining v_1 and v_2 become *loops* in $G/\{v_1, v_2\}$. The operation of identifying two vertices and deleting the adjacent edges is called *edge contraction*, and it is a combination of glueing v_1 and v_2 and deleting the adjacent edges $E(v_1, v_2)$.

If G is a finite graph, the *size* of the equivalence relation $\sim$ on $V(G)$ is defined as $|G| - |G/\sim|$.

1.2 Weighted Graphs

When a graph G is used to model some practical problem, one often needs to add some information to the combinatorial structure, such as costs associated with the edges or vertices. For example, in communications networks, some relevant factors could be the cost of the transmitting data or the numbers of computers in each communication centre. In this situation, the additional factors are modelled by putting *weight* on edges and/or vertices. Some application of weighted graphs can be found in [BE98].

Definition 1.2.1. A *weighted graph* (or *W-graph*) is an ordered pair $\boldsymbol{G} = (G, w)$ where $G = (V, E)$ is a graph and w is a weight associated with its vertices and its directed edges, i.e., w is a pair of functions (denoted with the same symbol) $w \colon V \to (0, \infty)$ and $w \colon E \to (0, \infty)$ such that $w(v)$ is the weight at the vertex v and w_e [1] is the weight at $e \in E$ with the property $w(e) = w(\bar{e})$.

Given the sets $V_0 \subset V$ and $E_0 \subset E$, it is natural to define the *weight of the sets* as:

$$w(V_0) := \sum_{v \in V_0} w(v) \qquad \text{and} \qquad w(E_0) := \sum_{e \in E_0} w_e \,. \tag{1.2.1}$$

The *relative weight* is a map $\rho \colon V \to (0, \infty)$ defined as

$$\rho(v) := \frac{w(E_v^-)}{w(v)} = \frac{w(E_v^+)}{w(v)} \,. \tag{1.2.2}$$

The weight is *normalized* if $\rho(v) = 1$ for all $v \in V$. If we need to stress the dependence of ρ of the weighted graph, we simply write ρ^G. We will assume throughout this dissertation that the relative weight is *uniformly bounded*, i.e.,

$$\rho_\infty := \sup_{v \in V} \rho(v) < \infty. \tag{1.2.3}$$

This condition will ensure in Proposition 1.4.4 that the discrete magnetic Laplacian is a bounded operator.

For each weighted graph $\boldsymbol{G} = (G, w)$, we associate the following Hilbert spaces

$$\ell_2(V, w) := \left\{ f \colon V \to \mathbb{C} \mid \|f\|^2_{V,w} = \sum_{v \in V} |f(v)|^2 w(v) < \infty \right\} \tag{1.2.4}$$

$$\ell_2(E, w) := \left\{ \eta \colon E \to \mathbb{C} \mid \|\eta\|^2_{E,w} = \frac{1}{2} \sum_{e \in E} |\eta_e|^2 w_e < \infty \quad \text{and} \quad -\eta_e = \eta_{\bar{e}} \right\}, \tag{1.2.5}$$

with inner products

$$\langle f, g \rangle_{\ell_2(V,w)} := \sum_{v \in V} f(v) \overline{g(v)} w(v) \quad \text{and} \quad \langle \eta, \zeta \rangle_{\ell_2(E,w)} := \frac{1}{2} \sum_{e \in E} \eta_e \overline{\zeta_e} w_e,$$

respectively. These spaces can be interpreted as 0- and 1-forms on the graph, respectively.

1.2.1 Examples of weights.

We present some important examples of weights which include the *intrinsic weights*, i.e., weights that depend only on the combinatorial structure of the graph: the combinatorial weight and the standard weights.

[1] Later, the virtualisation process of edges can also be interpreted allowing $w_e = 0$ on certain edges e.

Definition 1.2.2. Let $\boldsymbol{G} = (G, w)$ be a weighted graph.

(i) The weight $w = 1$, i.e., $w(v) = 1$ for all $v \in V$ and $w(e) = 1$ for all $e \in E$ is called the *combinatorial weight*. We denote a graph with combinatorial weights as $\boldsymbol{G} = (G, \mathbb{1})$.

(ii) The weight w given by $w(v) = \deg(v)$ for all $v \in V$ and $w(e) = 1$ for all $e \in E$ is called the *standard weight*. We denote a graph with standard weights as $\boldsymbol{G} = (G, \deg)$. Observe that the standard weight is a normalized weight.

(iii) The weight w such that $w(v) = 1$ for all $v \in V$ and $w(e)$ is the conductance (the reciprocal of the resistance) of the resistor represented by $e \in E$. In this case, the graph G represents a *resistive electric circuit*, i.e., is an electric circuit network consisting of resistors alone.

(iv) An edge weight on a graph determines a so-called *weighted degree* of a vertex defined by

$$\deg^w(v) := w(E_v^-) = \sum_{e \in E_v^-} w_e.$$

Recall that a loop counts twice in E_v. In particular, the standard weight $\deg(v)$ agrees with the weighted degree $\deg^w(v)$ if and only if the edge weight equals 1 for all edges. The weighted degree is *normalized* if

$$\deg^w(v) = w(v), \qquad \text{or, equivalently,} \qquad \sum_{e \in E_v^-} w_e = w(v), \quad \text{for all} \quad v \in V.$$

The next table summarises the most important weights and some related quantities:

Weight name	w_e	$w(v)$	$\rho(v)$	ρ_∞
standard	1	$\deg v$	1	1
combinatorial	1	1	$\deg v$	$\sup_{v \in V} \{\deg v\}$
normalized	w_e	$w(E_v^-)$	1	1
electric circuit	w_e	1	$w(E_v^-)$	$\sup_{v \in V} \{w(E_v^-)\}$

1.3 Magnetic Graphs

In this section, we present an additional structure on the graph: a magnetic potential that acts on the set of edges.

Let $G = (V, E)$ be a graph and R any subgroup of $\mathbb{R}/2\pi\mathbb{Z}$, which we write additively. We consider the *cochain groups* of R-valued functions on vertices and edges, which we denote by

$$C^0(G, R) := \left\{ \xi \colon V \to R \,\middle|\, \xi \text{ map} \right\} \qquad \text{and} \qquad C^1(G, R) := \left\{ \alpha \colon E \to R \,\middle|\, \forall e \in E \colon \alpha_{\bar{e}} = -\alpha_e \right\},$$

The so-called *coboundary operator* is given by

$$\mathrm{d} \colon C^0(G, R) \to C^1(G, R), \qquad (\mathrm{d}\xi)_e = \xi(\partial^+ e) - \xi(\partial - e).$$

Definition 1.3.1. Let $G = (V, E)$ be a discrete graph and R be a subgroup of $\mathbb{R}/2\pi\mathbb{Z}$.

(i) An *R-valued magnetic potential* α is an element of $C^1(G, R)$.
(ii) We say that $\alpha, \widetilde{\alpha} \in C^1(G, R)$ are *cohomologous* or *gauge-equivalent* (denote this as $\widetilde{\alpha} \sim \alpha$), if $\widetilde{\alpha} - \alpha$ is an *exact form*, i.e. if there is $\xi \in C^0(G, R)$ such that

$$(\mathrm{d}\xi)_e = \widetilde{\alpha}_e - \alpha_e \,, \quad \text{for all} \quad e \in E(G) \,,$$

and ξ is called the *gauge*. We denote the equivalence class or *cohomology class* by $[\alpha] = \{\widetilde{\alpha} \in C^1(G, R) \,|\, \widetilde{\alpha} \sim \alpha\}$. We say that α is a *trivial magnetic potential* if it is cohomologous to 0.

For a path $c = (e_1, e_2, \dots, e_n)$, we define the magnetic potential along c as

$$\int_c \alpha := \sum_{i=1}^{n} \alpha_e.$$

If the path c is closed, the integral corresponds to the *magnetic flux* of α through c.

Let $\xi \colon V \to R$ be a map, i.e. $\xi \in C^0(G, R)$ and c a path from the vertex u to the vertex v, then

$$\int_c \mathrm{d}\xi = \xi(v) - \xi(u) \,,$$

and if c is a closed path, then

$$\int_c \mathrm{d}\xi = 0 \,.$$

The next lemma shows that the magnetic potential is determined by the magnetic flux induced.

Lemma 1.3.2. *Let α_1 and α_2 two magnetic potentials acting on a connected graph G, i.e., $\alpha_1, \alpha_2 \in C^1(G, R)$. The magnetic flux of α_1 is equal to that of α_2 for every closed path c if and only if $\alpha_1 \sim \alpha_2$.*

Proof. Suppose that the magnetic flux of α_1 is equal to that of α_2 for every closed path c. Choose and fix $v_0 \in V(G)$. We define the function $\xi \colon V \to R$ as follows: for any vertex $v \in V(G)$, take a path from v_0 to v, i.e., $p = (e_1, e_2, \dots, e_n)$ such that $\partial^-(e_1) = v_0$ and $\partial^+(e_n) = v$, and define:

$$\xi(v) = \xi_p(v) := \int_p (\alpha_1 - \alpha_2) = \sum_{i=1}^{n} ((\alpha_1)_e - (\alpha_2)_e)$$

We will show that ξ does not depend on the choice of the path p from v_0 to v. Take p and q two paths from v_0 to v, and take the closed path $c = p\overline{q}$, where $\overline{q}$ is the inverse directed path of q. Then

$$\begin{aligned}
0 &= \int_c \alpha_1 - \int_c \alpha_2 \qquad \text{(magnetic flux of } \alpha_1 \text{ is equal to that of } \alpha_2 \text{)} \\
&= \int_c (\alpha_1 - \alpha_2) = \int_{p\overline{q}} (\alpha_1 - \alpha_2) = \int_p (\alpha_1 - \alpha_2) + \int_{\overline{q}} (\alpha_1 - \alpha_2) \\
&= \int_p (\alpha_1 - \alpha_2) - \int_q (\alpha_1 - \alpha_2) = \xi_p(v) - \xi_q(v) \,,
\end{aligned}$$

therefore $\xi_p(v) = \xi_q(v)$ and concluding ξ does not depend of the path. Let $e \in E$ an edge such that $\partial^- e = u$ and $\partial^+ e = v$, and consider a path p_1 from v_0 to u and p_2 from v_0 to v, then $c = e\overline{p_2}p_1$ is a closed path, then:

$$\begin{aligned} 0 &= \int_c \alpha_1 - \int_c \alpha_2 = \int_c (\alpha_1 - \alpha_2) = \int_{e\overline{p_2}p_1} (\alpha_1 - \alpha_2) \\ &= \int_e (\alpha_1 - \alpha_2) - \int_{p_2} (\alpha_1 - \alpha_2) + \int_{p_1} (\alpha_1 - \alpha_2) \\ &= (\alpha_1 - \alpha_2)_e - \xi(v) + \xi(u)\,, \end{aligned}$$

it follows that $(\alpha_2)_e + (\mathrm{d}\xi)_e = (\alpha_2)_e + \xi(v) - \xi(u) = (\alpha_1)_e$ and it concludes $\alpha_1 \sim \alpha_2$. Now suppose that $\alpha_1 \sim \alpha_2$, then it exists $\xi : V \to R$ such that

$$(\alpha_1)_e = (\alpha_2)_e + (\mathrm{d}\xi)_e, \qquad \text{for all} \quad e \in E\,,$$

then for any closed path c, it follows:

$$\int_c \alpha_1 = \int_c \alpha_2 + \int_c df = \int_c \alpha_2 + 0\,,$$

then, the magnetic flux of α_1 is equal to that of α_2 for every closed path c. □

The magnetic potential has a significant relation with the topology of the graph. In particular, the value of the magnetic potential on cut edges is irrelevant, i.e., the magnetic potential acts trivially on the edges such deletion increase the number of connected components.

Lemma 1.3.3. *Let G be graph and $e_0 \in E(G)$ a cut edge. Let α_1 and α_2 be two magnetic potentials acting on G. If $(\alpha_1)_e = (\alpha_2)_e$ for all $e \in E(G - e_0)$, then $\alpha_1 \sim \alpha_2$.*

Proof. If e_0 is a cut edge, then e_0 does not belong to any cycle, so the magnetic flux of α_1 and α_2 is the same for any cycle, then by Lemma 1.3.2 conclude $\alpha_1 \sim \alpha_2$. □

It can be shown that any magnetic potential on a finite graph can be supported in at most $b(G)$ many edges, where $b(G)$ is the Betti number of G (c.f. Eq. (1.1.2)). In fact, let G be a finite graph with α a vector potential acting on it and let T an induced tree of G. Then we can show that there exists a magnetic potential α' with support in $E(G) \setminus E(T)$ such that $\alpha \sim \alpha'$. Therefore, if G is a cycle, any vector potential is cohomologous to a vector potential supported in only one edge. Moreover, if the graph G is a tree, then any magnetic potential acting on G is cohomologous to 0.

1.4 Magnetic Weighted Graphs

In the following important definition, we collect all relevant structures needed in this dissertation: a discrete weighted graph with magnetic potential.

Definition 1.4.1. A *magnetic weighted graph* (or *MW-graph* for short) is a triple $\boldsymbol{G} = (G, \alpha, w)$, where $G = (V, E)$ is a discrete graph, w is a weight on G, and $\alpha \in C^1(G)$ is an R-valued magnetic potential, i.e. a map $\alpha\colon E \to R$ such that $\alpha_{\bar{e}} = -\alpha_e$ for all $e \in E$, where R is a subgroup of $\mathbb{R}/2\pi\mathbb{Z}$.

Let $\boldsymbol{G} = (G, \alpha, w)$ and $\boldsymbol{G}' = (G', \alpha', w')$ be two magnetic weighted graphs, we say that $\boldsymbol{G}$ and $\boldsymbol{G}'$ are isomorphic magnetic weighted graphs, which we denoted by $\boldsymbol{G} \cong \boldsymbol{G}'$, if it there exists a graph isomorphism $\varphi\colon G \to G'$ such that $\alpha = \alpha' \circ \varphi_E$, and $w = w' \circ \varphi$ for the weights in edges and vertices.

Note that R can be chosen a priori. If we choose $R = \{0\}$, then the corresponding Laplacian (see Definition 1.5.1) is the usual Laplacian (without magnetic potential). If we choose $R = \{0, \pi\}$, then the magnetic potential is also called a *signature*, and $\boldsymbol{G}$ is called a *signed graph* (see, e.g., [Lan+15] and references therein for details). This setting includes the so-called *signless Laplacian* (see Notation 1.5.2(iii)) by choosing $\alpha_e = \pi$ for all $e \in E$.

Notation 1.4.2 (Classes of magnetic weighted graphs)**.** We denote by $\mathscr{G}$ the class of all MW-graphs. We write the subclasses of MW-graphs with combinatorial respectively, standard weights just by $\mathscr{G}_{\mathbb{1}}$ respectively, $\mathscr{G}_{\deg}$. Moreover, for a symmetric subset R_0 of R (not necessarily a subgroup but satisfying if $t \in R_0$ then $-t \in R_0$), we will write

$$\mathscr{G}^{R_0} := \left\{ \boldsymbol{G} = (G, \alpha, w) \in \mathscr{G} \,\middle|\, \alpha_e \in R_0,\ e \in E(G) \right\} \qquad \text{and} \qquad \mathscr{G}^{t} := \mathscr{G}^{\{\pm t\}}$$

for the subclass of MW-graphs having magnetic potential with values in R_0 respectively with constant value $t \in R$. Similarly, we denote by $\mathscr{G}^{R_0}_{\deg}$ resp. $\mathscr{G}^{t}_{\deg}$ and $\mathscr{G}^{R_0}_{\mathbb{1}}$ resp. $\mathscr{G}^{t}_{\mathbb{1}}$ the MW-graphs with combinatorial and standard with vector potential with values in R_0 respectively with constant value t.

For a magnetic weighted graph, we can define an important operator between 0-forms and 1-forms.

Definition 1.4.3. Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph, the *(discrete) magnetic exterior derivative* d_α is a map $\mathrm{d}_\alpha\colon \ell_2(V, w) \to \ell_2(E, w)$ defined as:

$$(\mathrm{d}_\alpha \varphi)_e = \mathrm{e}^{\mathrm{i}\alpha_e/2} \varphi(\partial^+ e) - \mathrm{e}^{-\mathrm{i}\alpha_e/2} \varphi(\partial^- e) \qquad \text{for all} \qquad e \in E. \tag{1.4.1}$$

In [MY02], the derivative d_α is called a *coboundary operator* for a *twisted complex*. In particular, if $\alpha \sim 0$, then d_α is the usual coboundary operator. The next lemma proves some well-know properties of the twisted differential operator d_α.

Proposition 1.4.4. *Let* $\boldsymbol{G} = (G, \alpha, w)$ *be a magnetic weighted graph and* d_α *the magnetic exterior derivative.*

(i) $\|\mathrm{d}_\alpha\| \le \sqrt{2 p_\infty}$.
(ii) The operator $\mathrm{d}^*_\alpha\colon \ell_2(E, w) \to \ell_2(V, w)$*, given by*

$$\left(\mathrm{d}^*_\alpha \eta\right)(v) = \frac{-1}{w(v)} \sum_{e \in E^-_v} \mathrm{e}^{\mathrm{i}\alpha_e/2} \eta_e w_e\,, \qquad \textit{for all} \qquad \eta \in \ell_2(E, w), v \in V$$

is the adjoint operator of d_α*.*

(iii) $\|\mathrm{d}_\alpha^*\| \le \sqrt{2p_\infty}$.

(iv) $(\mathrm{d}_\alpha^*\mathrm{d}_\alpha f)(v) = \rho(v)f(v) - \dfrac{1}{w(v)}\sum_{e\in E_v^-} \mathrm{e}^{\mathrm{i}\alpha_e} f(\partial^+ e)w_e.$

Proof. (i) Let $f \in \ell_2(V,w)$ and recall the inequality, i.e., $(a+b)^2 \le 2(a^2+b^2)$ for any $a,b \in \mathbb{R}$, then

$$\begin{aligned}
\|\mathrm{d}_\alpha f\|^2_{E,w} &= \frac{1}{2}\sum_{e\in E} |(\mathrm{d}_\alpha f)_e|^2 w_e = \frac{1}{2}\sum_{e\in E} |\mathrm{e}^{\mathrm{i}\alpha_e/2} f(\partial^+(e)) - \mathrm{e}^{-\mathrm{i}\alpha_e/2} f(\partial^-(e))|^2 w_e \\
&\le \frac{1}{2}\sum_{e\in E} \left(|f(\partial^+(e))|^2 + |f(\partial^-(e))|^2 + 2|f(\partial^+(e))f(\partial^-(e))|^2\right) w_e \\
&= \frac{1}{2}\sum_{e\in E} (|f(\partial^+(e))| + |f(\partial^-(e))|)^2 w_e \\
&\le \sum_{e\in E} \left(|f(\partial^+(e))|^2 + |f(\partial^-(e))|^2\right) w_e \\
&= \sum_{v\in V}\left(\sum_{e\in E_v^+} |f(v)|^2 w_e + \sum_{e\in E_v^-} |f(v)|^2 w_e\right) \\
&= 2\sum_{v\in V} |f(v)|^2 \left(\sum_{e\in E_v} w_e\right) = 2\sum_{v\in V} |f(v)|^2 \rho(v) w(v) \\
&\le 2p_\infty \|f\|^2_{V,w}.
\end{aligned}$$

(ii) Let $f \in \ell_2(V,w)$ and $\eta \in \ell_2(E,w)$, then the following computation shows that d_α^* is, indeed, the adjoint of d_α.

$$\begin{aligned}
\langle f, \mathrm{d}_\alpha^*\eta\rangle_{\ell_2(V,w)} &= \sum_{v\in V} f(v)\overline{\mathrm{d}_\alpha^*\eta_e(v)}w(v) = -\sum_{v\in V} f(v)\sum_{e\in E_v^-} \mathrm{e}^{-\mathrm{i}\alpha_e/2}\overline{\eta_e}w_e \\
&= -\sum_{v\in V}\sum_{e\in E_v^-} f(v)\mathrm{e}^{-\mathrm{i}\alpha_e/2}\overline{\eta_e}w_e \\
&= -\frac{1}{2}\sum_{v\in V}\sum_{e\in E_v^-} f(v)\mathrm{e}^{-\mathrm{i}\alpha_e/2}\overline{\eta_e}w_e - \frac{1}{2}\sum_{v\in V}\sum_{e\in E_v^-} f(v)\mathrm{e}^{-\mathrm{i}\alpha_e/2}\overline{\eta_e}w_e \\
&= \frac{1}{2}\sum_{v\in V}\sum_{e\in E_v^+} \mathrm{e}^{\mathrm{i}\alpha_e/2} f(v)\overline{\eta_e}w_e - \frac{1}{2}\sum_{v\in V}\sum_{e\in E_v^-} \mathrm{e}^{-\mathrm{i}\alpha_e/2} f(v)\overline{\eta_e}w_e \\
&= \frac{1}{2}\sum_{e\in E} \mathrm{e}^{\mathrm{i}\alpha_e/2} f(\partial^+ e)\overline{\eta_e}w_e - \frac{1}{2}\sum_{e\in E} \mathrm{e}^{-\mathrm{i}\alpha_e/2} f(\partial^- e)\overline{\eta_e}w_e \\
&= \frac{1}{2}\sum_{e\in E} \left(\mathrm{e}^{\mathrm{i}\alpha_e/2} f(\partial^+ e) - \mathrm{e}^{-\mathrm{i}\alpha_e/2} f(\partial^- e)\right)\overline{\eta_e}w_e \\
&= \frac{1}{2}\sum_{e\in E} (\mathrm{d}_\alpha f)_e\overline{\eta_e}w_e = \langle \mathrm{d}_\alpha f, \eta\rangle_{\ell_2(E,w)}.
\end{aligned}$$

(iii) Let $\eta \in \ell_2(E, w)$, then

$$\begin{aligned}
\|d_\alpha^*\eta\|_{V,w}^2 &= \sum_{v\in V} |d_\alpha^*\eta(v)|^2 w(v) = \sum_{v\in V} \frac{1}{w(v)} \left| \sum_{e\in E_v^-} \mathrm{e}^{\mathrm{i}\alpha_e/2} \eta_e w_e \right|^2 \\
&\le \sum_{v\in V} \frac{1}{w(v)} \left(\sum_{e\in E_v^-} |\eta_e| w_e \right)^2 \\
&\le \sum_{v\in V} \frac{1}{w(v)} \left(\sum_{e\in E_v^-} |\eta_e|^2 w_e \sum_{e\in E_v^-} w_e \right) \qquad \text{(Using the Cauchy–Schwarz inequality)} \\
&= \sum_{v\in V} p(v) \left(\sum_{e\in E_v} |\eta_e|^2 w_e \right) \le p_\infty \left(\sum_{e\in E} |\eta_e|^2 w_e \right) = 2p_\infty \|\eta_e\|_{E,w}^2 .
\end{aligned}$$

(iv) A simple calculation shows:

$$\begin{aligned}
(\mathrm{d}_\alpha^* \mathrm{d}_\alpha f)(v) &= \frac{-1}{w(v)} \sum_{e\in E_v^-} \mathrm{e}^{\mathrm{i}\alpha_e/2} (\mathrm{d}_\alpha f)_e w_e \\
&= \frac{-1}{w(v)} \sum_{e\in E_v^-} \mathrm{e}^{\mathrm{i}\alpha_e/2} \left(\mathrm{e}^{\mathrm{i}\alpha_e/2} f(\partial^+ e) - \mathrm{e}^{-\mathrm{i}\alpha_e/2} f(\partial^- e) \right) w_e \\
&= \frac{-1}{w(v)} \sum_{e\in E_v^-} \left(\mathrm{e}^{\mathrm{i}\alpha_e} f(\partial^+ e) - f(\partial^- e) \right) w_e \\
&= \frac{1}{w(v)} \sum_{e\in E_v^-} \left(f(v) - \mathrm{e}^{\mathrm{i}\alpha_e} f(\partial^+ e) \right) w_e \\
&= \rho(v) f(v) - \frac{1}{w(v)} \sum_{e\in E_v^-} \mathrm{e}^{\mathrm{i}\alpha_e} f(\partial^+ e) w_e \,,
\end{aligned}$$

which concludes the proof. □

1.5 Discrete Magnetic Laplacian

The discrete analogue to the magnetic Schrödinger operator was introduced for the lattice in two dimensions $\mathbb{Z}^2$ as the Harper operator in [Har55]. In this case, a magnetic potential is defined in a way such that a constant flux through the cells. The generalisation has been introduced and studied by [Sun08], and is the following:

Definition 1.5.1. Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph, the *discrete magnetic Laplacian* (DML) is an operator $\Delta_\alpha \colon \ell_2(V, w) \to \ell_2(V, w)$ defined as $\Delta_\alpha = \mathrm{d}_\alpha^* \mathrm{d}_\alpha$, i.e., by

$$(\Delta_\alpha f)(v) = \rho(v) f(v) - \frac{1}{w(v)} \sum_{e\in E_v^-} \mathrm{e}^{\mathrm{i}\alpha_e} f(\partial^+ e) w_e \quad \forall f \in \ell_2(V, w), \quad \forall v \in V, \tag{1.5.1}$$

where the sum in Eq. (1.5.1) is taken over all edges starting in v and the loops are counted twice. If we need to stress the dependence on the weighted graph, we will denote the *DML* as $\Delta_\alpha = \Delta_\alpha^G$.

Notation 1.5.2 (Special cases of magnetic weighted Laplacians)**.**

(i) Let $\mathbf{G} = (G, \alpha, w) \in \mathcal{G}$ be an *MW*-graph (respectively, $\mathbf{G} \in \mathcal{G}_{\mathrm{deg}}$, $\mathbf{G} \in \mathcal{G}_{\mathbb{1}}$), then Δ_α is the magnetic weighted (respectively, standard, combinatorial) Laplacian.

(ii) Let $\mathbf{G} = (G, 0, w) \in \mathcal{G}^0$ be an *MW*-graph (respectively, $\mathbf{G} \in \mathcal{G}^0_{\mathrm{deg}}$, $\mathbf{G} \in \mathcal{G}^0_{\mathbb{1}}$), then Δ_0 is the weighted (respectively, standard, combinatorial) Laplacian.

(iii) Let $\mathbf{G} = (G, \pi, w) \in \mathcal{G}^\pi$ an *MW*-graph (respectively, $\mathbf{G} \in \mathcal{G}^\pi_{\mathrm{deg}}$, $\mathbf{G} \in \mathcal{G}^\pi_{\mathbb{1}}$), then Δ_π is the weighted (respectively, standard, combinatorial) *signless* Laplacian.

Remark 1.5.3. For the standard weight, it is convenient to associate to the graph with only one vertex and no edges the Laplace operator 0 with eigenvalue 0. Hence any isolated vertex of the standard Laplacian gives one eigenvalue 0 in its spectrum.

The next proposition proves some well-know properties of the *DML*.

Proposition 1.5.4. *Let $\mathbf{G} = (G, \alpha, w)$ be a magnetic weighted graph and Δ_α the* DML.

(i) Δ_α is a positive and self-adjoint operator.

(ii) $\|\Delta_\alpha\| \leq 2\rho_\infty$. In particular, if $\mathbf{G}$ is a uniformly bounded graph, then Δ_α is a bounded operator.

(iii) If $\alpha \sim \alpha'$, then Δ_α and $\Delta_{\alpha'}$ are unitary equivalent.

Proof. (i) By Definition 1.5.1, the *DML* is $\Delta_\alpha = d_\alpha^* d_\alpha$, then

$$\Delta_\alpha^* = (d_\alpha^* d_\alpha)^* = d_\alpha^* d_\alpha = \Delta_\alpha \,,$$

so Δ_α is self-adjoint. Also,

$$\langle f, \Delta_\alpha f \rangle = \langle d_\alpha f, d_\alpha f \rangle = \|d_\alpha f\| \geq 0 \,,$$

then Δ_α is positive.

(ii) Let $f \in \ell_2(V, w)$, using Proposition 1.4.4 (i) and (iii) it follows:

$$\|\Delta_\alpha f\| = \|d_\alpha^* d_\alpha f\| \leq \sqrt{2p_\infty}\, \|d_\alpha f\| \leq 2\rho_\infty \, \|f\|$$

then $\|\Delta_\alpha\| \leq 2p_\infty$. If $\mathbf{G}$ is uniformly bounded, then $\rho_\infty < \infty$ and we conclude that the operator Δ_α is bounded.

(iii) Suppose $\alpha' \sim \alpha$ are two cohomologous (gauge-equivalent) magnetic potentials for some gauge $\xi \colon V \to R$. Then the gauge ξ induces two unitary (multiplication) operators Ξ^0 and Ξ^1 on $\ell_2(V, w)$ and $\ell_2(E, w)$, respectively, defined by

$$(\Xi^0 \varphi)(v) := \mathrm{e}^{\mathrm{i}\xi(v)} \varphi(v) \quad \text{and} \quad (\Xi^1 \eta)_e := \mathrm{e}^{\mathrm{i}(\xi(\partial^+ e) + \xi(\partial^- e))/2} \eta_e. \tag{1.5.2}$$

Here, $\xi \mapsto \Xi^0$ and $\xi \mapsto \Xi^1$ are unitary representations of ξ seen as an additive group on $\ell_2(V, w)$ and $\ell_2(E, w)$. These representations commute with the twisted derivative as follows:

$$d_\alpha \Xi_0 = \Xi_1 d_{\alpha'} \qquad \text{and} \qquad \Delta_\alpha \Xi_0 = \Xi_0 \Delta_{\alpha'}.$$

The first equation follows by a straightforward calculation, namely

$$\begin{aligned}(d_\alpha \Xi_0 \varphi)_e &= \mathrm{e}^{\mathrm{i}\alpha_e/2+\mathrm{i}\xi(\partial^+ e)}\varphi(\partial^+ e) - \mathrm{e}^{-\mathrm{i}\alpha_e/2+\mathrm{i}\xi(\partial^- e)}\varphi(\partial^- e)\\ &= \mathrm{e}^{\mathrm{i}(\xi(\partial^+ e)+\xi(\partial^- e))/2}\left(\mathrm{e}^{\mathrm{i}\alpha_e/2}\varphi(\partial^+ e) - \mathrm{e}^{-\mathrm{i}\alpha_e/2}\varphi(\partial^- e)\right) = (\Xi_1 d_\alpha \varphi)_e.\end{aligned}$$

Then, we have the next intertwining relation

$$\Xi_0^* \Delta_\alpha \Xi_0 = \Xi_0^* d_\alpha^* d_\alpha \Xi_0 = (d_\alpha \Xi_0)^* \Xi_1 d_{\alpha'} = (\Xi_1 d_{\alpha'})^* \Xi_1 d_{\alpha'} = \Delta_{\alpha'}$$

using the fact that Ξ^0 and Ξ^1 are unitary. We conclude that Δ_α and $\Delta_{\alpha'}$ are unitary equivalents. □

In summary, the magnetic Laplacian Δ_α is a bounded, positive and self-adjoint operator, and its spectrum satisfies $\sigma(\Delta_\alpha) \subset [0, 2\rho_\infty]$. If $\alpha \sim \alpha'$, then Δ_α and $\Delta_{\alpha'}$ are unitary equivalent; in particular, $\sigma(\Delta_\alpha) = \sigma(\Delta_{\alpha'})$. Moreover, if $\alpha \sim 0$ then $\Delta_\alpha \cong \Delta$ where Δ denotes the discrete Laplacian with vector potential 0, i.e., the usual discrete Laplacian. For example, if $\boldsymbol{G} = (G, \alpha, w)$ where the graph G is a tree, then $\Delta_\alpha^G \cong \Delta^G$ for any vector potential.

Let $G = (V, E)$ be a graph. For all $v \in V$, consider $\mathbf{1}_v \colon V \to \mathbb{C}$ the indicator function for the set $\{v\}$ and define $\varphi_v = \mathbf{1}_v/\sqrt{w(v)}$. The set $\{\varphi_v\}_{v\in V}$ is the canonical orthonormal basis of the Hilbert space $\ell_2(V, w)$ defined in Eq. (1.2.4). Let $v_1, v_2 \in V$, then

$$\langle \varphi_{v_1}, \Delta_\alpha \varphi_{v_2}\rangle = \sum_{v\in V}\left(\varphi_{v_1}(v)\rho(v)\varphi_{v_2}(v) - \varphi_{v_1}(v)\frac{1}{w(v)}\sum_{e\in E_v^-}\mathrm{e}^{\mathrm{i}\alpha_e}\varphi_{v_2}(\partial^+ e)w_e\right)w(v)\,. \tag{1.5.3}$$

For the case that $v_1 = v_2$, then the Eq. (1.5.3) is simplify as follows:

$$\begin{aligned}\langle \varphi_{v_1}, \Delta_\alpha \varphi_{v_1}\rangle &= \left(\varphi_{v_1}(v_1)\rho(v_1)\varphi_{v_1}(v_1) - \varphi_{v_1}(v_1)\frac{1}{w(v_1)}\sum_{e\in E_{v_1}^-}\mathrm{e}^{\mathrm{i}\alpha_e}\varphi_{v_1}(\partial^+ e)w_e\right)w(v_1)\\ &= \rho(v_1) - \frac{1}{w(v_1)}\sum_{e\in E(v_1)}\cos(\alpha_e)\,,\end{aligned}$$

For the case $v_1 \neq v_2$, then the Eq. (1.5.3) is simplify as follows:

$$\begin{aligned}\langle \varphi_{v_1}, \Delta_\alpha \varphi_{v_2}\rangle &= -\varphi_{v_1}(v_1)\frac{1}{w(v_1)}\sum_{e\in E_{v_1}^-}\mathrm{e}^{\mathrm{i}\alpha_e}\varphi_{v_1}(\partial^+ e)w_e w(v_1)\\ &= -\frac{1}{\sqrt{w(v_1)w(v_2)}}\sum_{e\in E(v_1,v_2)}\mathrm{e}^{\mathrm{i}\alpha_e}w_e\,.\end{aligned}$$

In Proposition 1.5.4 (i), we showed that a necessary condition for Δ_α to be a bounded operator is that G is uniformly bounded. If G has no loops, now we prove that it is a sufficient condition. Therefore, the following proposition can be understood as a reverse of Proposition 1.5.4 (i).

Proposition 1.5.5. *Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph, where the graph G has no loops, and Δ_α is a bounded operator. Then the graph G is uniformly bounded.*

Proof. Let $\{\varphi_v\}_{v \in V}$ be the canonical orthonormal basis of the Hilbert space $\ell_2(V, w)$. If $\|\Delta_\alpha\|$ is finite, then

$$\|\Delta_\alpha\| = \sup_{\substack{\varphi \in \ell^2(V); \\ \|\varphi\|=1}} |\langle \varphi, \Delta_\alpha \varphi \rangle| \geq \sup_{v \in V} \langle \varphi_v, \Delta_\alpha \varphi_v \rangle = \sup_{v \in V} \rho(v) = \rho_\infty$$

and, therefore, G is uniformly bounded (cf. Eq. (1.2.3)). □

As a consequence of the previous results, we can finally give a matrix representation of the magnetic Laplacian. This representation is the basis of the program presented in Appendix B. Let $\boldsymbol{G} = (G, \alpha, w)$ be a finite magnetic weighted graph. For computing the eigenvalues of the *DML*, it is convenient to work with the associated matrix. Consider a numbering of the vertices as $V(G) = \{v_1, v_2, \ldots, v_n\}$. Then the *matrix representation* of Δ_α with respect to this orthonormal basis is given by

$$[\Delta_\alpha]_{jk} = \begin{cases} \rho(v_j) - \dfrac{1}{w(v_j)} \displaystyle\sum_{e \in E(v_j, v_j)} \mathrm{e}^{\mathrm{i}\alpha_e} w_e, & \text{if } j = k, \\ -\dfrac{1}{\sqrt{w(v_j) w(v_k)}} \displaystyle\sum_{e \in E(v_j, v_k)} \mathrm{e}^{\mathrm{i}\alpha_e} w_e, & \text{if } j \neq k \end{cases} \tag{1.5.4}$$

Note that this formula includes the case of graphs with multiple edges and loops.

1.6 Spectral Graph Theory

This section presents important results in spectral graph theory.

The *spectrum* of the discrete magnetic Laplacian is the set of λ such that $(\Delta_\alpha - \lambda\, I)$ is not invertible. The spectrum is denoted as $\sigma(\Delta_\alpha)$. The next lemma proves some of the most important properties of the spectrum of the *DML*.

Lemma 1.6.1. *Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph and Δ_α the discrete magnetic Laplacian.*

(i) The spectrum $\sigma(\Delta_\alpha) \subset [0, 2\rho_\infty]$.
(ii) If $\alpha \sim \alpha'$, then $\sigma(\Delta_\alpha) = \sigma(\Delta_{\alpha'})$.

Moreover, if the graph G is finite, then

(iii) $\alpha \sim 0$ implies $0 \in \sigma(\Delta_\alpha)$.
(iv) If G is connected and $0 \in \sigma(\Delta_\alpha)$, then $\alpha \sim 0$.

Proof. (i). By Proposition 1.5.4 (i), the operator Δ_α is self-adjoint, then $\sigma(\Delta_\alpha) \subset \mathbb{R}$, also is positive, the $\sigma(\Delta_\alpha) \subset [0,\infty)$. By Proposition 1.5.4 (ii), the magnetic Laplacian is bounded by $\|\Delta_\alpha\| \leq 2\rho_\infty$. We conclude $\sigma(\Delta_\alpha) \subset [0, 2\rho_\infty]$.

(ii). If $\alpha \sim \alpha'$, by Proposition 1.5.4 (iii) the operators Δ_α and $\Delta_{\alpha'}$ are unitary equivalents and, therefore, they have the same spectrum.

(iii). Consider the constant function $\mathbf{1}\colon V \to \mathbb{C}$ with $\mathbf{1}(v) = 1$ for all $v \in V$ and, because the graph is finite, it follows that $\mathbf{1} \in \ell_2(V,w)$. Therefore $d_0\mathbf{1} = 0$ and $0 \in \sigma(\Delta_0)$. By hypothesis $\alpha \sim 0$ together with (ii) follows that $\sigma(\Delta_0) = \sigma(\Delta_\alpha)$ and therefore $0 \in \sigma(\Delta_\alpha)$.

(iv). Suppose that $0 \in \sigma(\Delta_\alpha)$, then there exists a non-zero $\varphi \in \ell_2(V,w)$ such that $0 = \langle \Delta_\alpha\varphi, \varphi\rangle = \|\mathrm{d}_\alpha\varphi\|^2$. In particular, $d_\alpha\varphi = 0$, i.e., $\varphi(\partial^- e) = \mathrm{e}^{\mathrm{i}\alpha_e}\varphi(\partial^- e)$ for all $e \in E$. As the graph G is connected, we can define a function $\xi\colon V \to R$ adjusting the phases in such a way that $\varphi(v)\mathrm{e}^{\mathrm{i}\xi(v)}$ is constant on V. Then, we have $\alpha_e = (\mathrm{d}\xi)_e$ for all edge $e \in E$, hence $\alpha \sim 0$. □

1.6.1 Bipartiteness and the spectrum

The next theorem shows some important equivalences on the spectrum, in particular, the spectrum of a graph has a symmetry if and only if the graph G is bipartite.

Proposition 1.6.2. *Let $\mathbf{G} = (G, \alpha, w)$ a magnetic weighted graph where the graph G is finite and connected, and the weight w is a normalized weight. Then the following assertions are equivalent:*

(i) G is bipartite.
(ii) $\lambda \in \sigma(\Delta_\alpha)$ implies that $2 - \lambda \in \sigma(\Delta_\alpha)$.
(iii) $\alpha \sim 0$ implies $2 \in \sigma(\Delta_\alpha)$.

Proof. (i)⇒(ii) Let V_1 and V_2 be the bipartition of the vertices of the graph G and suppose $\lambda \in \sigma(\Delta_\alpha)$. Consider the eigenfunction $f \in \ell_2(V,w)$ that satisfies $\Delta_\alpha f = \lambda f$.

Define $g\colon \ell_2(V,w) \to \ell_2(V,w)$ given by:

$$g(v) = \begin{cases} f(v)\,, & \text{if } v \in V_1 \\ -f(v)\,, & \text{if } v \in V_2\,. \end{cases}$$

If $v \in V_1$, then $g(v) = f(v)$ and $\partial^\pm e \in V_2$ for all $e \in E_v^\mp$. The next calculation shows $(2-\lambda)g = \Delta_\alpha g$.

$$\begin{aligned}(2-\lambda)g(v) = 2g(v) - \lambda g(v) = 2f(v) - \Delta_\alpha f(v) &= f(v) + \frac{1}{w(v)}\sum_{e\in E_v^-} \mathrm{e}^{\mathrm{i}\alpha_e} f(\partial^+ e) w_e \\ &= g(v) - \frac{1}{w(v)}\sum_{e\in E_v^-} \mathrm{e}^{i\alpha_e} g(\partial^+ e) w_e = \Delta_\alpha g(v).\end{aligned}$$

Similarly, if $v \in V_2$ then $g(v) = -f(v)$ and $\partial^{\pm} e \in V_1$ for all $e \in E_v^{\mp}$, then

$$\begin{aligned}(2-\lambda)g(v) = 2g(v) - \lambda g(v) = -2f(v) + \Delta_\alpha f(v) &= f(v) + \frac{1}{w(v)} \sum_{e \in E_v^-} \mathrm{e}^{\mathrm{i}\alpha_e} f(\partial^+ e) w_e \\ &= g(v) - \frac{1}{w(v)} \sum_{e \in E_v^-} \mathrm{e}^{i\alpha_e} g(\partial^+ e) w_e = \Delta_\alpha g(v).\end{aligned}$$

We conclude that $2-\lambda$ is an eigenvalue of Δ_α with eigenfunction g.

(ii)⇒(iii) Suppose $\alpha \sim 0$, by Lemma 1.6.1 (iii) it follows $0 \in \sigma(\Delta_\alpha)$, this implies $2 \in \sigma(\Delta_\alpha)$ by hypothesis in (ii).

(iii)⇒(i) This part is proved in [Chu97, Lemma 1.7]. □

The next proposition will be useful in Chapter 2, where this additional symmetry related to the bipartite graph, allows us to obtain a better localisation of the spectrum of the magnetic Laplacian (see, e.g., Proposition 2.3 in [LP08b]).

Proposition 1.6.3. *Assume that $\mathbf{G} = (G, \alpha, w)$ is a magnetic weighted graph where G is a bipartite graph with normalized weight w. Then the spectrum of Δ_α is symmetric with respect to the map $\kappa \colon \mathbb{R} \to \mathbb{R}$, $\kappa(\lambda) = 2 - \lambda$, i.e.,*

$$\kappa(\sigma(\Delta_\alpha)) = \sigma(\Delta_\alpha).$$

In particular, if $J \subset [0,2]$ fulfils $\sigma(\Delta_\alpha) \subset J$, then we have the inclusion

$$\sigma(\Delta_\alpha) \subset J \cap \kappa(J).$$

Note that the set $J \cap \kappa(J)$ becomes smaller than J if J is *not* symmetric with respect to κ.

2 Graphs and preorders

In this chapter, we introduce two preorders on the set of magnetic weighted graphs. In Section 2.1, we define a preorder $\sqsubseteq$ on the set of infinite magnetic weighted graphs. We use a graph homomorphism to define $\sqsubseteq$, i.e., we use the geometry of the graph. If the graph is finite and with some particular weights (for example: for the standard and combinatorial), in Theorem 2.1.6 we prove that the relation $\sqsubseteq$ is a *partial order*.

The second preorder presented in Section 2.2, denoted by $\preccurlyeq$ is defined in the set of finite magnetic weighted graphs. In this case, we use the spectrum of the magnetic Laplacian. In particular, in Theorem 2.3.3, we show that the geometrical preorder $\sqsubseteq$ implies the spectral preorder $\preccurlyeq$.

Finally, in Section 2.4, we present some geometric perturbations and elementary operations on the graphs and some relation with the preorder defined previously. We studied three elementary operations: delete an edge (Subsection 2.4.1), contracting two vertices (Subsection 2.4.2) and the virtualisation of edges and vertices (Subsection 2.4.3). This spectral ordering and the virtualising operation on the graphs will be needed later to develop a discrete bracketing technique and show the existence of spectral gaps for Laplacians on periodic graphs in Chapter 4. Korotyaev and Saburova also present a discrete bracketing technique in [KS15] for combinatorial weights. Their Dirichlet upper bound of the bracketing is similar to the one we use here (vertex-virtualised). For the lower bound Korotyaev and Saburova use a Neumann type boundary condition. In this dissertation, we propose an alternative edge virtualisation process using the fact that we work with arbitrary weights.

2.1 Geometric preorder $\sqsubseteq$ for infinite MW-graph

Consider $\mathcal{G}$ the class of all magnetic weighted graphs. Let $\mathbf{G}, \mathbf{G}' \in \mathcal{G}$ be two magnetic weighted graphs, i.e., $\mathbf{G} = (G, \alpha, w)$ and $\mathbf{G}' = (G', \alpha', w')$. We say that $\mathbf{G}$ and $\mathbf{G}'$ are isomorphic (denoted as $\mathbf{G} \cong \mathbf{G}'$) if the following holds: there exists a graph isomorphism

$\varphi\colon G \to G'$ such $w_e = w'_{\varphi(e)}$, $\alpha_e = \alpha'_{\varphi(e)}$ for all $e \in E(G)$ and $w(v) = w'(\varphi(v))$ for all $v \in V(G)$.

Recall from notation 1.4.2, that we denote the class of all magnetic graphs with combinatorial weights as $\mathscr{G}_{\mathbb{1}}$ and the class of all magnetic graphs with standard weights as $\mathscr{G}_{\deg}$. In the following definition, we introduce the first preorder in the class of all magnetic weighted graphs.

Definition 2.1.1 (Geometric preorder $\sqsubseteq$). Let $\boldsymbol{G} = (G, \alpha, w)$ and $\boldsymbol{G}' = (G', \alpha', w')$ be two magnetic weighted graphs. We say that $\boldsymbol{G}$ is *geometrically smaller* than $\boldsymbol{G}'$, and we denoted as

$$\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$$

if it there exists an *MW*-graph homomorphism $\pi\colon \boldsymbol{G} \to \boldsymbol{G}'$, i.e., a graph homomorphism $\pi\colon G \to G'$ such that

(i) The magnetic potential is invariant: $\alpha = \alpha' \circ \pi$, i.e., then $\alpha_e = \alpha'_{\pi(e)}$ for all edge $e \in E(G)$.

(ii) The following vertex weight inequality holds:

$$(\pi_* w)(v) := \sum_{v \in V, \pi(v) = v'} w(v) \geq w'(v') \qquad \text{for all } v' \in V',$$

i.e., the push-forward vertex measure $\pi_* w$ is greater than or equal to w'.

(iii) The following edge weight inequality holds:

$$(\pi_* w)_e := \sum_{e \in E, \pi(e) = e'} w_e \leq w'_{e'} \qquad \text{for all } e' \in E',$$

i.e., the push-forward edge measure $\pi_* w$ is smaller than or equal to w'.

(iv) We say that π is *vertex* and *edge measure preserving* if equality holds in (ii) and (iii), respectively, i.e., $\pi_* w = w'$ for both the vertex and edge measure. We simply say that π is *measure preserving* if π is vertex *and* edge measure preserving.

Some example of *MW*-graph homomorphism for the geometrical preorder $\sqsubseteq$ are the following.

Example 2.1.2. Let $\boldsymbol{G} = (G, \alpha, w)$ and $\boldsymbol{G}' = (G', \alpha', w')$ be two *MW*-graphs.

(i) Suppose that $G = G'$, $\alpha = \alpha'$ and consider the identity graph homomorphism $\mathrm{id}_G\colon G \to G$. If $w(v) \geq w'(v)$ for all $v \in V(G)$ and $w_e \leq w'_e$ for all $e \in E(G)$, then $\mathrm{id}_{\boldsymbol{G}}\colon \boldsymbol{G} \to \boldsymbol{G}$ is an *MW*-graph homomorphism and hence $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$.
In particular, $(G, \alpha, \deg) \sqsubseteq (G, \alpha, \mathbb{1})$.

(ii) Suppose that $G' = G/\sim$ for some equivalence relation $\sim$ on $V(G)$ and $\alpha = \alpha'$. Consider the projection map given by the equivalence relation $\sim$, i.e., $\pi\colon G \to G/\sim$ defined in Eq. (1.1.4). If $\sum_{v \in \pi^{-1}(v')} w(v) \geq w'(v')$ for all $v \in V(G')$ and $w_e \leq w'_e$ for all $e \in E(G')$, then $\pi\colon \boldsymbol{G} \to \boldsymbol{G}$ is an *MW*-graph homomorphism and hence $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$.
This condition on weights is automatically true when both weighted graphs $\boldsymbol{G}$ and $\boldsymbol{G}'$ have combinatorial or standard weights, i.e., $(G, \alpha, \deg) \sqsubseteq (G/\sim, \alpha, \deg)$ and $(G, \alpha, \mathbb{1}) \sqsubseteq (G/\sim, \alpha, \mathbb{1})$.

(iii) Suppose that $G' = G - E_0$ for some $E_0 \in E(G)$, $\alpha' = \alpha\restriction_{E(G')}$ and $\iota_{E_0}: G' \to G$ be the inclusion map of Definition 1.1.4. If $w'(v) \geq w(v)$ for all $v \in V(G)$ and $w'_e \leq w_e$ for all $e \in E(G')$, then $\iota_{E_0}: \mathbf{G} \to \mathbf{G}$ is an *MW*-graph homomorphism and hence $\mathbf{G} \sqsubseteq \mathbf{G}'$. The condition on the edges is true when both magnetic weighted graphs $\mathbf{G}$ and $\mathbf{G}'$ have combinatorial or standard weights. However, for the vertices weights is valid only for the combinatorial case. Then, we have $(G', \alpha', \mathbb{1}) \sqsubseteq (G, \alpha, \mathbb{1})$ but not valid for the standard weight.

We state below some basic consequences. The most important is that the *MW*-graph homomorphism $\pi: \mathbf{G} \to \mathbf{G}'$ is injective on edges and surjective on vertices.

Lemma 2.1.3. *Let $\mathbf{G} = (G, \alpha, w)$ and $\mathbf{G}' = (G', \alpha', w')$ be two* MW*-graphs. If $\pi: G \to G'$ is an* MW*-graph homomorphism such that $\mathbf{G} \sqsubseteq \mathbf{G}'$, then:*

(i) The map $\pi: V(G) \to V(G')$ is surjective.

(ii) If for some $c > 0$ we have $w_e = w'_{e'} = c$ for all $e \in E(G)$ and $e' \in E(G')$ (e.g., if $\mathbf{G}$ has standard or combinatorial weights), then the map $\pi\restriction_E: E(G) \to E(G')$ is injective and

$$\sum_{v \in V, \pi(v) = v'} \deg_G(v) \leq \deg_{G'}(v') \quad \textit{for every } v' \in V'. \tag{2.1.1}$$

If π is not surjective on the edges, then there is a vertex $v' \in V'$ such that

$$\sum_{v \in V, \pi(v) = v'} \deg_G(v) < \deg_{G'}(v').$$

Proof. (i) Let $v' \in V(G')$, then $0 < w'(v') \leq \sum_{v \in \pi^{-1}(v')} w(v)$, and this implies the existence of $v \in \pi^{-1}(v')$ such that $w(v) > 0$, hence $\pi(v) = v'$, and we conclude that π is surjective on vertices.

(ii) If the edge weights on E and on E' have constant value $c > 0$, then $\sum_{e \in E, \pi(e) = e'} w_e \leq w'_{e'}$ is equivalent with the fact that $\{\, e \in E \mid \pi(e) = e' \,\}$ has at most one element, i.e., $\pi\restriction_E$ is injective. Let $v' \in V(G')$; then it exists $v \in V(G)$ such that $\pi(v) = v'$, and consider the restriction map $\pi_E\restriction_{E_v^+}: E_v^+ \to E_{v'}^+$, that is well-defined because π is graph homomorphism and *injective* because π is. Moreover, note that $\{E_v^+\}_{v \in V(G)}$ is a disjoint family of sets (as an edge only has one initial vertex); hence we have:

$$\sum_{v \in V, \pi(v) = v'} |E_v^+| = |\bigcup_{v \in V, \pi(v) = v'} \pi(E_v^+)| \leq |(E_{v'}^+)|\,.$$

Therefore

$$\sum_{v \in V, \pi(v) = v'} \deg_G(v) = \sum_{v \in V, \pi(v) = v'} |E_v^+| \leq |(E_{v'}^+)| = \deg_{G'}(v')\,.$$

Suppose that π is not surjective on the edges, choose an edge $e_0 \in E(G')$ and $v' \in \partial^+(e)$, such $\pi_E: E(G) \to E(G') \setminus e_0$ is injective and well defined as map; hence we conclude

$$\sum_{v \in V, \pi(v) = v'} \deg_G(v) = \sum_{v \in V, \pi(v) = v'} |E_v^+| \leq |\bigcup_{v \in V, \pi(v) = v'} \pi(E_v^+)| - 1 < |(E_{v'}^+)| = \deg_{G'}(v')$$

We have used the fact that π is surjective on the vertices. $\square$

For the combinatorial and for the standard weights, we have the following geometrical characterisation of the relation $\sqsubseteq$. The *geometrical* name is justified by the following fact: the relation $\sqsubseteq$ corresponds to an equivalence relation on the set of vertices.

Proposition 2.1.4. *Let $\boldsymbol{G} = \big(G, \alpha, \deg_G\big)$ and $\boldsymbol{G}' = (G', \alpha', \deg_{G'})$. The following are equivalent:*

(i) $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$.
(ii) There exists an MW*-graph homomorphism $\pi \colon \boldsymbol{G} \to \boldsymbol{G}'$ measure preserving.*
(iii) There exists an equivalence relation $\sim$ on $V(G)$ and a graph isomorphism $\pi' \colon G/\!\sim\, \to G'$ such that $\alpha = \alpha' \circ \pi'$.

Proof. (i)⇒(ii). Suppose that $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$, then there exists a graph homomorphism $\pi \colon G \to G'$, where π has the properties in Definition 2.1.1 (i)–(iii). We have to prove the equality in Definition 2.1.1 (ii) and (iii). By Lemma 2.1.3, the map π is surjective on vertices and injective on edges, hence the Eq. 2.1.1 gives the equality in (ii) of Definition 2.1.1, and the equality (iii) of Definition 2.1.1 follows by the injectivity on edges.

(ii)⇒(iii). Let $\pi \colon \boldsymbol{G} \to \boldsymbol{G}'$ be a measure preserving map, in particular, $\pi \colon G \to G'$ is a graph homomorphism. Define an equivalence relation in $V(G)$ as follows: $v_1 \sim v_2$ if and only if $\pi(v_1) = \pi(v_2)$, by Lemma 2.1.3 (i) π is surjective on the vertices then $\sim$ is an equivalence relation on $V(G)$. Consider the map $\pi' \colon G/\!\sim\, \to G'$ defined as follows: $\pi'([v]) = \pi(v)$ and $\pi'(e) = \pi(e)$. It is easy to see that π' is a graph homomorphism. Is clear that π' is bijective on the vertices and injective on the edges. If π' was not surjective on the edges, hence the Lemma 2.1.3 (ii) contradicts the fact that π is measure preserving on the vertices. Finally $\pi = \pi'$ on the edges, then $\alpha = \alpha' \circ \pi'$.

(iii)⇒(i). Let $\pi' \colon G/\!\sim\, \to G'$ be a graph isomorphism and let $\pi \colon G \to G/\!\sim$ be the projection given by $\sim$ defined in Eq. (1.1.4). It is straightforward to show that $\pi' \circ \pi$ fulfil the conditions in Definition 2.1.1 (i)–(iii), hence $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$. □

The next proposition states a characterisation for the combinatorial weight; its proof is similar to the previous proposition.

Proposition 2.1.5. *Let $\boldsymbol{G} = (G, \alpha, \mathbb{1})$ and $\boldsymbol{G}' = (G', \alpha', \mathbb{1})$, the following statement are equivalent:*

(i) $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$.
(ii) There exists an equivalence relation $\sim$ on $V(G)$, a subset of edges $E_0 \subset E(G')$ and a graph isomorphism $\pi' \colon G/\!\sim\, \to G' - E_0$ such that $\alpha = \alpha' \circ \pi'$.

For the class of magnetic graphs with normalized or combinatorial weights, the next theorem proves that the relation $\sqsubseteq$ is a partial order.

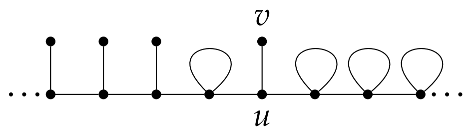
Theorem 2.1.6. *The relation $\sqsubseteq$ is a preorder on the class of all magnetic weighted graph $\mathcal{G}$, i.e., it is reflexive and transitive. Moreover, for finite magnetic weighted graphs, the relation $\sqsubseteq$ is a partial order on the equivalence classes of isomorphic* MW*-graphs in $\mathcal{G}_{\mathbb{1}}$ and in $\mathcal{G}_{\deg}$.*

Proof. Let $\boldsymbol{G} = (G, \alpha, w)$, $\boldsymbol{G}' = (G', \alpha', w')$ and $\boldsymbol{G}'' = (G'', \alpha'', w'')$ be three *MW*-graphs. It is trivial to show that $\boldsymbol{G} \sqsubseteq \boldsymbol{G}$ using the identity homomorphism $\iota \colon G \to G'$ as *MW*-graph homomorphism. If $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$ (with respect to π_1) and $\boldsymbol{G}' \sqsubseteq \boldsymbol{G}''$ (with respect to π_2), is easy to show that $\boldsymbol{G} \sqsubseteq \boldsymbol{G}''$ (with respect to $\pi_2 \circ \pi_1$).

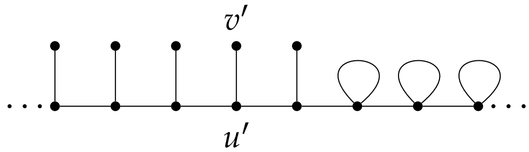
Consider two finite *MW*-graphs $\boldsymbol{G}$, $\boldsymbol{G}' \in \mathscr{G}_{\mathbb{1}}$ with $\pi \colon \boldsymbol{G} \to \boldsymbol{G}'$ and $\pi' \colon \boldsymbol{G}' \to \boldsymbol{G}$, then by Lemma 2.1.3 (i) follows that π and π' are surjective on the vertex sets. Since both sets are finite, it follows that π and π' are bijective on the vertex sets. Similarly, from Lemma 2.1.3 (ii) it follows that π and π' are bijective on the edge sets. In particular, $\boldsymbol{G}$ and $\boldsymbol{G}'$ are isomorphic, and hence $\sqsubseteq$ is a partial order on the equivalence classes of isomorphic *MW*-graphs in $\mathscr{G}_{\mathbb{1}}$. A similar argument is used to prove that $\sqsubseteq$ it is a partial order in $\mathscr{G}_{\deg}$. □

The previous result remains true on any subclass $\mathscr{G}'$ of $\mathscr{G}$ with edge weight given by a constant value.

Remark 2.1.7. In general, it is false that $\sqsubseteq$ is a partial order in $\mathscr{G}_{\mathbb{1}}$ and $\mathscr{G}_{\deg}$ for *infinite* magnetic weighted graphs. Consider $\boldsymbol{G} = (G, 0, \deg)$ and $\boldsymbol{G}' = (G', 0, \deg)$ where G and G' are the graphs in Figure 2.1. It is easy to see that $G' \cong G/\{u, v\}$ and $G \cong G'/\{u', v'\}$, therefore $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$ and $\boldsymbol{G}' \sqsubseteq \boldsymbol{G}$, but $\boldsymbol{G} \not\cong \boldsymbol{G}'$ because G and G' are not isomorphic as graphs. Therefore, $\sqsubseteq$ it is not antisymmetric for infinite graphs with standard weights; the same example works with the combinatorial weights.



(A) The infinite graph G.



(B) The infinite graph G'.

FIGURE 2.1: This example shows that $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$ and $\boldsymbol{G}' \sqsubseteq \boldsymbol{G}$, but $\boldsymbol{G} \not\cong \boldsymbol{G}'$

2.2 Spectral preorder $\preccurlyeq$ for finite *MW*-graphs

In this section, we consider only finite magnetic weighted graphs, i.e., $\boldsymbol{G} = (G, \alpha, w)$ of order n, i.e., $|G| = |\boldsymbol{G}| = |V(G)| = n$, denote the spectrum of the discrete magnetic Laplacian Δ_α of $\boldsymbol{G}$ as follow:

$$\sigma(\boldsymbol{G}) = \sigma(\Delta_\alpha) = (\lambda_1(\boldsymbol{G}), \lambda_2(\boldsymbol{G}), \ldots, \lambda_n(\boldsymbol{G})) \tag{2.2.1}$$

where the eigenvalues are written in ascending order and repeated according to their multiplicities.

We start with some general remarks about ordering finite increasing sequences of real numbers:

Definition 2.2.1. Let Λ and Λ' two finite sequence of real numbers in increasing order with length n (resp., n'), i.e.,

$$\Lambda := \{ (\lambda_1, \lambda_2 \ldots, \lambda_n) \,|\, \lambda_1 \leq \lambda_2 \leq \ldots \lambda_{n-1} \leq \lambda_n \};$$

$$\Lambda' := \{ (\lambda'_1, \lambda'_2 \ldots, \lambda'_{n'}) \,|\, \lambda'_1 \leq \lambda'_2 \leq \ldots \lambda'_{n'-1} \leq \lambda'_{n'} \}.$$

Given $r \in \mathbb{N}_0$, we say that Λ is *smaller than* Λ' *with shift* r (and denote this by $\Lambda \overset{r}{\preccurlyeq} \Lambda'$) if $n' - r \leq n$ and

$$\lambda_k \leq \lambda'_{k+r} \quad \text{for} \quad 1 \leq k \leq n' - r.$$

We define $|\Lambda| := n$ as the length of the sequence Λ.

We mention below some useful conventions and natural consequences of the above definition.

Remark 2.2.2. Let Λ, Λ' and Λ'' be sequences of real numbers as above.

(i) We denote $\Lambda \overset{0}{\preccurlyeq} \Lambda'$ simply by $\Lambda \preccurlyeq \Lambda'$.

(ii) If $\Lambda \overset{r}{\preccurlyeq} \Lambda'$ and $\Lambda' \overset{s}{\preccurlyeq} \Lambda''$, we will write $\Lambda \overset{r}{\preccurlyeq} \Lambda' \overset{s}{\preccurlyeq} \Lambda''$.

(iii) The case $\Lambda \overset{0}{\preccurlyeq} \Lambda' \overset{r}{\preccurlyeq} \Lambda$ implies that $n = |\Lambda| \geq |\Lambda'| \geq n - r$. If $|\Lambda'| = n - r$, then $\Lambda \preccurlyeq \Lambda' \overset{r}{\preccurlyeq} \Lambda$ is equivalent with the *interlacing* of Λ and Λ' similarly as in [BH12, Sec. 2.5], namely

$$\lambda_1 \leq \lambda'_1 \leq \lambda_{1+r}, \quad \lambda_2 \leq \lambda'_2 \leq \lambda_{2+r}, \quad \ldots, \quad \lambda_{n-r} \leq \lambda'_{n-r} \leq \lambda_n.$$

Especially if $r = 1$ it becomes the usual interlacing (explaining also the name)

$$\lambda_1 \leq \lambda'_1 \leq \lambda_2 \leq \lambda'_2 \leq \cdots \leq \lambda_{n-1} \leq \lambda'_{n-1} \leq \lambda_n.$$

(iv) If $\Lambda \overset{0}{\preccurlyeq} \Lambda'$, $n = |\Lambda| = |\Lambda'|$ and $\sum_{i=1}^{n} \lambda_i = \sum_{i=1}^{n} \lambda'_i$, then is trivial to prove that Λ' is majorized by Λ, see [MOA11] for additional results and motivation of majorization and its applications.

We state in the next lemma some direct consequences of the previous definition.

Lemma 2.2.3. *Let Λ, Λ' and Λ'' three sequences of real number written in increasing order.*

(i) If $r \in \mathbb{N}_0$, then $\Lambda \overset{r}{\preccurlyeq} \Lambda$ (reflexivity).

(ii) If $\Lambda \preccurlyeq \Lambda' \preccurlyeq \Lambda$, then $\Lambda = \Lambda'$ (antisymmetry).

(iii) If $\Lambda \overset{r}{\preccurlyeq} \Lambda'$ and $\Lambda' \overset{s}{\preccurlyeq} \Lambda''$, then $\Lambda \overset{r+s}{\preccurlyeq} \Lambda''$ (transitivity).

(iv) If $\Lambda \overset{r}{\preccurlyeq} \Lambda'$ and $r \leq s$, then $\Lambda \overset{s}{\preccurlyeq} \Lambda'$.

Proof. The reflexivity property and part (iv) follow from the fact that the sequence Λ is written in increasing order. The antisymmetry property (ii) is also a direct consequence of Definition 2.2.1. To show (iii), note that $|\Lambda| \geq |\Lambda'| - r$ and $\lambda_k \leq \lambda'_{k+r}$ for $1 \leq k \leq |\Lambda'| - r$, as well as $|\Lambda'| \geq |\Lambda''| - s$ and $\lambda_l \leq \lambda'_{l+s}$ for $1 \leq l \leq |\Lambda''| - s$. This implies $|\Lambda| \geq |\Lambda''| - r - s$ and $\lambda_k \leq \lambda'_{k+r+s}$ for $1 \leq k \leq |\Lambda''| - r - s$. □

We will now apply the relation $\preccurlyeq$ described before to relate the spectrum of the magnetic Laplacian of different *MW*-graphs.

Let $\boldsymbol{G} = (G, \alpha, w)$ be an *MW*-graph of order n, i.e. $|\boldsymbol{G}| = n$, denote the spectrum of the discrete magnetic Laplacian Δ_α of $\boldsymbol{G}$ as follows:

$$\sigma(\boldsymbol{G}) = \sigma(\Delta_\alpha) = (\lambda_1(\boldsymbol{G}), \lambda_2(\boldsymbol{G}), \ldots, \lambda_n(\boldsymbol{G})) \tag{2.2.2}$$

where the eigenvalues are written in ascending order and repeated according to their multiplicities.

Definition 2.2.4 (Spectral preorder $\preccurlyeq$). Let $\boldsymbol{G}, \boldsymbol{G}'$ be two finite magnetic weighted graphs. We say that $\boldsymbol{G}$ *is* (spectrally) *smaller than* $\boldsymbol{G}'$ *with shift* r, denoted by

$$\boldsymbol{G} \overset{r}{\preccurlyeq} \boldsymbol{G}'$$

if $\sigma(\boldsymbol{G}) \overset{r}{\preccurlyeq} \sigma(\boldsymbol{G}')$, where $\sigma(\boldsymbol{G})$ and $\sigma(\boldsymbol{G}')$ are the spectra of the corresponding discrete magnetic Laplacians as in Eq. (2.2.2), i.e., if $|\boldsymbol{G}| \geq |\boldsymbol{G}'| - r$ and if

$$\lambda_k(\boldsymbol{G}) \leq \lambda_{k+r}(\boldsymbol{G}') \qquad \text{for all } 1 \leq k \leq |\boldsymbol{G}'| - r.$$

If $r = 0$ we write again simply $\boldsymbol{G} \preccurlyeq \boldsymbol{G}'$.

Proposition 2.2.5. *The relation $\preccurlyeq$ is a preorder on $\mathscr{G}$.*

Proof. Lemma 2.2.3(i) and (iii) show the reflexivity and transitivity of $\preccurlyeq$ taking shift $s = r = 0$. □

Since there are non-isomorphic isospectral *MW*-graphs, it follows that $\preccurlyeq$ it is not anti-symmetric (i.e., equality of spectra does not imply that the *MW*-graphs are isomorphic). In particular, $\preccurlyeq$ it is not a partial order. See Chapter5.

Remark 2.2.6. The name *spectral order* has been introduced by Olson [Ols71] for two self-adjoint (bounded) operators T_1 and T_2 in a Hilbert space $\mathcal{H}$ with spectral resolutions $E_j(t) := \mathbf{1}_{(-\infty,t]}(T_j)$ $(j = 1, 2)$. Then $T_1 \preceq T_2$ if and only if $E_1(t) \leq E_2(t)$ for all $t \in \mathbb{R}$ (i.e. if $\langle E_1(t)\varphi, \varphi\rangle \leq \langle E_2(t)\varphi, \varphi\rangle$ for all $\varphi \in \mathcal{H}$). If $T_1 \geq 0$ and $T_2 \geq 0$, then $T_1 \preceq T_2$ is equivalent with $T_1^p \leq T_2^p$ for all $p \in \mathbb{N}$. If both operators have purely discrete spectrum $\lambda_k(T_j)$ (written in increasing order and repeated according to multiplicity) then we have the implications

$$T_1 \preceq T_2 \quad \Rightarrow \quad T_1 \leq T_2 \quad \Rightarrow \quad T_1 \preccurlyeq T_2,$$

where the latter means that $\lambda_k(T_1) \leq \lambda_k(T_2)$ for all k (the latter implication follows from the min-max principle as in Theorem 2.3.2).

Definition 2.2.7. For G_1 and G_2 two MW-graphs, with $G_1 \preccurlyeq G_2$ we define the *associated k-th* bracketing interval $J_k = J_k(G_1, G_2)$ by

$$J_k := \big[\lambda_k(G_1), \lambda_k(G_2)\big] \tag{2.2.3}$$

for $k = 1, \dots, |G_1|$.

If now G is an MW-graph with $G_1 \preccurlyeq G \preccurlyeq G_2$, then we have the following *eigenvalue bracketing*

$$\lambda_k(G) \in J_k \tag{2.2.4}$$

for all $k = 1, \dots, |G_1|$. Moreover,

$$\sigma(G) \subset J := \bigcup_{k=1}^{|G_1|} J_k \tag{2.2.5}$$

and we call $J = J(G_1, G_2)$ the *spectral localising set* of the pair G_1 and G_2, with the convention that $\lambda_k(G_1) = 2\rho_\infty^{G_1}$ for all $k = |G_2| + 1, \dots, |G_1|$.

The key observation for detecting spectral gaps in Chapter 4 using the eigenvalue bracketing technique is the following:

Proposition 2.2.8. *Let $\mathcal{G} = \{G_i\}_{i \in I}$ be a family of finite* MW*-graphs together with H_1 and H_2 be two* MW*-graphs and suppose that $H_1 \preccurlyeq G_i \preccurlyeq H_2$ with $|H_1| = |G_i| \geq |H_2|$ for all $i \in I$. If $c = \sup_{i \in I} \rho_\infty^{G_i} < \infty$, then*

$$\mu\Big(\bigcup_{i \in I} \sigma(G_i)\Big) \leq \mathrm{Tr}(H_2) - \mathrm{Tr}(H_1) + c\,(|H_1| - |H_2|) \tag{2.2.6}$$

where μ denotes the 1-dimensional Lebesgue measure. In particular, if $|H_1| - |H_2| = 1$ and $\mathrm{Tr}(H_2) - \mathrm{Tr}(H_1) < 0$, then $\bigcup_{i \in I} \sigma(G_i)$ cannot be the entire interval $[0, c]$.

Proof. We have

$$\begin{aligned}\mu\Big(\bigcup_{i \in I} \sigma(G_i)\Big) &\leq \mu\Big(\bigcup_{k=1}^{|H_1|} J_k\Big) \leq \sum_{k=1}^{|H_1|} \big(\lambda_k(H_2) - \lambda_k(H_1)\big) \\ &\leq Tr(H_2) - \mathrm{Tr}(H_1) + c(|H_1| - |H_2|).\end{aligned}$$

The inequality in Eq. (2.2.6) is a direct consequence of the preceding equalities. □

The relation between the preorder $\sqsubseteq$ and $\preccurlyeq$ is presented in the next section.

2.3 Geometric preorder $\sqsubseteq$ implies spectral preorder $\preccurlyeq$ for finite *MW*-graphs

We begin lifting maps between vertices and edges to the ℓ_2-spaces. Recall the geometric preorder in Definition 2.1.1 as well as its consequences in Lemma 2.1.3.

Lemma 2.3.1. *Let $\mathbf{G} = (G,\alpha,w)$ and $\mathbf{G}' = (G',\alpha',w')$ be two* MW*-graphs and $\pi\colon \mathbf{G} \to \mathbf{G}'$ an* MW*-graph homomorphism. If $G = (V,E)$ and $G' = (V',E')$, define the identification operators on functions over vertices $J^0\colon \ell_2(V',w') \to \ell_2(V,w)$ and on edges $J^1\colon \ell_2(E',w') \to \ell_2(E,w)$ given by $J^0\varphi := \varphi\circ\pi$ and $J^1\eta := \eta\circ\pi$, respectively. Then the following holds:*

(i) We have $\|J^0\varphi\|_{\ell_2(V,w)} \geq \|\varphi\|_{\ell_2(V',w')}$ for all $\varphi \in \ell_2(V',w')$. In particular, J^0 is injective. If π is vertex measure preserving, then J^0 is an isometry.

(ii) We have $\|J^1\eta\|_{\ell_2(E,w)} \leq \|\eta\|_{\ell_2(E',w')}$ for all $\eta \in \ell_2(E',w')$. If π is edge measure preserving, then J^1 is an isometry.

(iii) We have $d_\alpha J^0 = J^1 d_{\alpha'}$.

Proof. (i) From Definition 2.1.1 (ii) we have:

$$\begin{aligned}
\|J^0\varphi\|^2_{\ell_2(V,w)} &= \sum_{v\in V} |(\varphi\circ\pi)(v)|^2 w(v)\\
&= \sum_{v'\in V'}\Big(\sum_{v\in\pi^{-1}(v')} w(v)\Big)|\varphi(v')|^2 = \sum_{v'\in V'}(\pi_* w)(v')|\varphi(v')|^2\\
&\geq \sum_{v'\in V'} w'(v')|\varphi(v')|^2 = \|\varphi\|^2_{\ell_2(V',w')}.
\end{aligned}$$

Clearly, if π is vertex measure preserving, then $\pi_* w = w'$ on V', and equality in the above estimate holds.

(ii) The assertion of the identification map J^1 on the edges follows similarly from Definition 2.1.1 (iii), i.e.,

$$\begin{aligned}
\|J^1\eta\|^2_{\ell_2(E,w)} &= \frac{1}{2}\sum_{e\in E} |(\varphi\circ\eta)(e)|^2 w_e\\
&= \frac{1}{2}\sum_{e'\in E'}\Big(\sum_{e\in\pi^{-1}(e')} w_e\Big)|\eta_{e'}|^2 = \frac{1}{2}\sum_{e'\in E'}(\pi_* w)_{e'}|\eta_{e'}|^2\\
&\leq \frac{1}{2}\sum_{e'\in E'} w'_{e'}|\eta_{e'}|^2 = \|\eta\|^2_{\ell_2(E',w')}.
\end{aligned}$$

(iii) This intertwining equation follows immediately from the properties given in Definition 2.1.1 (i). □

Now, we recall some variations of the well-known variational characterisation of the eigenvalues, this theorem is fundamental for some relevant results in this dissertation, for the proof we reference [HJ85].

Theorem 2.3.2 (Courant-Hilbert)**.** *Let $\mathcal{H}$ be an n-dimensional (complex) Hilbert space and $A\colon\mathcal{H}\to\mathcal{H}$ linear and $A^* = A$. Moreover, denote by $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be the eigenvalues of A written in ascending order and repeated according to their multiplicities. Let $k \in \{1,2,\ldots,n\}$, then*

$$\lambda_k = \min_{S\in\mathcal{S}_{n-k}} \max_{\substack{\varphi\perp S\\ \varphi\neq 0}} \frac{\langle A\varphi,\varphi\rangle}{\langle A\varphi,\varphi\rangle} \qquad \textit{and} \qquad \lambda_k = \max_{S\in\mathcal{S}_{k-1}} \min_{\substack{\varphi\perp S\\ \varphi\neq 0}} \frac{\langle A\varphi,\varphi\rangle}{\langle A\varphi,\varphi\rangle}, \tag{2.3.1}$$

and

$$\lambda_k = \min_{S \in \mathcal{S}_k} \max_{\substack{\varphi \in S \\ \varphi \neq 0}} \frac{\langle A\varphi, \varphi \rangle}{\langle A\varphi, \varphi \rangle} \qquad \text{and} \qquad \lambda_k = \max_{S \in \mathcal{S}_{n-k+1}} \min_{\substack{\varphi \in S \\ \varphi \neq 0}} \frac{\langle A\varphi, \varphi \rangle}{\langle A\varphi, \varphi \rangle}, \tag{2.3.2}$$

where $\mathcal{S}_k$ denotes the set of k-dimensional subspaces of $\mathcal{H}$.

The following result for *MW*-graphs is just a simple consequence of the previous Theorem 2.3.2; in the case of $|\boldsymbol{G}| = |\boldsymbol{G}'| + 1$ with a measure preserving it is just known as the *eigenvalue interlacing*.

Theorem 2.3.3. *Let $\boldsymbol{G}, \boldsymbol{G}'$ be two finite* MW*-graphs, if $\boldsymbol{G}$ is geometrically smaller than $\boldsymbol{G}'$, then $\boldsymbol{G}$ is spectrally smaller than $\boldsymbol{G}'$, i.e.,*

$$\boldsymbol{G} \sqsubseteq \boldsymbol{G}' \quad \text{implies} \quad \boldsymbol{G} \preccurlyeq \boldsymbol{G}'.$$

Moreover, if there exists a map $\pi \colon \boldsymbol{G} \to \boldsymbol{G}'$ which is (vertex and edge) measure preserving, then we have, in addition,

$$\boldsymbol{G}' \overset{r}{\preccurlyeq} \boldsymbol{G}, \quad \text{where} \quad r = |\boldsymbol{G}| - |\boldsymbol{G}'| \geq 0.$$

Proof. First, note that π is surjective on the set of vertices by Lemma 2.1.3 (i) hence $|\boldsymbol{G}| \geq |\boldsymbol{G}'|$ and therefore $r \geq 0$. From Lemma 2.3.1 we conclude

$$\frac{\|d_\alpha J^0 \varphi'\|^2_{\ell_2(E,w)}}{\|J^0 \varphi'\|^2_{\ell_2(V,w)}} = \frac{\|J^1 d_{\alpha'} \varphi'\|^2_{\ell_2(E,w)}}{\|J^0 \varphi'\|^2_{\ell_2(V,w)}} \leq \frac{\|d_{\alpha'} \varphi'\|^2_{\ell_2(E',w')}}{\|\varphi'\|^2_{\ell_2(V',w')}}. \tag{2.3.3}$$

Denote by S'_k the k-dimensional subspace of $\ell_2(V', w')$ spanned by the first k eigenfunctions of $\Delta(\boldsymbol{G}')$. From the min-max characterisation of the k-th eigenvalue (first equality in Eq. (2.3.2)), we then have by the previous estimation:

$$\begin{aligned} \lambda_k(\boldsymbol{G}) = \min_{S \in \mathcal{S}_k} \max_{\substack{\varphi \in S \\ \varphi \neq 0}} \frac{\|d_\alpha \varphi\|^2_{\ell_2(E,w)}}{\|\varphi\|^2_{\ell_2(V,w)}} &\leq \max_{\substack{\varphi' \in S'_k \\ \varphi' \neq 0}} \frac{\|d_\alpha J^0 \varphi'\|^2_{\ell_2(E,w)}}{\|J^0 \varphi'\|^2_{\ell_2(V,w)}} \\ &\leq \max_{\substack{\varphi' \in S'_k \\ \varphi' \neq 0}} \frac{\|d_{\alpha'} \varphi'\|^2_{\ell_2(E',w')}}{\|\varphi'\|^2_{\ell_2(V',w')}} = \lambda_k(\boldsymbol{G}') \end{aligned}$$

for all $1 \leq k \leq |\boldsymbol{G}'|$, where $\mathcal{S}_k$ is the set of all k-dimensional subspaces of $\ell_2(V, w)$. Moreover, as J^0 is injective, $S = J^0(S'_k)$ is also k-dimensional, i.e., $J^0(S'_k) \in \mathcal{S}_k$. This shows $\boldsymbol{G} \preccurlyeq \boldsymbol{G}'$.

If π is measure preserving, then J^0 and J^1 are isometries, hence we have equality in Eq. (2.3.3). Moreover, let $n = |\boldsymbol{G}|$, $n' = |\boldsymbol{G}'|$ and denote by T'_k the space generated by the $n - k + 1$ eigenfunctions $\varphi'_{n'-n+k}, \dots, \varphi'_{n'}$ of the Laplacian on $\boldsymbol{G}'$, then we have similarly as before (second equality in Eq. (2.3.2))

$$\lambda_k(\boldsymbol{G}) = \max_{S\in\mathcal{S}_{n-k+1}} \min_{\substack{\varphi\in S\\ \varphi\neq 0}} \frac{\|d_\alpha \varphi\|^2_{\ell_2(E,w)}}{\|\varphi\|^2_{\ell_2(V,w)}} \geq \min_{\substack{\varphi'\in T'_k\\ \varphi'\neq 0}} \frac{\|d_\alpha J^0\varphi'\|^2_{\ell_2(E,w)}}{\|J^0\varphi'\|^2_{\ell_2(V,w)}}$$

$$= \min_{\substack{\varphi'\in T'_k\\ \varphi'\neq 0}} \frac{\|d_{\alpha'} \varphi'\|^2_{\ell_2(E',w')}}{\|\varphi'\|^2_{\ell_2(V',w')}} = \lambda_{n'-(n-k+1)+1}(\boldsymbol{G}') = \lambda_{k-r}(\boldsymbol{G}'),$$

where $S = J^0(T'_k)$ is $(n-k+1)$-dimensional since J^0 is injective. From Definition 2.2.1 and 2.2.4 it follows that $\boldsymbol{G}' \overset{r}{\preccurlyeq} \boldsymbol{G}$. □

We have the following simple consequence of the previous theorem and Example 2.1.2 (i).

Corollary 2.3.4. *Let* $\boldsymbol{G} = (G, \alpha, \deg)$ *and* $\boldsymbol{G}' = (G, \alpha, \mathbb{1})$*, then* $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$*. In particular,* $\boldsymbol{G} \preccurlyeq \boldsymbol{G}'$*, i.e. the (magnetic) eigenvalues of the standard Laplacian are always lower or equal than the (magnetic) eigenvalues of the combinatorial Laplacian.*

Proof. By Example 2.1.2 (i), we obtain $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$ and by Theorem 2.3.3, we conclude $\boldsymbol{G} \preccurlyeq \boldsymbol{G}'$. □

Remark 2.3.5. Note that the converse statement of Theorem 2.3.3 is false, i.e., there are *MW*-graphs such that $\boldsymbol{G} \preccurlyeq \boldsymbol{G}'$ but not $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$. Choose two non-isomorphic graphs G and G' such that their standard Laplacians have the same spectrum (see future Chapter 4). If $\boldsymbol{G} \sqsubseteq \boldsymbol{G}'$, then by Proposition 2.1.4 we have $\boldsymbol{G}' \cong \boldsymbol{G}/\!\sim$ for some $\sim$ equivalence relation on the vertices of $\boldsymbol{G}$. As the number of vertices for isospectral graphs are the same, each equivalence class contains only one element, and hence π is a graph isomorphism.

Another counterexample for the converse statement of Theorem 2.3.3 is given by $\boldsymbol{G} = \boldsymbol{G}_9$ and $\boldsymbol{G}' = \boldsymbol{G}_{10}$ in Figure 6.3.

2.4 Geometric perturbations and elementary operations

In this section, we consider some elementary operations on the *MW*-graphs, and we study the behaviour of the spectrum of the corresponding magnetic Laplacian. We will obtain some consequences for general weights, but more precise results are obtained for the combinatorial and standard weights.

We begin the study of elementary operations with edge deletion.

2.4.1 Deleting an edge

The following theorem generalises some well knows interlacing results. Some particular cases are proved in the next references: for the standard and combinatorial weights without vector potential, i.e. if $\boldsymbol{G} \in \mathscr{G}^0_{\text{deg}}$ or if $\boldsymbol{G} \in \mathscr{G}^0_{\mathbb{1}}$ see [Che+04]; for the standard signless Laplacian, i.e. if $\boldsymbol{G} \in \mathscr{G}^\pi_{\text{deg}}$ see [AT14, Thm.8] in relation to Corollary 2.4.2 (i). The next result is the generalisation of the ideas in the previous articles, but now we consider any vector potential acting on the magnetic weighted graph.

Let $\boldsymbol{G} = (G, \alpha, w)$ and $\boldsymbol{G}' = (G', \alpha', w')$ be two MW-graphs and $e_0 \in E(G)$. Suppose that $G' = G - \{e_0\}$ as in Definition 1.1.4 with the same magnetic potential acting on both graphs, i.e., $\alpha_e = \alpha'_e$ for all edge $e \in E(G') = E(G - e_0) \subset E(G)$. We say that $\boldsymbol{G}'$ is the edge e_0 deletion from $\boldsymbol{G}$ and we denote as $\boldsymbol{G}' = \boldsymbol{G} - \{e_0\}$. The Theorem 2.4.1 shows the relation between the spectrum of $\boldsymbol{G}$ and $\boldsymbol{G}'$ and respect to their weights. This result complete and generalise a similar result of [FLP18], where it is considered the virtualisation of the edge e_0.

Theorem 2.4.1 (General weights). *Let $\boldsymbol{G} = (G, \alpha, w)$ and $\boldsymbol{G}' = (G', \alpha', w')$ be two* MW-*graphs where $\boldsymbol{G}' = \boldsymbol{G} - e_0$ for some $e_0 \in E(G)$.*

(i) Suppose that $w'_e \le w_e$ for all edge $e \in E(G')$ and $w(v) \le w'(v)$ for all $v \neq \partial^\pm e_0 \in V(G)$.
  (a) If $w(v) \le w'(v)$ for $v = \partial^\pm e_0$, then $\boldsymbol{G}' \sqsubseteq \boldsymbol{G}$ (and hence $\boldsymbol{G}' \preccurlyeq \boldsymbol{G}$).
  (b) If $w(v) - w_{e_0} \le w'(v)$ for $v = \partial^\pm e_0$ and $\rho_\infty \le 1$, then $\boldsymbol{G}' \overset{1}{\preccurlyeq} \boldsymbol{G}$. Moreover if e_0 is a loop and $\alpha_{e_0} = \pi$ then $\boldsymbol{G}' \preccurlyeq \boldsymbol{G}$.

(ii) Suppose that $w_e \le w'_e$ for all edge $e \in E(G')$ and $w'(v) \le w(v)$ for all $v \in V(G)$, then $\boldsymbol{G} \overset{1}{\preccurlyeq} \boldsymbol{G}'$. Moreover, if e_0 is a loop with $\alpha_{e_0} = 0$ then $\boldsymbol{G} \preccurlyeq \boldsymbol{G}'$.

(iii) If $w_e = w'_e$ for all edge $e \in E(G')$, $w'(v) = w(v)$ for all $v \in V(G)$ and e_0 is a loop with $\alpha_{e_0} = 0$ then $\boldsymbol{G}$ and $\boldsymbol{G}'$ are isospectral.

Proof. (ia) Consider the inclusion map $\iota_{e_0} : G' \to G$ defined in Subsection 1.1.2. Then, the map ι_{e_0} fulfilled the conditions in Definition 2.1.1, and we conclude $\boldsymbol{G}' \sqsubseteq \boldsymbol{G}$. Finally, by Theorem 2.3.3 we obtain $\boldsymbol{G}' \preccurlyeq \boldsymbol{G}$.

(ib) We prove the relation $\boldsymbol{G}' \overset{1}{\preccurlyeq} \boldsymbol{G}$. We will use Theorem 2.3.2 twice,

$$\begin{aligned}
\lambda_k(\boldsymbol{G}') &= \max_{S \in \mathcal{S}_{k-1}} \min_{\substack{\varphi \perp S \\ \varphi \neq 0}} \frac{\|d_{\alpha'}\varphi\|^2_{\ell_2(E',w')}}{\|\varphi\|^2_{\ell_2(V',w')}} \\
&= \max_{S \in \mathcal{S}_{k-1}} \min_{\substack{\varphi \perp S \\ \varphi \neq 0}} \frac{\|d_\alpha \varphi\|^2_{\ell_2(E,w)} - |(d_\alpha\varphi)_{e_0}|^2 w_{e_0}}{\|\varphi\|^2_{\ell_2(V,w)} - |\varphi(\partial^- e_0)|^2 w_{e_0} - |\varphi(\partial^+ e_0)|^2 w_{e_0}} \\
&\le \max_{S \in \mathcal{S}_{k-1}} \min_{\substack{\varphi \perp S \cup L'(e_0) \\ \varphi \neq 0}} \frac{\|d_\alpha \varphi\|^2_{\ell_2(E,w)} - |(d_\alpha\varphi)_{e_0}|^2 w_{e_0}}{\|\varphi\|^2_{\ell_2(V,w)} - \left(|\varphi(\partial^- e_0)|^2 + |\varphi(\partial^+ e_0)|^2\right) w_{e_0}} \\
&= \max_{S \in \mathcal{S}_{k-1}} \min_{\substack{\varphi \perp S \cup L'(e_0) \\ \varphi \neq 0}} \frac{\|d_\alpha \varphi\|^2_{\ell_2(E)} - 4|\varphi(\partial^+ e_0)|^2 w_{e_0}}{\|\varphi\|^2_{\ell_2(V,w)} - 2|\varphi(\partial^+ e_0)|^2 w_{e_0}}
\end{aligned}$$

$$\leq \max_{S\in\mathcal{S}_{k-1}} \min_{\substack{\varphi\perp S\cup L'(e_0)\\ \varphi\neq 0}} \frac{\|d_\alpha\varphi\|^2_{\ell_2(E,w)}}{\|\varphi\|^2_{\ell_2(V,w)}}$$

$$\leq \max_{S\in\mathcal{S}_k} \min_{\substack{\varphi\perp S\\ \varphi\neq 0}} \frac{\|d_\alpha\varphi\|^2_{\ell_2(E,w)}}{\|\varphi\|^2_{\ell_2(V,w)}} = \lambda_{k+1}(\boldsymbol{G}),$$

for $k = 1,\dots,n-1$, where $L'(e_0) = \mathbb{C}\{\psi'\}$ denotes the linear space generated by

$$\psi' = \frac{1}{(w(\partial^+e_0))^{1/2}}\delta_{\partial^+e_0} + \mathrm{e}^{\mathrm{i}\alpha_{e_0}}\frac{1}{(w(\partial^-e_0))^{1/2}}\delta_{\partial^-e_0}, \tag{2.4.1}$$

and where we used the fact that $\varphi' \perp L'(e_0)$ implies $|(d_\alpha\varphi)_{e_0}|^2 = 4|\varphi(\partial_+e_0)|^2$ and $|\varphi(\partial_-e_0)|^2 = |\varphi(\partial_+e_0)|^2$ in the third equality. Moreover, for the second inequality, we use the following inequality between real numbers a, b and γ (see [Che+04]), namely

$$a^2-2\gamma^2 \geq 0, \qquad b^2-\gamma^2 > 0, \qquad \text{and} \qquad \frac{a^2}{b^2}\leq 2\,, \qquad \text{then} \qquad \frac{a^2-2\gamma^2}{b^2-\gamma^2}\leq \frac{a^2}{b^2}\,.$$

We also used the fact that $\rho_\infty \leq 1$ as a^2/b^2 is the Rayleigh quotient for the graph $\boldsymbol{G}$ and hence $a^2/b^2 \leq 2$.

The proof of the second part is very similar to the previous. We observe if $\alpha_{e_0} = \pi$ for a loop e_0, then $\psi' = 0$ in Eq. (2.4.1) and $L'(e_0) = 0$. In particular, we do not have to introduce the function ψ', hence $\lambda_k(\boldsymbol{G}') \leq \lambda_k(\boldsymbol{G})$.

(ii) Now, we prove $\boldsymbol{G} \overset{1}{\preccurlyeq} \boldsymbol{G}'$. We use Theorem 2.3.2 twice, and we obtain

$$\lambda_{k+1}(\boldsymbol{G}') = \min_{S\in\mathcal{S}_{n-(k+1)}} \max_{\substack{\varphi\perp S\\ \varphi\neq 0}} \frac{\|d_{\alpha'}\varphi\|^2_{\ell_2(E',w')}}{\|\varphi\|^2_{\ell_2(V',w')}}$$

$$\geq \min_{S\in\mathcal{S}_{n-(k+1)}} \max_{\substack{\varphi\perp S\cup L(e_0)\\ \varphi\neq 0}} \frac{\|d_{\alpha'}\varphi\|^2_{\ell_2(E',w')}}{\|\varphi\|^2_{\ell_2(V',w')}}$$

$$= \min_{S\in\mathcal{S}_{n-(k+1)}} \max_{\substack{\varphi\perp S\cup L(e_0)\\ \varphi\neq 0}} \frac{\|d_{\alpha}\varphi\|^2_{\ell_2(E,w)}}{\|\varphi\|^2_{\ell_2(V,w)}}$$

$$\geq \min_{S\in\mathcal{S}_{n-k}} \max_{\substack{\varphi\perp S\\ \varphi\neq 0}} \frac{\|d_{\alpha}\varphi\|^2_{\ell_2(E,w)}}{\|\varphi\|^2_{\ell_2(V,w)}} = \lambda_k(\boldsymbol{G})$$

for $k = 1,\dots,n-1$, where $L(e_0) = \mathbb{C}\{\psi\}$ denotes the linear space generated by

$$\psi = \frac{1}{(w(\partial^+e_0))^{1/2}}\delta_{\partial^+e_0} - \mathrm{e}^{\mathrm{i}\alpha_{e_0}}\frac{1}{(w(\partial^-e_0))^{1/2}}\delta_{\partial^-e_0} \tag{2.4.2}$$

for the canonical orthonormal basis $(\delta_v)_v$ of $\ell_2(V,w)$; and where we used the fact that $(d_\alpha\varphi)_{e_0}=0$ if $\varphi\perp L(e_0)$, hence we can just take the norm over E' instead of E for the second equality.

The proof of the second part is very similar to the previous, we observe that $(d_\alpha\varphi)_{e_0}=0$ if $\alpha_{e_0}=0$ for a loop e_0, and $\psi=0$ in Eq. (2.4.2). In particular, we do not have to introduce the function ψ, hence $\lambda_k(\boldsymbol{G}')\leq\lambda_k(\boldsymbol{G})$.

(iii) The weights in edges and vertices fulfil the conditions in part (ia), then we conclude that $\boldsymbol{G}'\preccurlyeq\boldsymbol{G}$ and by part (ii) follows $\boldsymbol{G}\preccurlyeq\boldsymbol{G}'$. Finally, observe that G and G' have the same number of vertices, then $\boldsymbol{G}$ and $\boldsymbol{G}'$ are isospectral. □

For standard and combinatorial weights, we immediately obtain more precise results:

Corollary 2.4.2. *Let $\boldsymbol{G}=(G,\alpha,w)$ and $\boldsymbol{G}'=(G',\alpha',w')$ be two* MW*-graphs where $\boldsymbol{G}'=\boldsymbol{G}-e_0$ for some $e_0\in E(G)$.*

(i) If $\boldsymbol{G},\boldsymbol{G}'\in\mathscr{G}_{\deg}$, then $\boldsymbol{G}\overset{1}{\preccurlyeq}\boldsymbol{G}'\overset{1}{\preccurlyeq}\boldsymbol{G}$.
Moreover, if e_0 is a loop and $\alpha_{e_0}=0$ then $\boldsymbol{G}'\preccurlyeq\boldsymbol{G}$ and if $\alpha_{e_0}=\pi$ then $\boldsymbol{G}\preccurlyeq\boldsymbol{G}'$.

(ii) If $\boldsymbol{G},\boldsymbol{G}'\in\mathscr{G}_{\mathbb{1}}$, then $\boldsymbol{G}\overset{1}{\preccurlyeq}\boldsymbol{G}'$ and $\boldsymbol{G}'\sqsubseteq\boldsymbol{G}$, hence $\boldsymbol{G}\overset{1}{\preccurlyeq}\boldsymbol{G}'\preccurlyeq\boldsymbol{G}$.
If e_0 is not a loop, then there exists $1\leq k\leq|\boldsymbol{G}|$ such that $\lambda_k(\boldsymbol{G}')<\lambda_k(\boldsymbol{G})$.
If e_0 is a loop with $\alpha_{e_0}=0$ then $\boldsymbol{G}$ and $\boldsymbol{G}'$ are isospectral, i.e., their Laplacians have the same spectrum.

Proof. (i) Observe that $\deg_{G'}(v)=\deg_G(v)-1$ for $v=\partial^\pm e_0$ and $\deg_{G'}(v)=\deg_G(v)$ for all other vertices, hence by Theorem 2.4.1 (ia) follows that $\boldsymbol{G}'\overset{1}{\preccurlyeq}\boldsymbol{G}$ and by Theorem 2.4.1 (ii) follows that $\boldsymbol{G}\overset{1}{\preccurlyeq}\boldsymbol{G}'$. We conclude $\boldsymbol{G}\overset{1}{\preccurlyeq}\boldsymbol{G}'\overset{1}{\preccurlyeq}\boldsymbol{G}$. Now, suppose that e_0 is a loop. If $\alpha_{e_0}=0$, then then $\boldsymbol{G}'\preccurlyeq\boldsymbol{G}$ by Theorem 2.4.1 (ii) and if $\alpha_{e_0}=\pi$ then $\boldsymbol{G}\preccurlyeq\boldsymbol{G}'$ by Theorem 2.4.1 (ia).

(ii) By Theorem 2.4.1 (i) follows $\boldsymbol{G}'\sqsubseteq\boldsymbol{G}$ (and hence $\boldsymbol{G}'\preccurlyeq\boldsymbol{G}$) and by Theorem 2.4.1 (ii) follows that $\boldsymbol{G}\overset{1}{\preccurlyeq}\boldsymbol{G}'$. Suppose that e_0 is not a loop, note that

$$\sum_{k=1}^{n}\lambda_k(\boldsymbol{G})=tr(\Delta_\alpha)=\sum_{v\in V}\deg_G(v)>\sum_{v\in V'}\deg_{G'}(v)=tr(\Delta_{\alpha'})=\sum_{k=1}^{n}\lambda_k(\boldsymbol{G}'),$$

hence there exists an index $k\in\{1,\dots,n\}$ such that $\lambda_k(\boldsymbol{G}')<\lambda_k(\boldsymbol{G})$. If If e_0 is a loop with $\alpha_{e_0}=0$ then $\boldsymbol{G}$ and $\boldsymbol{G}'$ are isospectral by Theorem 2.4.1 (iii). □

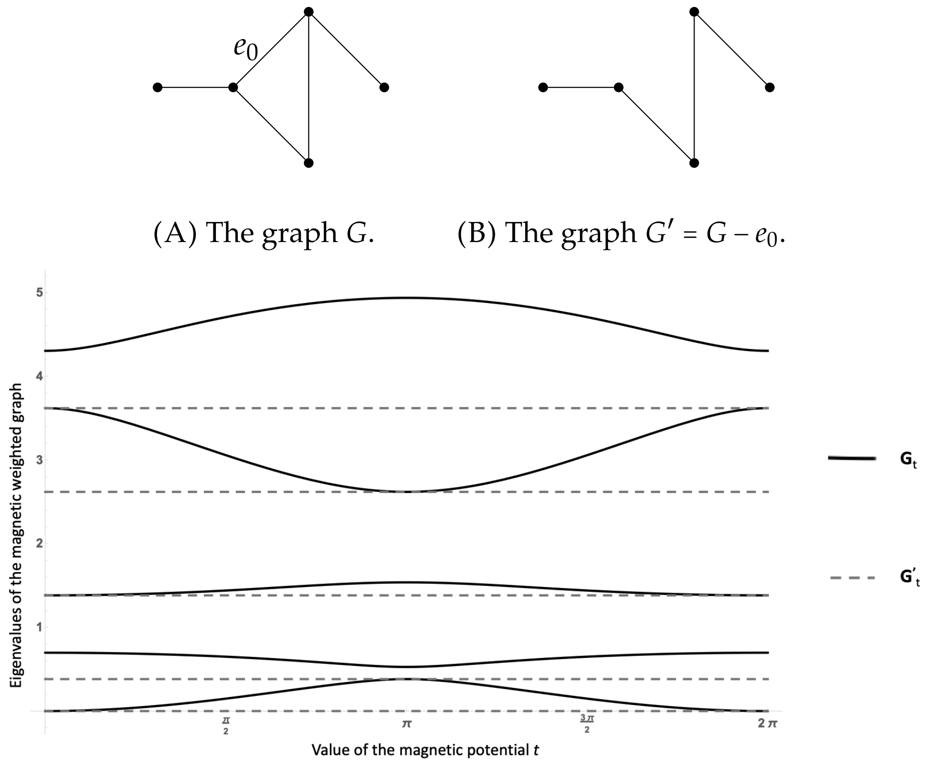
Remark 2.4.3. Corollary 2.4.2(ii) is sharp in the sense that one cannot lower the shift 1: for example, the relation $\boldsymbol{G}\preccurlyeq\boldsymbol{G}'$ is false in Example 2.4.4. Similarly, one can find counterexamples that other shifts cannot be smaller.

Example 2.4.4. For all $t\in[0,2\pi]$, and using the Notation 1.4.2, we consider the *MW*-graph $\boldsymbol{G}_t\in\mathscr{G}_{\mathbb{1}}^t$ defined by G in Figure 2.2A. Note that the flux through the closed path adds up to t. The spectrum $\sigma(\boldsymbol{G}_t)$ consists of five eigenvalues plotted as a solid line in Figure 2.2C (the spectrum depends on the value of t). Let $\boldsymbol{G}_t'\in\mathscr{G}_{\mathbb{1}}^t$ defined by $G'=G-e_0$ (see Figure 2.2B). Because G' is a tree, then $\sigma(\boldsymbol{G}_t')=\sigma(\boldsymbol{G}_0')$ for any t. In particular, $\sigma(\boldsymbol{G}_0')$

consists of five eigenvalues (dotted lines in Figure 2.2C). From Corollary 2.4.2(ii) we conclude $\boldsymbol{G}_t \overset{1}{\preccurlyeq} \boldsymbol{G}'_0 \preccurlyeq \boldsymbol{G}_t$ for all $t \in [0, 2\pi]$, and

$$\sigma(\boldsymbol{G}'_0) = \left\{0, \frac{3-\sqrt{5}}{2}, \frac{5-\sqrt{5}}{2}, \frac{3+\sqrt{5}}{2}, \frac{5+\sqrt{5}}{2}\right\} \approx \{0, 0.381, 1.382, 2.618, 3.618\} .$$

Finally, we can give a localisation of the spectrum of $\sigma(\boldsymbol{G}'_t)$ for any $t \in [0, 2\pi]$, i.e., $\lambda_i(\boldsymbol{G}_t) \in [\lambda_i(\boldsymbol{G}'), \lambda_{i+1}(\boldsymbol{G}')]$ for $i = 1, 2, 3$ and 4.



(A) The graph G.

(B) The graph $G' = G - e_0$.

(C)

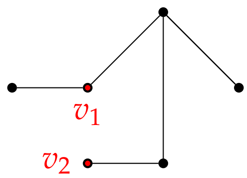
FIGURE 2.2: If we delete the edge e_0 from graph G in Figure 2.2A, we obtain the graph $G' = G - e_0$ in Figure 2.2B. Let $\boldsymbol{G}_t$ (respectively $\boldsymbol{G}'_t$) be in $\mathscr{G}^t_{\mathbb{1}}$ with underlying graphs G (respectively, G'). In Figure 2.2C, we plot $\sigma(\boldsymbol{G}_t)$ (respectively, $\sigma(\boldsymbol{G}'_t)$) as a solid (respectively, dashed) line for all $t \in [0, 2\pi]$. Note that $\boldsymbol{G}_t \overset{1}{\preccurlyeq} \boldsymbol{G}'_t \preccurlyeq \boldsymbol{G}_t$.

2.4.2 Vertex contraction

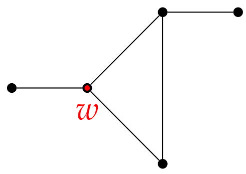
The second operation considered in this section is the contraction of vertices or glueing vertices.

Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph and consider two different vertices $v_1, v_2 \in V(G)$. Consider the graph $G' = G/\{v_1, v_2\}$ as in Definition 1.1.5, i.e., consider an equivalence relation $\sim$ on $V(G)$ that identify (or *glueing*) the vertices v_1 and v_2. In particular $E(G) = E(G')$, then the magnetic potential acting on G induces a magnetic potential on G'. Recall the definition in Subsection 1.1.2 of the *projection* of the equivalence relation $\sim$, i.e., $\pi\colon V \to V/\!\sim$ defined by $\pi(v) = [v]$. The vertices that belongs to the same equivalence relation, will be also known as glued vertices.

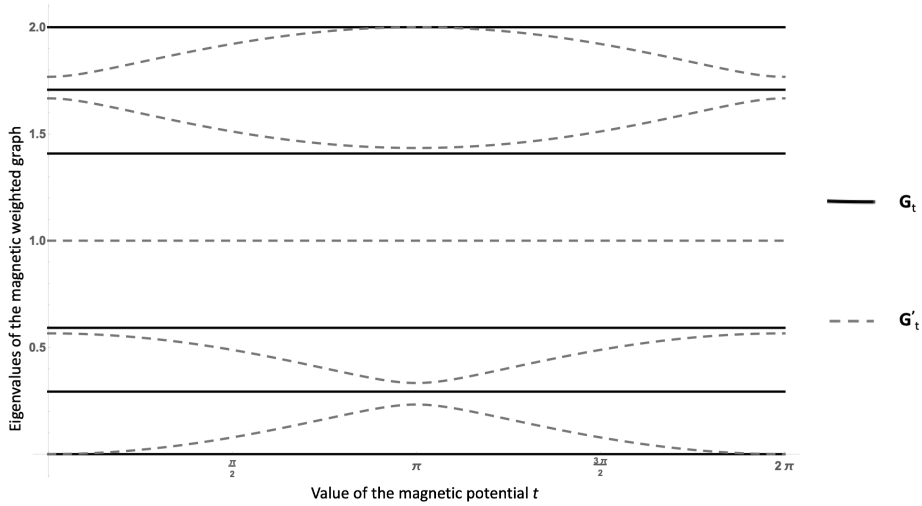
Let $\mathbf{G} = (G, \alpha, w)$ and $\mathbf{G}' = (G', \alpha', w')$ be two *MW*-graphs and $v_1, v_2 \in V(G)$. Suppose that $G' = G/\{v_1, v_2\}$ as in Definition 1.1.5 with the same magnetic potential acting on both graphs, i.e., $\alpha_e = \alpha'_e$ for all edge $e \in E(G') = E(G)$. We say that $\mathbf{G}'$ is the vertex contraction from $\mathbf{G}$ and we denote as $\mathbf{G}' = \mathbf{G}/\{v_1, v_2\}$. The next theorem shows some relation between the spectrum of the *MW*-graphs $\mathbf{G}$ and $\mathbf{G}'$ and their weights.



(A) The graph G.



(B) The graph $G' = G/\{v_1, v_2\}$ where $w = [v_1] = [v_2]$.



(C)

FIGURE 2.3: Contracting the vertices v_1 and v_2 of the *MW*-graph $\mathbf{G}$ in 2.3A gives the graph $\mathbf{G}' = \mathbf{G}/\{v_1, v_2\}$ in Figure 2.3B. Let $\mathbf{G}_t, \mathbf{G}'_t \in \mathscr{G}_{\mathrm{deg}}$ defined by $\mathbf{G}$ (respectively, $\mathbf{G}'$), then in Figure 2.3C we plot as solid lines $\sigma(\mathbf{G}_t)$ and as dashed lines $\sigma(\mathbf{G}'_t)$ for $t \in [0, 2\pi]$.

Theorem 2.4.5. *Let $\mathbf{G}, \mathbf{G}'$ be two* MW*-graphs where $\mathbf{G} = (G, \alpha, w)$ and $\mathbf{G}' = (G', \alpha', w')$ with $G' = G/\{v_1, v_2\}$ for some $v_1, v_2 \in V(G)$ and $\alpha = \alpha'$.*

(i) Suppose $w_e \leq w'_e$ for all $e \in E(G)$ with $w'([v]) \leq w(v)$ for all $v \neq v_1, v_2 \in V(G)$ and $w'([v_1]) \leq w(v_1) + w(v_2)$, then $\mathbf{G} \sqsubseteq \mathbf{G}'$ (and hence $\mathbf{G} \preccurlyeq \mathbf{G}'$).

(ii) Suppose $w_e = w'_e$ for each $e \in E(G)$ and $w'(v) = w(v)$ for all $v \neq v_1, v_2 \in V(G)$.

(a) If $w'([v_1]) = w(v_1) + w(v_2)$, then $\mathbf{G} \sqsubseteq \mathbf{G}'$ and $\mathbf{G}' \overset{1}{\preccurlyeq} \mathbf{G}$(and hence $\mathbf{G} \preccurlyeq \mathbf{G}' \overset{1}{\preccurlyeq} \mathbf{G}$).

(b) *If $w'([v_1]) = w(v_1) = w(v_2)$, then $\mathbf{G} \sqsubseteq \mathbf{G}'$ and $\mathbf{G}' \overset{r+1}{\preccurlyeq} \mathbf{G}$ (and hence $\mathbf{G} \preccurlyeq \mathbf{G}' \overset{r+1}{\preccurlyeq} \mathbf{G}$) where $r = \min\{deg_G(v_1), deg_G(v_2)\}$.*

Proof. (i) Consider π the projection graph homomorphism that identifies v_1 and v_2 in the same equivalence relation, i.e., $\pi: G \to G/\sim$ defined in Eq. (1.1.4) where $v_1 \sim v_2$. Then π fulfil the conditions in Definition 2.1.1, and this shows that $\mathbf{G} \sqsubseteq \mathbf{G}'$. Hence, $\mathbf{G} \preccurlyeq \mathbf{G}'$ follows from Theorem 2.3.3.

(iia) This part is similar, but in this case, the map $\pi: G \to G'$ is measure preserving, hence we also conclude $\mathbf{G}' \overset{1}{\preccurlyeq} \mathbf{G}$ from Theorem 2.3.3 as $|\mathbf{G}| - |\mathbf{G}'| = 1$.

(iib) By (i) it follows $\mathbf{G} \sqsubseteq \mathbf{G}'$. Suppose $r = \deg(v_1)$ is the minimal degree of v_1 and v_2, and we proceed by induction on r to prove $\mathbf{G}' \overset{r+1}{\preccurlyeq} \mathbf{G}$. If $r = 0$, then v_1 is an isolated vertex in $\mathbf{G}$, then $\mathbf{G}' = \mathbf{G}/\{v_1, v_2\}$, so the spectrum of $\mathbf{G}$ is just the one of $\mathbf{G}'$ with an extra 0, then $\mathbf{G}' \overset{1}{\preccurlyeq} \mathbf{G}$. Suppose that the statement is true for $r = k$. Now, we prove the case $r = k+1$. Consider $\mathbf{G}'' = (G'', \alpha'', w'')$ where $G'' = G' - e_0$ for any $e_0 \in E_{v_1}$, $\alpha''_e = \alpha_e$ and $w''_e = w_e$ for all $e \in E(G'')$ and $w''(v) = w(v)$ for all $v \in V(G')$. By (iia) follows $\mathbf{G}' \overset{1}{\preccurlyeq} \mathbf{G}''$ and by construction $deg_{G''}(v_1) = r$, hence by inductive hypothesis $\mathbf{G}'' \overset{r+1}{\preccurlyeq} \mathbf{G}$, therefore, $\mathbf{G}'' \overset{r+2}{\preccurlyeq} \mathbf{G}$. □

As a corollary, we obtain again for the combinatorial and standard weight. Note that our result improves Theorem 10 of [AT14]:

Corollary 2.4.6. *Let $\mathbf{G}, \mathbf{G}'$ be two* MW*-graphs where $\mathbf{G} = (G, \alpha, w)$ and $\mathbf{G}' = (G', \alpha', w')$ with $G' = G/\{v_1, v_2\}$ for some $v_1, v_2 \in V(G)$ and $\alpha = \alpha'$.*

(i) If $\mathbf{G}, \mathbf{G}' \in \mathscr{G}_{\mathrm{deg}}$, then $\mathbf{G} \sqsubseteq \mathbf{G}'$ (hence $\mathbf{G} \preccurlyeq \mathbf{G}'$) and $\mathbf{G}' \overset{1}{\preccurlyeq} \mathbf{G}$.

(ii) If $\mathbf{G}, \mathbf{G}' \in \mathscr{G}_{\mathbb{1}}$, then $\mathbf{G} \sqsubseteq \mathbf{G}'$ (hence $\mathbf{G} \preccurlyeq \mathbf{G}'$) and $\mathbf{G}' \overset{r+1}{\preccurlyeq} \mathbf{G}$ where $r = \min\{deg_G(v_1), deg_G(v_2)\}$.

Proof. (i) If $\mathbf{G}, \mathbf{G}' \in \mathscr{G}_{\mathrm{deg}}$, and the standard weights fulfil the condition in Theorem 2.4.5 (i)–(iia), then $\mathbf{G} \sqsubseteq \mathbf{G}'$ and $\mathbf{G}' \overset{1}{\preccurlyeq} \mathbf{G}$.

(ii) If $\mathbf{G}, \mathbf{G}' \in \mathscr{G}_{\mathrm{deg}}$, and the combinatorial weights fulfil the condition in Theorem 2.4.5 (i)–(iib), then $\mathbf{G} \preccurlyeq \mathbf{G}' \overset{r+1}{\preccurlyeq} \mathbf{G}$. □

Example 2.4.7. For any $t \in [0, 2\pi]$, consider the *MW*-graph $\mathbf{G}_t = (G, \alpha^t, \deg)$ defined by G in Figure 2.3A. The magnetic potential α^t is defined as follow: $\alpha^t_{e_1} = t$, $\alpha^t_{\bar{e}_1} = -t$ and zero in all the other edges. Since G is a tree, then $\sigma(\mathbf{G}_t) = \sigma(\mathbf{G}_0)$ and $\sigma(\mathbf{G}_0)$ consists of the six eigenvalues (solid lines in Figure 2.3C). For any $t \in [0, 2\pi]$, consider the $\mathbf{G}'_t = \mathbf{G}_t/\{v_1, v_2\}$ with the standard weights, i.e. $\mathbf{G}' \in \mathscr{G}_{\mathrm{deg}}$ defined by the graph G' in Figure 2.3B. Figure 2.3C shows the five eigenvalues of $\sigma(W'_t)$ changing t from 0 to 2π in dashed lines. By Theorem 2.4.5 we have $\mathbf{G}_t \preccurlyeq W'_t \overset{1}{\preccurlyeq} \mathbf{G}_t$ for any t, then $\mathbf{G}_0 \preccurlyeq \mathbf{G}'_t \overset{1}{\preccurlyeq} \mathbf{G}_0$. We can use the spectrum of tree $\boldsymbol{G}$ to localised the spectrum of $\boldsymbol{G}'$ for any vector potential, i.e.

$$\lambda_1(\boldsymbol{G}'_t) \in \left[0, 1 - \frac{1}{\sqrt{2}}\right], \quad \lambda_2(\boldsymbol{G}'_t) \in \left[1 - \frac{1}{\sqrt{2}}, 1 - \frac{1}{\sqrt{6}}\right], \quad \lambda_3(\boldsymbol{G}'_t) \in \left[1 - \frac{1}{\sqrt{6}}, 1 + \frac{1}{\sqrt{6}}\right],$$
$$\lambda_4(\boldsymbol{G}'_t) \in \left[1 + \frac{1}{\sqrt{6}}, 1 + \frac{1}{\sqrt{2}}\right] \quad \text{and} \quad \lambda_5(\boldsymbol{G}'_t) \in \left[1 + \frac{1}{\sqrt{2}}, 2\right].$$

The previous bracketing is also the same if we contracting any other vertices, i.e. $\boldsymbol{G}_0 \preccurlyeq \boldsymbol{G}''_t \overset{1}{\preccurlyeq} \boldsymbol{G}_0$ where $\boldsymbol{G}''_t = \boldsymbol{G}/\{u,v\}$ for all $u, v \in V(G)$.

2.4.3 Virtualising edges and vertices

Let $\boldsymbol{G} = (G, \alpha, w)$ be an *MW*-graph with a set of edges E_0 and a set of vertices V_0. It can be thought the *edge virtualisation* of the set E_0 as putting the weights on the edges E_0 to zero, and the *vertex virtualisation* of V_0 as changing the weights of V_0 to zero. By definition of weights, it allows weight zero at the edges, but not on the vertices. So we need to explain what does it mean to have zero weight vertex.

Definition 2.4.8 (*virtualising* edges)**.** Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph and $E_0 \subset E(G)$. We denote by $\mathbf{G}^- = (G^-, \alpha^-, w^-)$ the weighted graph such that

(i) $G^- := G$ and $\alpha^- := \alpha$.
(ii) $w^-(v) := w(v)$ for all $v \in V(G)$;
(iii) $w^-_e := w_e$ for all $e \in E(G^-) = E(G) \setminus E_0$; and $w^-_e := 0$ for all $e \in E_0$

We call $\mathbf{G}^-$ the weighted subgraph obtained from $\boldsymbol{G}$ by *virtualising the edges* E_0. We will sometimes also use the suggestive notation $\mathbf{G}^- := \boldsymbol{G} - E_0$.

The corresponding discrete magnetic Laplacian is denoted by $\Delta_{\alpha^-}^{\mathbf{G}^-}$.

Some useful facts are collected in the next remark.

Remark 2.4.9.

(i) Note that $\Delta_{\alpha^-}^{\mathbf{G}^-} = (d_{\alpha^-})^* d_{\alpha^-}$, where $d_{\alpha^-} := \pi \circ d_\alpha$ and $\pi \colon \ell_2(E(G), w) \to \ell_2(E(G^-), w^-)$ is the orthogonal projection onto the functions on the non-virtualised edges. Note that $\pi = \iota^*$ with $\iota \colon \ell_2(E(G^-), w^-) \to \ell_2(E(G), w)$ being the natural inclusion, i.e., for $\eta \in \ell_2(E(G^-), w^-)$ $\iota\eta$ is extended by 0 on $E(G^-) = E(G) \setminus E_0$. Note that the process of virtualisation of edges can also be described by changing the weights on $\boldsymbol{G}$: set $m_{e_0} = 0$ for $e_0 \in E_0$, and leave all other weights unchanged.
(ii) The process of *virtualising* edges has consequences for various quantities related to the graph. The most important for us here refers to the spectrum (see the following proposition). If ρ^- denotes the relative weight of $\mathbf{G}^-$, then $\rho^-(v) \le \rho(v)$ for $v \in V$. Let $\boldsymbol{G} = (G, \alpha, \deg_G)$ be a magnetic weighted graph with standard weights, and denote by $\boldsymbol{G}' = (G^-, \alpha, \deg_{G^-})$ the graph G^- with standard weights. If $E_0 \neq \emptyset$, then there exists a $v \in V(G)$ such that $w^-(v) > w'(v)$, i.e., the new weight w^- is not standard anymore. More generally, if $\boldsymbol{G} = (G, \alpha, w)$ has a normalized

weight, then w^- is no longer normalized; the relative weights of $\mathbf{G}^-$ and $\boldsymbol{G}'$ fulfil $\rho^-(v) \leq \rho'(v) = 1$ with strict inequality for $v \in V(G^-)$ incident with an edge in E_0. If $\boldsymbol{G} = (G, w, \mathbb{1})$ is a weighted graph with combinatorial weight w, then w^- as well has the combinatorial weight, i.e., combinatorial weights are preserved under edge virtualisation.

(iii) It is also clear that if G is connected, then G^- need not to be connected any more. Moreover, the homology of the graph changes under edge virtualisation. This is perhaps an important motivation for this definition. Later we will exploit the fact that deleting a suitable set of edges the graph will turn it into a tree. The graph G^- is sometimes also called spanning subgraph.

The next corollary shows that the process of virtualising edges produces a DML which is spectrally smaller (cf., Definition 2.2.4).

Corollary 2.4.10. *Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph and $E_0 \subset E(G)$. Let $\boldsymbol{G}^- = (G^-, \alpha^-, w^-)$ where $G^- = G - E_0$ the edge virtualised graph (cf. Definition 2.4.8), then*

$$\boldsymbol{G}^- \preccurlyeq \boldsymbol{G}\,.$$

Proof. By definition of the virtualised magnetic weighted graph $\boldsymbol{G}^-$ (see Definition 2.4.8), then $w_e = w'_e$ for all edge and $w(v) = w'(v)$ for all $v \in V(G)$. Then, by Theorem 2.4.1 (ia) it follows $\boldsymbol{G}' \sqsubseteq \boldsymbol{G}$ and hence by Theorem 2.3.3 conclude $\boldsymbol{G}^- \preccurlyeq \boldsymbol{G}$.

□

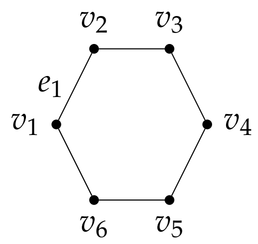
Example 2.4.11. Let $\boldsymbol{G} = (G, \alpha, w)$ be the 6-cycle with standard weights as in Figure 2.4A. Let $\mathbf{G}^- = (G^-, \alpha^-, w^-)$ be the graph with the edge e_1 virtualised (i.e., $\boldsymbol{G}^- = \boldsymbol{G} - e_1$, see Definition 2.4.8, and w^- being the restriction of w to $E(G^-) = E(G) \setminus \{e_1, \overline{e_1}\}$. If α is any vector potential on G, then α can be supported on e_1, so α^- is trivial on $\boldsymbol{G}^-$. Therefore $\Delta_{\alpha^-}^{\mathbf{G}^-}$ is unitarily equivalent with $\Delta^{\mathbf{G}^-}$ (usual Laplacian with $\alpha = 0$). Finally, we plot the six eigenvalues of $\Delta_\alpha^{\boldsymbol{G}}$ and $\Delta^{\mathbf{G}^-}$, when α_{e_1} runs through $[0, 2\pi]$. This example illustrates $\sigma(\Delta_{\alpha^-}^{\mathbf{G}^-}) \preccurlyeq \sigma(\Delta_\alpha^{\boldsymbol{G}})$ hence, by unitary equivalence, also $\sigma(\Delta^{\mathbf{G}^-}) \preccurlyeq \sigma(\Delta_\alpha^{\boldsymbol{G}})$.

Remark 2.4.12. Example 2.4.11 shows that Corollary 2.4.10 is not valid if we insist on having standard weights both in $\boldsymbol{G}$ and $\boldsymbol{G}^-$ (cf., Remark 2.4.9 (ii)). Take G and $G^- = C_6 - e_1$ both with the standard weights (Figure 2.4). Consider the vector potential supported on e_1 such that $\alpha_{e_1} = \pi/2$. In this case, we have $\lambda_4(\Delta_{\alpha^-}^{\boldsymbol{G}^-}) = \lambda_4(\Delta_0^{\boldsymbol{G}^-}) \approx 1.31 \nleq 1.26 \approx \lambda_4(\Delta_\alpha^{\boldsymbol{G}})$, hence $\Delta_{\alpha^-}^{\boldsymbol{G}^-}$ is not spectrally smaller than $\Delta_\alpha^{\boldsymbol{G}}$.

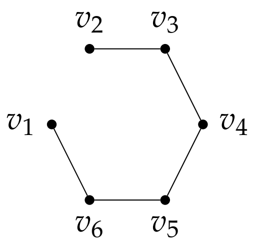
The next graph operation is dual to edge virtualising.

Definition 2.4.13 (*virtualising vertices*)**.** Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph with $V_0 \subset V(G)$. We denote by $\mathbf{G}^+ = (G^+, \alpha^+, w^+)$ the magnetic weighted partial subgraph defined as follows:

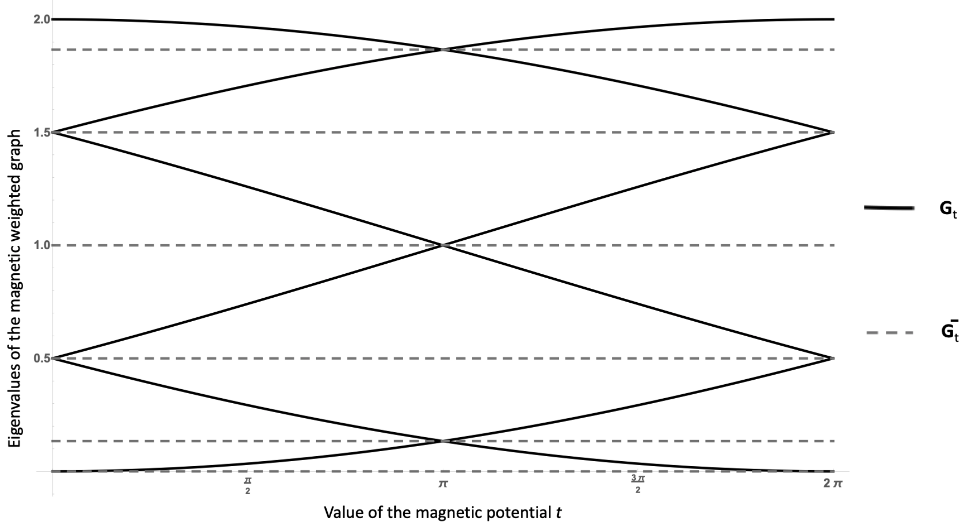
(i) $V(G^+) = V(G) \setminus V_0$ with $w^+(v) := w(v)$ for all $v \in V(G^+)$;
(ii) $E(G^+) = E(G) \setminus E(V_0)$ with $w_e^+ := w_e$ for all $e \in E(G^+)$;
(iii) $\alpha_e^+ = \alpha_e$, for all $e \in E(G^+)$.



(A) The graph $G = C - 6$.



(B) $G^- = C_6 - \{e_1\}$.



(C) Spectra of $\Delta_\alpha^{C_6}$ (black lines) and $\Delta_{\alpha^-}^{G^-}$ (dashed lines).

FIGURE 2.4: Virtualisation of an edge in the cycle with six vertices denoted as C_6.

We call $\mathbf{G}^+$ the magnetic weighted open subgraph obtained from $\boldsymbol{G}$ by *virtualising* the vertices V_0. We will also use the suggestive notation $G^+ = G - V_0$.

The corresponding discrete magnetic Laplacian is defined by

$$\Delta_{\alpha^+}^{\mathbf{G}^+} = (d_{\alpha^+})^* d_{\alpha^+}, \qquad \text{where} \qquad d_{\alpha^+} := d_\alpha \circ \iota$$

with

$$\iota\colon \ell_2(V(G^+), w^+) \to \ell_2(V(G), w), \qquad (\iota f)(v) = \begin{cases} f(v), & v \in V(G^+), \\ 0, & v \in V_0. \end{cases}$$

Remark 2.4.14.

(i) Here, we use the notion of G^+ being an *open subgraph* of G. Then G^+ have edges with only one vertex in the $V(G^+)$, the other one being in $V_0 \subset V(G)$; one can also call the vertices in V_0 *virtual*. Formally, $\partial_{G^+}\colon E(G^+) \to V(G) \times V(G)$ still maps into the product of the vertex set, but of the *original* graph G, not into $V(G^+) \times V(G^+)$. In general, $G^+ = (V(G^+), E(G^+))$ is not a graph in the classical sense anymore, as some edges have initial or terminal vertices no longer in $V(G^+)$. One can actually see that there is no such proper weighted graph $\boldsymbol{G}_1 = (G^+, 0, \deg)$. In fact, the corresponding Laplacian $\Delta^{\boldsymbol{G}_1}$ has 0 as lowest eigenvalue, but $\Delta^{\mathbf{G}^+}$ does not have 0 as lowest eigenvalue (provided $V_0 \neq \emptyset$) since any function with $\Delta^{\mathbf{G}^+} f = 0$ has to be constant on V, and 0 on V_0, hence $f = 0$.

(ii) The definition of $d_{\alpha^+} = d_\alpha \circ \iota$ is consistent with the natural definition of d_{α^+} for a partial subgraph, namely we set

$$(d_{\alpha^+} f)_e = \begin{cases} \mathrm{e}^{\mathrm{i}\alpha_e/2} f(\partial^+ e) - \mathrm{e}^{-\mathrm{i}\alpha_e/2} f(\partial^- e), & \text{if } \partial^\pm e \in V(G^+), \\ \mathrm{e}^{\mathrm{i}\alpha_e/2} f(\partial^+ e), & \text{if } \partial_+ e \in V(G^+), \partial^- e \in V_0, \\ -\mathrm{e}^{-\mathrm{i}\alpha_e/2} f(\partial^- e), & \text{if } \partial^- e \in V(G^+), \partial^+ e \in V_0, \end{cases}$$

see Eq. (1.4.1). This is the same as extending $f \in \ell_2(V(G^+), w^+)$ by 0. In particular, the notation d_{α^+} is justified. Actually, the magnetic potential on connecting bridges edges can be gauged away.

(iii) The nature of virtualising vertices is different from the process of virtualising edges, but dual in the sense that for virtualising edges, we use $d_{\alpha^-} = \iota^* \circ d_\alpha$, and for virtualising vertices, we use $d_{\alpha^+} = d_\alpha \circ \iota$ with ι being the natural embedding on the space of edges and vertices, respectively. As a consequence, $\Delta_{\alpha^+}^{\mathbf{G}^+} = d_{\alpha^+}^* d_{\alpha^+} = \iota^* \Delta_\alpha^{\boldsymbol{G}} \iota$, i.e., $\Delta_{\alpha^+}^{\mathbf{G}^+}$ is a compression of $\Delta_\alpha^{\boldsymbol{G}}$. If we number the vertices $V(G)$ such that the vertices of V_0 appear at the end, then a matrix representation of $\Delta_\alpha^{\boldsymbol{G}}$ (cf. Subsection Eq. (1.5.4)) has the block structure

$$\Delta_\alpha^{\boldsymbol{G}} = \begin{bmatrix} \Delta_{\alpha^+}^{\mathbf{G}^+} & C_{12} \\ C_{21} & C_{22} \end{bmatrix},$$

i.e., $\Delta_{\alpha^+}^{\mathbf{G}^+}$ corresponds to a principal sub-matrix of $\Delta_\alpha^{\boldsymbol{G}}$. In particular, we have the following inequality for traces:

$$Tr\left[\Delta_{\alpha^+}^{\mathbf{G}^+}\right] \leq Tr\left[\Delta_\alpha^{\boldsymbol{G}}\right].$$

We show next, that the process of vertex virtualisation makes a DML spectrally larger (cf., Definition 2.2.4).

Corollary 2.4.15. *Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph and $V_0 \subset V(G)$. Denote by $\mathbf{G}^+ = (G^+, \alpha^+, w^+)$ the vertex-virtualised graph with $G^+ = G - V_0$ (cf. Definition 2.4.13), then*

$$\boldsymbol{G} \preccurlyeq \boldsymbol{G}^+.$$

Proof. Let $n = |V|$ and $r = |V_0|$. Since $\Delta_{\alpha^+}^{\mathbf{G}^+} = \iota^* \Delta_\alpha^{\boldsymbol{G}} \iota$ is a compression of $\Delta_\alpha^{\boldsymbol{G}}$ we can apply Cauchy's Interlacing Theorem (see, e.g. [Bha07, Corollary II.1.5]) and obtain

$$\lambda_k(\Delta_\alpha^{\boldsymbol{G}}) \leq \lambda_k(\Delta_{\alpha^+}^{\mathbf{G}^+}) \leq \lambda_{k+r}(\Delta_\alpha^{\boldsymbol{G}}), \qquad k = 1, 2, \ldots, n - r.$$

Since $\Delta_{\alpha^+}^{\mathbf{G}^+}$ acts on an $(n - r)$-dimensional Hilbert space, we have shown that $\sigma(\Delta_\alpha^{\boldsymbol{G}}) \preccurlyeq \sigma(\Delta_{\alpha^+}^{\mathbf{G}^+})$ and hence $\boldsymbol{G} \preccurlyeq \boldsymbol{G}^+$ (cf., Definition 2.2.4) using only the first inequality. □

Summarising, given a magnetic weighted graph $\boldsymbol{G} = (G, \alpha, w)$ the process of edge and vertex virtualisation produces two different magnetic weighted graphs $\mathbf{G}^- = (G^-, \alpha^-, w^-)$ respectively $\mathbf{G}^+ = (G^+, \alpha^+, w^+)$ with induced potentials and such that the corresponding DMLs are spectrally smaller respectively larger than the original one, i.e.,

$$\boldsymbol{G}^- \preccurlyeq \boldsymbol{G} \preccurlyeq \boldsymbol{G}^+.$$

This will be the basis for the next bracketing technique used later on.

Corollary 2.4.16. *Let $\boldsymbol{G} = (G, \alpha, w)$ be a magnetic weighted graph with $E_0 \subset E(G)$ and $V_0 \subset V(G)$. Then*

$$\boldsymbol{G}^- \preccurlyeq \boldsymbol{G} \preccurlyeq \boldsymbol{G}^+ .$$

where $\mathbf{G}^- = (G^-, \alpha^-, w^-)$ with $G^- = G - E_0$ the edge virtualised graph (cf. Definition 2.4.8) and denote by $\mathbf{G}^+ = (G^+, \alpha^+, w^+)$ the vertex-virtualised graph with $G^+ = G - V_0$ (cf.Definition 2.4.13). In particular, we have the spectral localising inclusion

$$\sigma(\Delta_\alpha^{\boldsymbol{G}}) \subset \bigcup_{k=1}^{n} \underbrace{[\lambda_k(\Delta_{\alpha^-}^{\boldsymbol{G}^-}), \lambda_k(\Delta_{\alpha^+}^{\boldsymbol{G}^+})]}_{=:J_k} \subset [0, 2\rho_\infty] \tag{2.4.3}$$

where $n = |G^-|$ and the convention that $\lambda_k(\Delta_{\alpha^+}^{\boldsymbol{G}^+}) = 2\rho_\infty$ for all $|G^-| < k \leq |G^+|$.

Proof. The Corollary 2.4.10 proves $\boldsymbol{G}^- \preccurlyeq \boldsymbol{G}$ and the Corollary 2.4.15 proves $\boldsymbol{G} \preccurlyeq \boldsymbol{G}^+$ and together with Definition 2.2.7 and Eq. (2.2.5) is obtained the localising inclusion. □

Later on, the set E_0 will be the set of connecting edges of a periodic graph (Chapter 3), and we will choose V_0 to be as small as possible to guarantee the existence of spectral gaps (in general, this set is not unique).

3 Periodic and Covering Graphs

The analysis of Schrödinger operators (in particular Laplacians) and its spectrum on periodic structures is one of the most important features in solid state physics. Periodicity here means that there is a discrete group Γ (typically Abelian) acting on the underlying structure, e.g., a manifold or a graph with compact quotient, that commutes with the operator. Using Floquet theory, the analysis of the operator can be reduced to the analysis of a related family of operators on the quotient. In the case of graphs, the family of operators corresponds to a family of finite dimensional operators, i.e., matrices. The study of periodic structures in all fields of mathematics is quite natural, for examples periodic manifolds [Pos03], periodic differential equations [Eas73], periodic groups [Zel92], periodic elliptic operators [HP03] to mention only a few.

In order to study the magnetic Laplacian on infinite periodic graphs, we use the concept of covering maps [Sun13]. A *covering map* is a morphism between two graphs that, locally, are essentially the same. Given a covering map, we form an important group: the *covering transformation groups*. This concept is fundamental for the Topological Crystallography [Sun13], and it has an important role in the study of crystals and its symmetries. The structure of the crystal (or any molecule) is model by a periodic graph, in which each atom is represented by a vertex on the graph and each edge of the graph represents a *bond*.

One application of the theory of covering graphs can be found in [MSS15]. In this remarkable paper is proved that there exist infinite families of regular bipartite Ramanujan graphs (for every degree greater than 2). This result solves (partially) a conjecture of Lubotzky. They use the notion of 2-covering and interlacing families of polynomials to construct infinite families of irregular Ramanujan graphs. Years after, in [HPS18] is generalised the case $r = 2$, and it is proved that bipartite Ramanujan graph has a Ramanujan r-covering for every r using an r-covering. Also, a crucial component of the proof is the existence polynomials (with the property of interlacing families) for complex reflection symmetry.

In this chapter, we introduce the formal definition of *covering graph* in Section 3.1 and *periodic graph* in Section 3.2, together with some important properties and examples.

The basic introduction of the discrete Floquet Theory is presented in Section 3.3 (we have included more technical results in Appendix A). The principal result from this section is presented in Theorem 3.4.2. This theorem interprets the magnetic potential as a Floquet parameter. The result is going to be crucial for proving the existence of spectral gaps in Chapter 4.

3.1 Covering graphs

The concept of *covering graph* is fundamental in the theory of Topological crystallography. A *topological crystal* G is an infinite-fold regular covering (possibly with parallel edges or loops) over a finite graph G_0 (see [Sun13] for the details), whose covering transformation group is *free* Abelian group.

In this section, we present the basic theory of covering maps. Roughly speaking, a covering map is a continuous map between two topological spaces. This map has two properties: it is surjective, and it preserves the local topological structure. A discrete version of covering graphs is presented in the next definition.

Definition 3.1.1. Let $G = (V, E)$ and $G_0 = (V_0, E_0)$ be two connected graphs with $\varpi\colon G \to G_0$ a graph homomorphism. We say that ϖ is a *covering map* if it preserves local adjacency relations between vertices and edges; more precisely,

(i) The function $\varpi_V\colon V \to V_0$ is surjective.
(ii) For every $v \in V$, the restriction $\varpi\restriction_{E_v}\colon E_v \to E_{0,\varpi(v)}$ is a bijection.

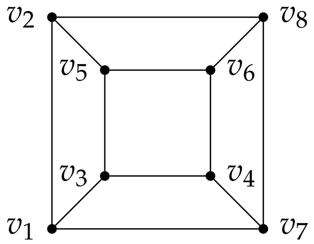
The graph G is *finite covering* (resp. *infinite covering*) of G_0, if G is a finite graph (resp. infinite graph).

Example 3.1.2. We show two simple examples of covering maps. The first example can be found in [Sun13]. Consider the graph G in Figure 3.1A and the graph G_0 in Figure 3.1B. It is easy to see that G is a covering of G_0 with the next covering map:

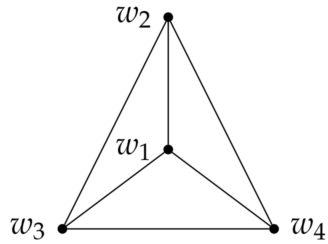
$$\varpi(v) = \begin{cases} w_1, & \text{if } v = v_5, v_7 \\ w_2, & \text{if } v = v_2, v_4 \\ w_3, & \text{if } v = v_3, v_8 \\ w_4, & \text{if } v = v_1, v_6\ . \end{cases}$$

Observe that for simple graphs, the graph homomorphism is defined by the function on the vertices, because it determines the function on the edges.

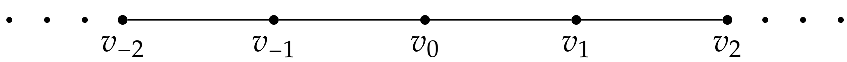
The second example shows an infinite covering. In this case, the infinite lattice in one dimension (or the infinity path) in Figure 3.1C is an infinity cover of the graph in Figure 3.1D, that is a loop. The covering map is given by $\omega(v_i) = v$ for $i \in \mathbb{Z}$.



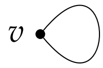
(A) The finite graph G.



(B) The graph G_0



(C) The infinite graph G'.



(D) The graph G_0'

FIGURE 3.1: Examples of covering graphs. The graph G is a finite covering of G_0 and the graph G' is an infinite covering of G_0'.

3.2 Periodic graphs

Another way to explain the *covering map* is by using the periodicity of the graph. To define a periodic graph, we need to see how a group acts on a graph. A group Γ is said to *act* on a set S when is given a map $\varphi\colon \Gamma \times S \to S$ satisfying the following conditions for all $s \in S$:

(i) If 1_Γ is the identity element of Γ, then $\varphi(1_\Gamma, s) = s$.
(ii) $\varphi(\gamma, \varphi(\gamma', s)) = \varphi(\gamma\gamma', s)$ for all $\gamma, \gamma' \in \Gamma$.

In this case, the group Γ is called a *transformation group*, S is called a Γ-set and φ is called the *group action*. For simplicity, we write γs instead of $\varphi(\gamma, s)$. An *action* of Γ in S is *transitive* if, for any $s_1, s_2 \in S$, there exists $\gamma \in \Gamma$ with $\gamma s_1 = s_2$. We also say that Γ acts *freely* on S if $\gamma s = s$ for some $s \in S$, then $\gamma = 1_\Gamma$.

If A and B are two Γ-sets, a map $f\colon A \to B$ is said to be Γ-*equivariant* if holds $f(\gamma a) = \gamma f(a)$ for all $a \in A$ and $\gamma \in \Gamma$.

Given a graph G and a group Γ acting on G (on vertices and edges), we can define the *quotient graph*, which we denote by G/Γ in a unique way by the next theorem:

Theorem 3.2.1 ([Sun08]). *Let $G = (V, E)$ be a graph on which a group Γ acts without inversion, and let $V_1 := V/\Gamma$ and $E_1 := E/\Gamma$, the orbit spaces for the Γ-actions. Then there exists a unique graph structure on the pair $G_1 := (V_1, E_1)$ such that the pair $\varphi := (\varphi_V, \varphi_E)$ of the canonical projections*

$$\varphi_V\colon V \to V_1, \qquad \textit{and} \qquad \varphi_E\colon E \to E_1$$

form a graph homomorphism.

Now, we can extend this construction to the magnetic weighted graph. Intuitively, it is a periodic structure with a translation action which quotient is a finite magnetic weighted graph.

Definition 3.2.2. Let $\widetilde{\mathbf{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ be a magnetic weighted graph and Γ a group. We say that $\widetilde{\mathbf{G}}$ is Γ-periodic if the graph, weights and magnetic potential are periodic in the following sense:

(i) *Graph periodicity*. The graph $\widetilde{G} = (\widetilde{V}, \widetilde{E})$ is Γ-*periodic*, if the following holds:
  (a) The group Γ acts freely on the graph $\widetilde{G}$ without inversion, i.e., Γ acts freely on both sets of vertices $\widetilde{V}$ and edges $\widetilde{E}$ such that $\gamma e \neq \bar{e}$ for all $e \in \widetilde{E}$.
  (b) The quotient $G = \widetilde{G}/\Gamma$ is a finite graph.

(ii) *Operator periodicity*. The weight $\widetilde{w}$ and the magnetic potential $\widetilde{\alpha}$ are Γ-periodic (or invariant under the action of G), i.e.,

$$w(\gamma v) = w(v)\ ,\ v \in \widetilde{V}\ ,\ w_{\gamma e} = w_e\ ,\ e \in \widetilde{E} \qquad \text{and} \qquad \widetilde{\alpha}_{\gamma e} = \widetilde{\alpha}_e\ ,\ e \in \widetilde{E}\ .$$

Remark 3.2.3. Note that any Γ-periodic graph $\widetilde{G}$ is, in fact, a covering graph of $G = \widetilde{G}/\Gamma$ and the canonical map, i.e., the quotient map $\pi \colon \widetilde{G} \to G$ is a covering map. If we consider a periodic graph $\widetilde{G}$, then, by definition, the standard or combinatorial weights acting on $\widetilde{G}$ satisfy the invariance conditions on the weights.

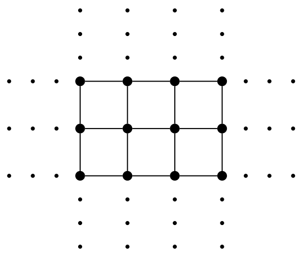
Let $\widetilde{\mathbf{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ be a Γ-periodic graph, we can consider the finite magnetic weighted graph $\mathbf{G} = (G, \alpha, w)$ as follow: $G = \widetilde{G}/\Gamma$ and the induced weight w and magnetic potential α on the quotient graph is given by $w = \widetilde{w} \circ \pi^{-1}$ and $\alpha = \widetilde{\alpha} \circ \pi^{-1}$. We denote this *MW*-graph as $\mathbf{G} = \widetilde{\mathbf{G}}/\Gamma$.

Example 3.2.4. Let $\widetilde{\mathbf{G}} = (\widetilde{G}, 0, \deg)$ be a magnetic weighted graph, where $\widetilde{G}$ is either the $\mathbb{Z}^n$-lattice or the graphene lattice (hexagonal lattice consisting of carbon atoms, see Figure 3.2A and 3.2B) both with standard weights, then $\sigma(\Delta^{\widetilde{G}}) = [0, 2]$. Hence, the set of spectral gaps is empty.

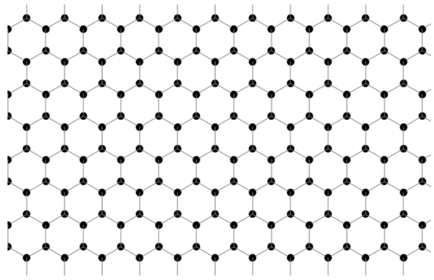
The graph*a*ne is just the decoration of the graph*e*ne adding a hydrogen atom for each carbon atom (see Figure 3.2C). Here, in the case when $\widetilde{G}$ is the graph that models the graph*a*ne, the $\sigma(\Delta^{\widetilde{G}}) = [0, 3/4] \cup [5/4, 2]$ for the standard weight, hence the interval $(3/4, 5/4)$ is a spectral gap. The study of spectral gaps is going to be a fundamental part of Chapter 4.

We define next some useful notions in relation to periodic graphs (see, e.g., [FLP18], Section 5, [FL19], Section 4 as well as ([KS14], Sections 1.2 and 1.3) and [LP08b]). The idea behind the periodic structure, it is the existence of a fundamental domain that repeated with the action of the group acting on it. Then, for the discrete case of the periodic graph, we have the following definition of a fundamental domain of vertices and fundamental domain of edges.

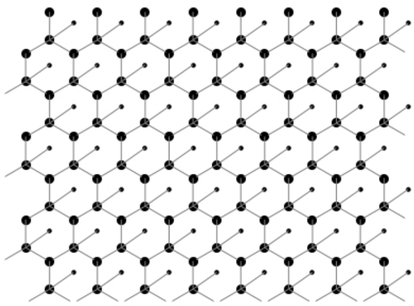
Definition 3.2.5. Let $\widetilde{G} = (\widetilde{V}, \widetilde{E})$ be a Γ-periodic graph.



(A) The $\mathbb{Z}^2$-lattice.



(B) The graphene.



(C) The Graphane.

FIGURE 3.2: Examples of $\mathbb{Z}^2$ periodic graphs.

(i) A *vertex fundamental domain*, respectively *edge fundamental domain* on a Γ-periodic graph is given by two subsets $D^V \subset \widetilde{V}$ and $D^E \subset \widetilde{E}$ satisfying

$$\widetilde{V} = \bigcup_{\gamma\in\Gamma} \gamma D^V \quad \text{and} \quad \gamma_1 D^V \cap \gamma_2 D^V = \emptyset \quad \text{if } \gamma_1 \neq \gamma_2,$$
$$\widetilde{E} = \bigcup_{\gamma\in\Gamma} \gamma D^E \quad \text{and} \quad \gamma_1 D^E \cap \gamma_2 D^E = \emptyset \quad \text{if } \gamma_1 \neq \gamma_2$$

with the restriction that $D^E \cap E(\widetilde{V} \setminus D^V) = \emptyset$, i.e., an edge in D^E has at least one endpoint in D^V, using the definition given with Eq. (1.1.1). We often simply write D for a fundamental domain.

(ii) A fundamental domain of a periodic graph $\widetilde{G}$ is an open subgraph (cf., Definition 1.1.2)

$$D := (D^V, D^E),$$

where D^V and D^E are vertex and edge fundamental domains, respectively, and the connection map $\partial_D = \partial_{\widetilde{G}} \restriction_{D^E}$. We call

$$E(\widetilde{G}, D) := E(D^V, \widetilde{V} \setminus D^V)$$

the set of connecting edges of the fundamental domain D in $\widetilde{G}$.

We collect some important observations on periodic graphs in the next remark.

Remark 3.2.6.

(i) Note that once a fundamental domain D^V has been specified in a Γ-periodic graph $\widetilde{G}$, we can write any $v \in V(\widetilde{G})$ uniquely as $v = \xi(v)v_0$ for a unique pair

$(\xi(v), v_0) \in \Gamma \times D^V$. This follows from the fact that the action is free. We call $\xi(v)$ the Γ-*coordinate of* v (with respect to the fundamental domain D^V). Similarly, we can define the coordinates for the edges: any $e \in E(\widetilde{G})$ can be written as $e = \xi(e)e_0$ for a unique pair $(\xi(e), e_0) \in \Gamma \times D^E$. In particular, we have

$$\xi(\gamma v) = \gamma\xi(v) \qquad \text{and} \qquad \xi(\gamma e) = \gamma\xi(e).$$

(ii) Once we have chosen a fundamental domain $D = (D^V, D^E)$, we can embed D it into the quotient $G = \widetilde{G}/\Gamma$ of the covering $\pi\colon \widetilde{G} \to G = \widetilde{G}/\Gamma$ by

$$D^V \to V(G) = V/\Gamma, \quad v \mapsto [v] \qquad \text{and} \qquad D^E \to E(G) = E/\Gamma, \quad e \mapsto [e],$$

where $[v]$ and $[e]$ denote the Γ-orbits of v and e, respectively. By definition of a fundamental domain, these maps are bijective. Moreover, if $\partial(e) \subset D^V$ in D, then also $\partial([e]) \subset V(G)$, i.e., the embedding is an (open) graph homomorphism.

We introduce now, a way to localise the edges in the periodic graph, so we define the *index* of an edge in the following definition, see, e.g.,[KS14; KS15; KS16].

Definition 3.2.7. Let $\widetilde{G} = (\widetilde{V}, \widetilde{E})$ be a Γ-periodic graph with fundamental domain $D = (D^V, D^E)$. We define the *index* of an edge $e \in E$ as

$$\mathrm{ind}_D(e) := \xi(\partial^+ e)\,(\xi(\partial^- e))^{-1} \in \Gamma.$$

In particular, we have $\mathrm{ind}_D\colon E \mapsto \Gamma$, and $\mathrm{ind}_D(e) \neq 1_\Gamma$ if and only if $e \in \bigcup_{\gamma\in\Gamma} \gamma E(D, \widetilde{G})$, i.e., the index is only non-trivial on the (translates of the) connecting edges. Moreover, the set of indices and its inverses generate the group Γ.

Since the index fulfils $\mathrm{ind}_D(\gamma e) = \gamma \mathrm{ind}_D(e)$ for all $\gamma \in \Gamma$ and by Remark 3.2.6 (i), we can extend the definition to the quotient $G = \widetilde{G}/\Gamma$ by setting $\mathrm{ind}_G([e]) = \mathrm{ind}_D(e)$ for all $e \in E(\widetilde{G})$. We denote by $[E(D, \widetilde{G})] := \{[e] \mid e \in E(D, \widetilde{G})\}$.

3.3 Discrete Floquet Theory

Let $\widetilde{\boldsymbol{G}} = (\widetilde{G}, \widetilde{w})$ be a weighted Γ-periodic graph where $\widetilde{G} = (\widetilde{V}, \widetilde{E})$ and fundamental domain $D = (D^V, D^E)$ with corresponding weights inherited from $\widetilde{G}$. In this context, one has the natural Hilbert space identifications (the details can be founded in Appendix A)

$$\ell_2(\widetilde{V}, \widetilde{w}) \cong \ell_2(\Gamma) \otimes \ell_2(D^V, \widetilde{w}) \cong \ell_2\left(\Gamma, \ell_2(D^V, \widetilde{w})\right).$$

Floquet theory uses a partial Fourier transformation on the Abelian group that can be understood as putting coordinates on the periodic structure and allows to decompose the corresponding operators as direct integrals. Concretely, we consider

$$F\colon \ell_2(\Gamma) \to L_2(\widehat{\Gamma}), \qquad (F\mathbf{a})\,(\chi) := \sum_{\gamma\in\Gamma} \overline{\chi(\gamma)} a_\gamma$$

for $\mathbf{a} = \{a_\gamma\}_{\gamma\in\Gamma} \in \ell_2(\Gamma)$ and where $\widehat{\Gamma}$ denotes the character group of Γ. We adapt to the discrete context of graphs with periodic magnetic potential $\widetilde{\alpha}$ the main results concerning Floquet theory needed later. See, e.g., ([LP07] Section 3) or [KS14] for details, additional motivation and references.

For any character $\chi \in \widehat{\Gamma}$, consider the space of *equivariant functions* on vertices and edges

$$\begin{aligned} \ell_2^\chi(V,\widetilde{w}) &:= \{g\colon V \to \mathbb{C} \mid g(\gamma v) = \chi(\gamma)g(v) \text{ for all } v \in V \text{ and } \gamma \in \Gamma\}, \\ \ell_2^\chi(E,\widetilde{w}) &:= \left\{\eta\colon E \to \mathbb{C} \mid \eta_{\gamma e} = \chi(\gamma)\eta_e \text{ for all } e \in E \text{ and } \gamma \in \Gamma\right\}. \end{aligned}$$

These spaces have the natural inner product defined on the fundamental domains D^V and D^E:

$$\langle g_1, g_2\rangle := \sum_{v\in D^V} g_1(v)\overline{g_2(v)}\widetilde{w}(v) \quad \text{and} \quad \langle \eta_1,\eta_2\rangle := \sum_{e\in D^E} \eta_{1,e}\overline{\eta_{2,e}}\widetilde{w}_e\,.$$

The definition of the inner product is independent of the choice of the fundamental domain (due to the equivariance). We extend the standard decomposition to the case of the DML with periodic magnetic potential (see, for example, [KS14; HS99]).

Proposition 3.3.1. *Let $\widetilde{\mathbf{G}} = (\widetilde{G},\widetilde{\alpha},\widetilde{w})$ be a Γ-periodic magnetic weighted graph where $\widetilde{G} = (\widetilde{V},\widetilde{E})$. Then there are unitary transformations*

$$\begin{aligned} \Phi\colon \ell_2(\widetilde{V},\widetilde{w}) &\to \int_{\widehat{\Gamma}}^{\oplus} \ell_2^\chi(\widetilde{V},\widetilde{w})d\chi \quad \textit{given by} \quad (\Phi f)_\chi(v) := \sum_{\gamma\in\Gamma} \overline{\chi(\gamma)} f(\gamma v) \\ \Phi\colon \ell_2(\widetilde{E},\widetilde{w}) &\to \int_{\widehat{\Gamma}}^{\oplus} \ell_2^\chi(\widetilde{E},\widetilde{w})d\chi \quad \textit{given by} \quad (\Phi\eta)_\chi(v) := \sum_{\gamma\in\Gamma} \overline{\chi(\gamma)}\eta_{\gamma e}\,, \end{aligned}$$

such that

$$\sigma\left(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}\right) = \bigcup_{\chi\in\widehat{\Gamma}} \sigma\left(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}(\chi)\right),$$

where equivariant Laplacian (fibre operators) is defined as $\left(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}(\chi)\right) := \Delta_{\widetilde{\alpha}}^{\widetilde{G}} \restriction_{\ell_2^\chi(\widetilde{V})}$.

Proof. Consider the twisted derivative $d_{\widetilde{\alpha}}\colon \ell_2(\widetilde{V},\widetilde{w}) \to \ell_2(\widetilde{E},\widetilde{w})$ specified in Eq. (1.4.1) and the equivariant twisted derivative on the fibre spaces defined by $d_{\widetilde{\alpha}}^\chi\colon \ell_2^\chi(\widetilde{V},\widetilde{w}) \to \ell_2^\chi(\widetilde{E},\widetilde{w})$

$$(d_{\widetilde{\alpha}}^\chi g)_e := e^{i\widetilde{\alpha}_e/2}g(\partial^+e) - e^{-i\widetilde{\alpha}_e/2}g(\partial^-e)\,, \quad g \in \ell_2^\chi(\widetilde{V},\widetilde{w})\,.$$

It is straightforward to check that if $g \in \ell_2^\chi(\widetilde{V},\widetilde{w})$, then $d_{\widetilde{\alpha}}^\chi g \in \ell_2^\chi(\widetilde{E})$ and that $\Delta_{\widetilde{\alpha}}^{\widetilde{G}} = (d_{\widetilde{\alpha}}^\chi)^* d_{\widetilde{\alpha}}^\chi$. Moreover, we will show that the unitary transformations Φ intertwine these two first order operators, i.e.,

$$\Phi d_{\widetilde{\alpha}} f = \int_{\widehat{\Gamma}}^{\oplus} d_{\widetilde{\alpha}}^\chi(\Phi f)_\chi d\chi\,, \quad f \in \ell_2(\widetilde{V})\,.$$

In fact, this is a consequence of the following computation that uses the invariance of the magnetic potential. For any $f \in \ell_2(\widetilde{V}, \widetilde{w})$ and $\chi \in \widehat{\Gamma}$

$$\begin{aligned}
(\Phi\,(d_{\widetilde{\alpha}} f))_{\chi,e} &= \sum_{\gamma\in\Gamma} \overline{\chi(\gamma)}\;(d_{\widetilde{\alpha}} f)_{\gamma e} \\
&= \sum_{\gamma\in\Gamma} \overline{\chi(\gamma)}\left[e^{i\widetilde{\alpha}_{\gamma e}/2} f(\partial^+\gamma e) - e^{-i\widetilde{\alpha}_{\gamma e}/2} f(\partial^-\gamma e)\right] \\
&= \sum_{\gamma\in\Gamma} \overline{\chi(\gamma)}\left[e^{i\widetilde{\alpha}_{e}/2} f(\gamma\partial^+ e) - e^{-i\widetilde{\alpha}_{e}/2} f(\gamma\partial^- e)\right] \\
&= \left(d^{\chi}_{\widetilde{\alpha}}\,(\Phi f)_{\chi}\right)_e .
\end{aligned}$$

This shows that

$$\Delta^{\widetilde{G}}_{\widetilde{\alpha}} = \int_{\widehat{\Gamma}}^{\oplus} \Delta^{\widetilde{G}}_{\widetilde{\alpha}}(\chi)\, d\chi$$

hence, $\sigma\left(\Delta^{\widetilde{G}}_{\widetilde{\alpha}}\right) = \bigcup_{\chi\in\widehat{\Gamma}} \sigma\left(\Delta^{\widetilde{G}}_{\widetilde{\alpha}}(\chi)\right)$. □

3.4 Vector Potential as a Floquet Parameter

The following result shows that in the case of Abelian groups Γ, we can interpret the magnetic potential α on the quotient graph partially as a Floquet parameter for the covering graph $\pi\colon \widetilde{\mathbf{G}} \to \mathbf{G}$ (see part (b) in Remark 3.2.6). Moreover, recalling the definition of coordinate giving in part (a) of Remark 3.2.6) we can define the following unitary maps (see also [KOS89] for a similar definition in the context of manifolds):

$$\begin{aligned}
U^V&\colon \ell_2(V,w) \to \ell_2^{\chi}(\widetilde{V},\widetilde{w}), &\qquad (U^V f)(v) &:= \chi(\xi(v)) f([v]),\\
U^E&\colon \ell_2(E,w) \to \ell_2^{\chi}(\widetilde{E},\widetilde{w}), &\qquad (U^E \eta)_e &:= \chi(\xi(e))\,(\eta)_{[e]}\,.
\end{aligned}$$

It is straightforward to check that U^V and U^E are well defined and unitary.

Definition 3.4.1. Let $\widetilde{\mathbf{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ a Γ-periodic magnetic graph with fundamental domain D. We denote by α a magnetic potential acting on the quotient $G = G/\Gamma$. We say that α has the ***lifting property*** if there exists $\chi \in \widehat{\Gamma}$ such that:

$$\mathrm{e}^{i\alpha_{[e]}} = \chi\,(\mathrm{ind}_D(e))\,\mathrm{e}^{i\widetilde{\alpha}_e} \quad \text{for all } e \in E(\widetilde{G}). \tag{3.4.1}$$

We denote the set of all the magnetic potentials with the lifting property as $\mathcal{A}_D$.

We conclude with the most important theorem of the chapter. This result is going to be fundamental in the following chapters.

Theorem 3.4.2. *Consider a Γ-periodic magnetic weighted graph $\widetilde{\mathbf{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ with D a fundamental domain. If $\mathbf{G} = (G, \alpha, w)$ where $\pi\colon \widetilde{G} \to G = \widetilde{G}/\Gamma$ and $w = \widetilde{w} \circ \pi^{-1}$, then*

$$\sigma(\Delta^{\widetilde{G}}_{\widetilde{\alpha}}) = \bigcup_{\alpha\in\mathcal{A}_D} \sigma(\Delta^{G}_{\alpha}). \tag{3.4.2}$$

Proof. By Proposition 3.3.1, it is enough to show

$$\bigcup_{\chi\in\widehat{\Gamma}} \sigma\left(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}\right) = \bigcup_{\alpha\in\mathcal{A}_D} \sigma\left(\Delta_{\alpha}^{G}\right)$$

To show the inclusion "$\subset$" consider a character $\chi\in\widehat{\Gamma}$ and define a magnetic potential on $\boldsymbol{G}$ as follows

$$\mathrm{e}^{i\alpha_{[e]}} := \chi\left(\mathrm{ind}_D(e)\right) e^{i\widetilde{\alpha}_e}, \qquad \text{for all } e\in E(\widetilde{G}). \tag{3.4.3}$$

Then we have

$$\begin{aligned}\left(d_{\widetilde{\alpha}}^{\chi}(U^V f)\right)_e =& \mathrm{e}^{i\widetilde{\alpha}_e/2}(U^V f)(\partial^+ e) - e^{-i\widetilde{\alpha}_e/2}(U^V f)(\partial^- e)\\ =& \mathrm{e}^{i\widetilde{\alpha}_e/2}\chi(\xi(\partial^+ e)) f([\partial^+ e]) - e^{-i\widetilde{\alpha}_e/2}\chi(\xi(\partial^- e)) f([\partial^- e]).\end{aligned}$$

On the other hand, we have

$$(U^E d_\alpha f)_e = \chi(\xi(e))\left(\mathrm{e}^{\mathrm{i}\alpha_{[e]}/2} f([\partial^+ e]) - \mathrm{e}^{-\mathrm{i}\alpha_{[e]}/2} f([\partial^- e])\right).$$

Therefore, the intertwining equation $d_{\widetilde{\alpha}}^{\chi} U = U^E d_\alpha$ holds if

$$e^{i\widetilde{\alpha}_e/2}\chi(\xi(\partial^+ e)) = \chi(\xi(e))\mathrm{e}^{\mathrm{i}\alpha_{[e]}/2} \quad \text{and} \quad e^{-i\widetilde{\alpha}_e/2}\chi(\xi(\partial^- e)) = \chi(\xi(e))\mathrm{e}^{-\mathrm{i}\alpha_{[e]}/2}$$

or, equivalently, if

$$\mathrm{e}^{\mathrm{i}\alpha_{[e]}} = \chi(\xi(\partial^+ e))\chi(\xi(\partial^- e))^{-1} e^{i\widetilde{\alpha}_{[e]}} = \chi(\mathrm{ind}_D(e))\, e^{i\widetilde{\alpha}_{[e]}}\ .$$

However, this equation is true by definition of the magnetic potential on $\boldsymbol{G}$ given in Equation (3.4.3). Finally, since $\Delta_{\widetilde{\alpha}}^{\widetilde{G}}(\chi) = (d_{\widetilde{\alpha}}^{\chi})^* d_{\widetilde{\alpha}}^{\chi}$ and $\Delta_\alpha^G = d_\alpha^* d_\alpha$, then it is clear that these Laplacians are unitary equivalent.

To show the reverse inclusion "$\supset$" let $\alpha\in\mathcal{A}_D$ and $D^E\subset E(\widetilde{G})$ is such that $\{\mathrm{ind}_D(e) \mid [e]\in D^E\}$ is a basis of the group Γ. Then define

$$\chi(\mathrm{ind}_D(e)) := \mathrm{e}^{\mathrm{i}\alpha_{[e]}} e^{-i\widetilde{\alpha}_{[e]}}\ , \quad e\in D^E \tag{3.4.4}$$

and we can extend χ to all Γ multiplicatively, so that $\chi\in\widehat{\Gamma}$. As before, we can show then $\sigma\left(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}(\chi)\right) = \sigma\left(\Delta_\alpha^G\right)$ and the proof is concluded. □

We conclude the present section, mentioning an important conjecture that will be partially solved in the next chapter. We have seen that periodic graphs can also be understood as covering graphs (see, e.g., [Sun08; Sun13]) and the existence of spectral gaps is related with the *full spectrum conjecture* (*FSP*) stating that the discrete Laplacian on a maximal Abelian covering $\pi\colon \widetilde{\boldsymbol{G}}\to\boldsymbol{G}=\widetilde{\boldsymbol{G}}/\Gamma$ has maximal possible spectrum. A covering is *maximal Abelian* if the covering group is $\Gamma=\mathbb{Z}^b$ with $b=b(G)=|V(G)|-|E(G)|+1$, the first Betti number of G (see [Sun13, Chapter 6] for details; as usual, $V(G)$ and $E(G)$ denote the set of vertices and edges of G, respectively). The conjecture states that the (standard) Laplacian on a maximal Abelian covering has maximal possible spectrum $[0,2]$, i.e., it has no spectral gaps (see [HS99, Conjecture 3.5]) — at least when there is no vertex of degree *one*. This conjecture was partially solved by [HS99, Proposition 3.6 and 3.8] for graphs where all vertices have *even* degree, and certain regular graphs with odd degree. Such graphs allow so-called *Euler paths*, related to the famous Königsberg bridges problem due to Euler. Besides, Higuchi and Shirai [HS04b] realise that one needs additional conditions for the conjecture to be true; namely that there is no vertex of degree *one*. We prove this conjecture for periodic trees in Corollary 4.1.6 (i.e., when the quotient graph has Betti number *one*). Moreover, Higuchi and Nomura [HN09] show that the normalised Laplacian on a maximal Abelian covering graph of a finite even-regular graph respectively odd-regular and bipartite graph has an absolutely continuous spectrum and no eigenvalues.

4 Application I: Spectral gaps

We this chapter, we apply the spectral ordering studied in Chapter 2 to localise the spectrum of the magnetic Laplacian on certain bracketing intervals. With this technique, we can prove the existence of spectral gaps for Laplacians in periodic graphs.

In Section 4.1, we introduce the notion of *spectral gap* and *magnetic spectral gap* (for finite and infinite graphs), and we give a sufficient geometrical condition on the weighted graph such that the set of magnetic spectral gaps is non-empty (see Theorem 4.1.3). As a consequence of this result, we give several characterisations of non empty magnetic spectral gaps for finite weighted graphs with Betti number 1 (cf., Corollary 4.1.6) and using the magnetic potential as a Floquet parameter (Theorem 3.4.2) we will show the existence of spectral gaps in periodic graphs. We also present here several examples of finite graphs with non-empty magnetic spectral gaps and show spectral localisation of the spectrum of the DMLs in the bracketing intervals.

An essential result of this chapter is the partial solution that we give for the Higuchi-Shirai's conjecture in [HS04b] or know as the *full spectrum conjecture*, more precisely the Theorem 4.1.10 solve the conjecture for $\mathbb{Z}$-periodic trees.

In solid-state physics, the Laplacian is the operator modelling the dynamics of particles, and then the spectral gap represents forbidden energy regions (see, e.g., [Kuc01; KK02]). Spectral gaps may be produced by geometry (cf., [LP07; LP08b; Pos03]), by decoration (see, e.g., [SA00; KS15; LP08a; Suz13] and [Kuc05, Section 4] or in nanoribbons with temperature [Han+07].

In this chapter, we generalise the geometric condition obtained in [FLP18, Theorem 4.4], for $\widetilde{\alpha} \sim 0$ to non-trivial periodic magnetic potentials. In particular, if $\widetilde{\boldsymbol{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ is a Γ-periodic magnetic weighted graph, we will give in Theorem 4.1.3 a simple geometric condition on the quotient graph $\widetilde{\boldsymbol{G}} = \boldsymbol{G}/\Gamma$ that guarantees the existence of non-trivial spectral gaps on the spectrum of the discrete magnetic Laplacian $\Delta_{\widetilde{\alpha}}^{\widetilde{G}}$. To show the existence of spectral gaps, we use the purely discrete spectral localisation technique based on the virtualisation of edge and vertices on quotient $\boldsymbol{G}$ developed in Chapter 2. These operations produce new graphs with, in general, different weights that allow localising the eigenvalues of the original Laplacian inside certain intervals. We call this procedure discrete bracketing, and we refer to [FL19] for additional motivation.

4.1 Spectral gaps

We begin by making several precise notions of spectral gaps. Denote by $\sigma(T)$ and $\rho(T) = \mathbb{C} \setminus \sigma(T)$ the spectra and the resolvent set of a self-adjoint operator T, respectively. Recall that $\sigma(\Delta_\alpha^G) \subset [0, 2\rho_\infty]$, where ρ_∞ denotes the supremum of the relative weight, see Equation (1.2.3). We have the following natural question: when do we have $J \subsetneq [0, 2\rho_\infty]$? This question motivates the following definition.

Definition 4.1.1. Let $\boldsymbol{G} = (G, \alpha, w)$ a magnetic weighted graph.

(i) The *spectral gap* set of the DML acting on $\boldsymbol{G}$ is defined by

$$\mathcal{S}_\alpha^G := [0, 2\rho_\infty] \setminus \sigma(\Delta^{\boldsymbol{G}}) = [0, 2\rho_\infty] \cap \rho(\Delta^{\boldsymbol{G}}).$$

If $\alpha \sim 0$, we write $\mathcal{S}^G$ instead of $\mathcal{S}_0^G$.

(ii) Let $\mathcal{A}$ be a set of magnetic potentials acting on G, i.e.,

$$\mathcal{A} \subset \{\, \alpha \colon E \to R \,|\, \alpha_e = -\alpha_{\bar{e}} \quad \text{for all} \quad e \in E(G)\,\}\,,$$

the *magnetic spectral gaps set* (with respect to the family $\mathcal{A}$) of $\boldsymbol{G}$ is defined by

$$\mathcal{MS}_\mathcal{A}^{\boldsymbol{G}} = [0, 2\rho_\infty] \setminus \bigcup_{\alpha \in \mathcal{A}} \sigma(\Delta_\alpha^G) = \bigcap_{\alpha \in \mathcal{A}} \rho(\Delta_\alpha^G) \cap [0, 2\rho_\infty].$$

If $\mathcal{A}$ is the set of all the magnetic potentials acting on G, i.e., if $\mathcal{A} = C^1(G, R)$ as in Eq. (1.3), we write just simply $\mathcal{MS}^{\boldsymbol{G}}$ and know as the *magnetic spectral gaps set*.

We have the following elementary properties:

- If $\mathcal{A}_1 \subset \mathcal{A}_2$, then $\mathcal{MS}_{\mathcal{A}_2}^{\boldsymbol{G}} \subset \mathcal{MS}_{\mathcal{A}_1}^{\boldsymbol{G}}$ and in particular if $\mathcal{A}_2 = C^1(G, R)$ hence $\mathcal{MS}^{\boldsymbol{G}} \subset \mathcal{MS}_{\mathcal{A}_1}^{\boldsymbol{G}}$.
- If $\mathcal{A}$ contains the trivial magnetic potential, then $\mathcal{MS}_\mathcal{A}^{\boldsymbol{G}} \subset \mathcal{S}^G$. In particular, if $\mathcal{S}^G = \varnothing$, then $\mathcal{MS}_\mathcal{A}^{\boldsymbol{G}} = \varnothing$. Moreover, if $\mathcal{MS}_\mathcal{A}^{\boldsymbol{G}} \neq \varnothing$, then $\mathcal{S}^G \neq \varnothing$.
- If G is a tree, then $\mathcal{MS}_\mathcal{A}^G = \mathcal{S}^G$ for any family $\mathcal{A}$ of magnetic potentials (because any magnetic potential on G acts trivially), as all DMLs are unitarily equivalent with Δ^G (the usual Laplacian).

4.1.1 Magnetic spectral gaps on finite graphs

We are now able to prove the following sufficient condition for the existence of magnetic spectral gaps for a family of magnetic potentials $\mathcal{A}$ (i.e., for $\mathcal{MS}_\mathcal{A}^{\boldsymbol{G}} \neq \varnothing$). We will use this result (in the case of standard weights) in the examples presented in Section 4.2. Recall that we allow loops and multiples edges in the graph G. We define an important family of magnetic potential.

Definition 4.1.2. Let $\mathbf{G} = (G, \alpha, w)$ be a magnetic weighted graph and let $E_0 \subset E(G)$ a subset of edges that contain both orientations for each edge, i.e., $e \in E_0$ implies that $\bar{e} \in E_0$.

(i) We say that a vertices subset $V_0 \subset V(G)$ is in the *neighbourhood* of E_0 if $E_0 \subset \bigcup_{v \in V_0} E_v$, i.e., if $\partial^+ e \in V_0$ or $\partial^- e \in V_0$ for all $e \in E_0$. If $V_0 = \{v_0\}$, the vertex v_0 is called *center vertex*.

(ii) Let $\mathcal{A}$ be a family of magnetic potentials acting on G is said to be *centralised* on E_0, if the following holds: for all $\alpha' \in \mathcal{A}$ we have that $\alpha'_e = \alpha_e$ for all $e \in E(G) \setminus E_0$.

The next theorem gives us a simple geometric condition on an *MW*-graph $\mathbf{G}$ for the existence of magnetic spectral gaps for a set of magnetic potentials $\mathcal{A}$.

Theorem 4.1.3. *Let $\mathbf{G} = (G, \alpha, w)$ be a magnetic weighted finite graph and let $E_0 \subset E_{v_0}$ (without loops) for some $v_0 \in V(G)$. Let $\mathcal{A}$ be any set of magnetic potentials acting on G centralised on E_0. If we define $\mathbf{G}^-$ as the magnetic weighted graph getting from virtualisation of the set of edges E_0,*

$$\delta := \rho^{\mathbf{G}}(v_0) - \frac{w(E_0 \cap E_v^-)}{w(v_0)} - \sum_{e \in E_0 \cap E_{v_0}^-} \frac{w_e}{w(\partial^+ e)} - \lambda_1(\Delta^{\mathbf{G}^-}) > 0\,, \tag{4.1.1}$$

then $\mathcal{MS}_{\mathcal{A}}^{\mathbf{G}} \neq \varnothing$.

Proof. Consider the following edges and vertex virtualised weighted graphs:

$$\mathbf{G}^- := \mathbf{G} - E_0 \qquad \text{and} \qquad \mathbf{G}^+ := \mathbf{G} - \{v_0\}\,,$$

where $\mathbf{G}^-$ and $\mathbf{G}^+$ are graphs as in Definition 1.1.4 and Definition 2.4.13, then by Corollary 2.4.16 follows that

$$\mathbf{G}^- \preccurlyeq \mathbf{G} \preccurlyeq \mathbf{G}^+\,,$$

then, if $n = |V(G)|$ we obtain

$$\sigma(\Delta_\alpha^G) \subset \bigcup_{k=1}^{n} \underbrace{[\lambda_k(\Delta_{\alpha^-}^{G^-}), \lambda_k(\Delta_{\alpha^+}^{G^+})]}_{=:J_k} \subset [0, 2\rho_\infty].$$

with the convention that $\lambda_n(\Delta_{\alpha^+}^{G^+}) = 2\rho_\infty$. But, for any $\alpha_1 \in \mathcal{A}$ follows that $\alpha_1^- = \alpha^-$ and $\alpha_1^+ = \alpha^+$ (because $\mathcal{A}$ is centralised in E_0), hence

$$\bigcup_{\alpha \in \mathcal{A}} \sigma(\Delta_\alpha^G) \subset \bigcup_{k=1}^{n} \underbrace{[\lambda_k(\Delta_{\alpha^-}^{G^-}), \lambda_k(\Delta_{\alpha^+}^{G^+})]}_{=:J_k} \subset [0, 2\rho_\infty].$$

To prove that $\mathcal{MS}_{\mathcal{A}}^{\mathbf{G}} \neq \varnothing$, it is enough to show that the measure of $[0, 2\rho_\infty] \setminus J$ is positive. Furthermore, J it can be estimated from below by:

$$\begin{aligned} \sum_{k=1}^{n-1} \Big(\lambda_{k+1}\big(\Delta_{\alpha^-}^{G^-}\big) - \lambda_k\big(\Delta_{\alpha^+}^{G^+}\big)\Big) &= \sum_{k=2}^{n} \lambda_k\big(\Delta_{\alpha^-}^{G^-}\big) - \sum_{k=1}^{n-1} \lambda_k\big(\Delta_{\alpha^+}^{G^+}\big) \\ &= Tr\big(\Delta_{\alpha^-}^{G^-}\big) - Tr\big(\Delta_{\alpha^+}^{G^+}\big) - \lambda_1\big(\Delta_{\alpha^-}^{G^-}\big). \end{aligned} \tag{4.1.2}$$

Therefore it is enough to calculate $Tr(\Delta_{\alpha^+}^{G^+})$ and $Tr(\Delta_{\alpha^-}^{G^-})$

Step 1: Trace of $\Delta_{\alpha^-}^{G^-}$. We define $\mathbf{G}^- = (G^-, \alpha^-, w^-)$ where $G^- = G - E_0$. Recall that $V(G^-) = V(G)$, $E(G^-) = E(G) \setminus E_0$; the weights on $V(G^-)$ and $E(G^-)$ coincide with the corresponding weights on $\boldsymbol{G}$. The relative weights of $\mathbf{G}^-$ are

$$\rho^{\boldsymbol{G}^-}(v) = \begin{cases} \rho^{\boldsymbol{G}}(v) - \dfrac{w\,(E_0 \cap E_v^-)}{w(v)}, & \text{if } v = v_0, \\ \rho^{\boldsymbol{G}}(v) - \dfrac{w\,(E_0 \cap E_v^-)}{w(v)}, & \text{if } v \in B_{v_0}, \\ \rho^{\boldsymbol{G}}(v), & \text{otherwise}, \end{cases}$$

where

$$B_{v_0} = \{v \in V(G) \mid v = \partial^+ e \text{ for some } e \in E_0 \text{ with } v \neq v_0\}.$$

The trace of $\Delta_{\alpha^-}^{G^-}$ is now

$$\begin{aligned} \operatorname{Tr}\bigl(\Delta_{\alpha^-}^{G^-}\bigr) &= \sum_{k=1}^{n} \lambda_k\bigl(\Delta_{\alpha^-}^{G^-}\bigr) = \sum_{v \in V(G)} \rho^{\boldsymbol{G}^-}(v) \\ &= \sum_{v \in V(G)} \rho^{\boldsymbol{G}}(v) - \frac{w\,(E_0 \cap E_v^-)}{w(v)} - \sum_{v \in B_{v_0}} \frac{w\,(E_0 \cap E_v^-)}{w(v)}. \end{aligned} \tag{4.1.3}$$

Step 2: Trace of $\Delta_{\alpha^+}^{G^+}$. Let $\boldsymbol{G}^+ = (G^+, \alpha^+, w^+)$, then the trace of $\Delta_{\alpha^+}^{G^+}$ is given by

$$\operatorname{Tr}\bigl(\Delta_{\alpha^+}^{G^+}\bigr) = \sum_{k=1}^{n-1} \lambda_k\bigl(\Delta_{\alpha^+}^{G}\bigr) = \sum_{\substack{v \in V(G) \\ v \neq v_0}} \rho^{\boldsymbol{G}}(v). \tag{4.1.4}$$

Combining Equations (4.1.2)–(4.1.4) we obtain

$$\begin{aligned} \operatorname{Tr}\bigl(\Delta_{\alpha^-}^{G^-}\bigr) - \operatorname{Tr}\bigl(\Delta_{\alpha^+}^{G^+}\bigr) - \lambda_1\bigl(\Delta_{\alpha^-}^{G^-}\bigr) &= \rho^{\boldsymbol{G}}(v_0) - \frac{w(E_0 \cap E_v^-)}{w(v_0)} - \sum_{v \in B_{v_0}} \frac{w(E_0 \cap E_v^-)}{w(v)} - \lambda_1\bigl(\Delta_{\alpha^-}^{G^-}\bigr) \\ &= \rho^{\boldsymbol{G}}(v_0) - \frac{w(E_0 \cap E_v^-)}{w(v_0)} - \sum_{e \in E_0 \cap E_{v_0}^-} \frac{w_e}{w(\partial^+ e)} - \lambda_1(\Delta^{\boldsymbol{G}^-}) = \delta \end{aligned}$$

as defined in Equation (4.1.11). This shows that if $\delta > 0$, then the spectrum of the DML is not the full interval. □

Remark 4.1.4.

(i) In the proof, we used the spectral localising inclusion 2.2.3. If the graph is bipartite and with normalized weights (or more generally if the relative weight is constant), and if we find $B \subset \mathcal{MS}_{\mathcal{A}}^{\boldsymbol{G}}$, then we have also $\kappa(B) \subset \mathcal{MS}_{\mathcal{A}}^{\boldsymbol{G}}$ by Proposition 1.6.3.

(ii) For applications, in particular, for the examples of Section 4.2, we explicitly write Condition 4.1.11 for the most important weights (see Section 1.2.1).

(a) If the graph has the *standard weights*, the condition becomes:

$$\delta = 1 - \sum_{e \in E_0 \cap E_{v_0}^-} \frac{1}{\deg(\partial^+ e)} - \frac{|E_0 \cap E_{v_0}^-|}{\deg(v_0)} - \lambda_1(\Delta_{\alpha^-}^{G^-}) \,, \tag{4.1.5}$$

where $|E_0 \cap E_{v_0}^-|$ denote the cardinality of the set $E_0 \cap E_{v_0}^-$.

(b) If we have the *combinatorial weights*, the condition becomes simply:

$$\delta = \deg(v_0) - \ |E_0| - \lambda_1(\Delta_{\alpha^-}^{G^-}) \,. \tag{4.1.6}$$

(c) For the *electric circuit weights*, the condition is:

$$\delta = w(E_{v_0}) - \ w(E_0) - \lambda_1(\Delta_{\alpha^-}^{G^-}) \,. \tag{4.1.7}$$

(d) For the *normalized weights*, the condition is:

$$\delta = 1 - \sum_{e \in E_0 \cap E_{v_0}^-} \frac{w_e}{w(E_{\partial^+ e})} - \frac{w(E_0 \cap E_{v_0}^-)}{w(E_{\partial^+ e})} \,. \tag{4.1.8}$$

In all of the previous cases, if $\boldsymbol{G}$ is a graph with the corresponding weights and meets the condition $\delta > 0$, then we can assure the existence of magnetic spectral gaps, i.e., $\mathcal{MS}_{\mathcal{A}}^{\boldsymbol{G}} \neq \varnothing$.

(iii) In all the previous cases, if the graph G^- is a tree or/and $\alpha^- \sim 0$, then $\lambda_1(\Delta_{\alpha^-}^{G^-}) = 0$.

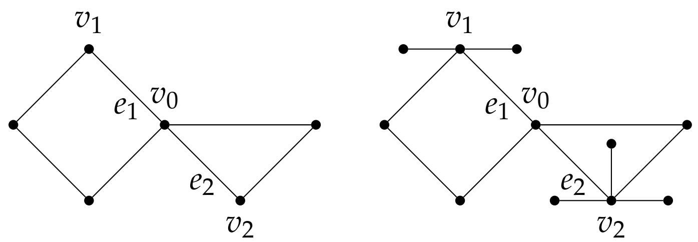
Example 4.1.5. Consider the next two graphs in Figure 4.1, both with the standard weights, and we want to know if the graphs have magnetic spectral gaps (for all magnetic potential), i.e., $\mathcal{MS}^{\boldsymbol{G}}$ is empty or not. In the first case of Figure 4.1A, we have no magnetic spectral gaps, i.e., $\mathcal{MS}^{G_1} = \varnothing$. The strategy to produce gaps is to raise the degree of the vertices v_1 and v_2. Let α be a magnetic potential acting on the graphs, without loss of generality, we can suppose that α is supported in $E_0 = \{e_1, e_2\}$ (and in its inverse edges). In both graphs, consider v_0 is a centre vertex, define the family

$$\mathcal{A}' = \{\, \alpha' \colon E(G_2) \to R \,|\, \alpha'_e = -\alpha'_{\bar{e}} \text{ for all } e \in E(G) \text{ with } \alpha'_e = \alpha_e \text{ for all } e \in E(G) \setminus E_0 \,\} \,,$$

then, $\mathcal{A}'$ is centralised in the set of edges E_0. Because for any magnetic potential α_1 acting on the graph G_2, we can find $\alpha_2 \in \mathcal{A}'$ such that $\alpha_1 \sim \alpha_2$, then $\mathcal{MS}^{G_2} = \mathcal{MS}_{\mathcal{A}'}^{G_2}$, but for the second graph 4.1B we have

$$\delta = 1 - \frac{1}{\deg(v_1)} - \frac{1}{\deg(v_2)} - \frac{2}{\deg(v_0)} = 1 - \frac{1}{4} - \frac{1}{5} - \frac{2}{4} = \frac{1}{20} > 0,$$

then $\mathcal{MS}^{G_2} = \mathcal{MS}_{\mathcal{A}'}^{G_2} \neq \varnothing$ as a consequence of Theorem 4.1.3. This example also shows that Condition (4.1.11) is sufficient but not necessary: consider the graph G_2 with only one decorating edge at each vertex v_1 and v_2. The corresponding graph still has a spectral gap, although $\delta = 1 - 1/3 - 1/3 - 2/4 = -1/6 < 0$.



(A) The graph G_1. (B) The graph G_2.

FIGURE 4.1: Producing magnetic spectral gaps by decoration. The graph G_2 is obtained from G_1 by adding pendant edges.

As a consequence, we have the following topological characterisation for the existence of magnetic spectral gaps for finite graphs with Betti number 1:

Corollary 4.1.6. *Let* $\mathbf{G} = (G, w)$ *be an weighted graph with the standard or the combinatorial weights (i.e.,* $w = \deg$ *or* $w = \mathbb{1}$*) and Betti number* $b(G) = 1$*. Then the following conditions are equivalent:*

(i) $\mathbf{G}$ *has a magnetic spectral gap (i.e.,* $\mathcal{MS}^G_{\mathcal{A}} \neq \emptyset$*) for any set* $\mathcal{A}$ *of magnetic potential.*
(ii) G *is not a cycle graph;*
(iii) G *has a vertex of degree* 1.

Proof. "(i)⇒(ii)": Suppose that $G = C_n$. Let now $\lambda \in [0, 2]$ and $t \in [0, 2\pi]$ be such that $\cos t = 1 - \lambda$. Consider a sequence of (directed) edges such that $c = (e_1, e_2, \ldots, e_n)$ is a (directed) cycle and define the magnetic potential α given by $\alpha_e = t$ for all $e \in c$, then $\alpha_{\bar{e}} = -t$. We will show that $\lambda \in \sigma(\Delta^G_\alpha)$. In fact, consider the constant function on the vertices equal to one, i.e., $\mathbf{1}(v) = 1$ for all $v \in V(G)$, then

$$(\Delta^G_\alpha \mathbf{1})(v) = 1 - \frac{\mathrm{e}^{-it} + \mathrm{e}^{it}}{2} = 1 - \cos t = \lambda \cdot \mathbf{1}(v).$$

We have shown that $[0, 2] \subset \bigcup_{\alpha \in \mathcal{A}} \sigma(\Delta^G_\alpha)$, i.e., $\mathcal{MS}^G_{\mathcal{A}} = \emptyset$.

"(ii)⇒(iii)": Using the fact that $b(G) = 1$, one can prove this by induction on the number of vertices.

"(iii)⇒(i)": Since G has Betti number $b(G) = 1$ and since G has a vertex of degree 1, there exists $v_0 \in V(G)$ such that v_0 belongs to the cycle with $\deg v_0 \geq 3$, and it is adjacent with $v_1 \in V(G)$ by an edge $e_1 \in E(G)$ with $\deg v_1 \geq 2$. Consider the family $\mathcal{A}$ the set of all vector potentials supported on the edge (and in its inverse) e_0, i.e.

$$\mathcal{A} \subset \{\, \alpha : E(G) \to R \,|\, \alpha(e) = -\alpha(\bar{e}) \quad \text{and} \quad \alpha(e) = 0 \quad \text{for} \quad e \neq e_0 \,\},$$

hence $\mathcal{A}$ is centralised on e_0. Then if $E_0 = \{e_0, \overline{e_0}\}$,

$$1 - \sum_{e \in E_0 \cap E^-_{v_0}} \frac{1}{\deg(\partial^+ e)} - \frac{|E_0 \cap E^-_{v_0}|}{\deg(v_0)} = 1 - \frac{1}{\deg_G v_1} - \frac{1}{\deg_G v_0} \geq 1 - \frac{1}{2} - \frac{1}{3} = \frac{1}{6} > 0,$$

we conclude by Theorem 4.1.3 that $\mathcal{MS}_{\mathcal{A}}^{G} \neq \emptyset$ and hence (i).

□

Remark 4.1.7.

(i) Corollary 4.1.6 also holds for combinatorial weights: for "(i)⇒(ii)" note that C_n is a regular graph, hence a simple scaling just relates the spectrum of the standard weight and the combinatorial weight. For "(iii)⇒(i)" note that the condition on the weights becomes $2 = |E_0| < 3 \leq \deg v_0$ (choose v_0 to be the vertex of degree larger than 2). Finally "(ii)⇒(iii)" is independent of the weights.

(ii) If the graph G has the electric circuit weights, then "(i)⇒(iii)" is no longer true. In fact choose $G = C_6$ as in Figure 2.4 with $w_e = 1$ if $e \neq e_1$ and $w_{e_1} = 2$. For example, an easy calculation shows that 0 and $1 \in \sigma(\Delta^{\mathbf{G}})$ but $0.3 \in \mathcal{MS}^{\mathbf{G}}$, then $\mathcal{MS}^{\mathbf{G}} \neq \emptyset$ even if there is no vertex of degree 1.

(iii) If the graph G has normalized weights, then in general "(i)⇒(iii)" is not true. Choose $G = C_6$ as in Figure 2.4 with the following weights: on the edges $w_e = 1$ if $e \neq e_1$ and $w_{e_1} = 2$, on the vertices $w(v_i) = 2$ for $i = 1,2$ and $w(v_i) = 1$ for $i = 3,4,5,6$. It is easy to check that 0 and $1 \in \sigma(\Delta^{\mathbf{G}})$ with $1/2 \in \mathcal{MS}^{\mathbf{G}}$. Then $\mathcal{MS}^{\mathbf{G}} \neq \emptyset$ but again, there is no vertex of degree 1.

The next example shows how decoration creates magnetic spectral gaps.

Example 4.1.8. Let $\mathbf{G}' = (G', w')$ a weighted graph, where $G' = C_6$ and w' are the standard weights, then by Corollary 4.1.6 we have $\mathcal{MS}^{\mathbf{G}'} = \emptyset$. To create magnetic spectral gaps, we add a new edge. Let now $\mathbf{G} = (G, w)$ be a weighted graph, where G is the graph C_6 with an edge added to the cycle (see Figure 4.2) and w the standard weights. Then the Laplacian on G has a magnetic spectral gap by Corollary 4.1.6. Now, using the bracketing technique of Corollary 2.4.16, we can localise the position of the gaps.

Consider $E_0 = \{e_1, \overline{e_1}\}$, and recall that any vector potential α can be supported on e_1. Consider also the edge virtualised weighted graph $\mathbf{G}^- = (G^-, w^-)$ with $G^- = G - E_0$. Then its spectrum is:

$$\sigma\left(\Delta^{G^-}\right) \approx \{0, 0.116, 0.5, 0.713, 1.145, 1.638, 1.889\}.$$

Now, we have that $V_0 = \{v_1\}$ is a central vertex for E_0. Now consider the vertex virtualised weighted graph $\mathbf{G}^+ = (G^+, w^+)$ with $G^+ = G - V_0$, then its spectrum is:

$$\sigma\left(\Delta^{G^+}\right) \approx \{0.121, 0.358, 0.744, 1.256, 1.642, 1.879, 2\}.$$

Therefore, the bracketing intervals in which we can localise the spectrum is given by (see Figure 4.2):

$$J_1 \approx [0, 0.121], \quad J_2 \approx [0.116, 0.358], \quad J_3 \approx [0.5, 0.744], \quad J_4 \approx [0.713, 1.256],$$
$$J_5 \approx [1.145, 1.642], \quad J_6 \approx [1.638, 1.879], \quad \textit{and} \quad J_7 \approx [1.889, 2].$$

In conclusion, we have the following spectral localising inclusion for any vector potential α, i.e. if $\mathcal{A} = C(G, R)$, then

$$\bigcup_{\alpha \in \mathcal{A}} \sigma(\Delta_\alpha^G) \subset J = \bigcup_{k=1}^{7} J_i \subsetneq [0, 2]. \tag{4.1.9}$$

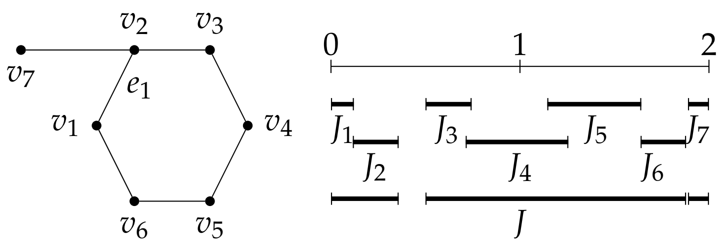


FIGURE 4.2: Examples of bracketing intervals for the cycle graph C_6 with one pendant edge.

4.1.2 Spectral gaps in Γ-periodic graphs

Consider a Γ-periodic weighted graph $\widetilde{\boldsymbol{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ with D a fundamental domain. If $\boldsymbol{G} = (G, \alpha, w)$ where $\boldsymbol{G} = \widetilde{\boldsymbol{G}}/\Gamma$, then to the Eq. 3.4.2, we can add the definition of magnetic spectral gap from Definition 4.1.1 as follow:

$$\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{\boldsymbol{G}}}) = \bigcup_{\alpha \in \mathcal{A}_D} \sigma(\Delta_\alpha^{\boldsymbol{G}}) \subset [0, 2p_\infty] \setminus \mathcal{MS}_{\mathcal{A}_D}^{\boldsymbol{G}}. \tag{4.1.10}$$

Remark 4.1.9.

(i) If $\widetilde{G} \to G$ is a maximal Abelian covering, then we have $\sigma(\Delta^{\widetilde{G}}) = [0, 2p_\infty] \setminus \mathcal{MS}^G$. In particular, this is true if $\widetilde{G}$ is a tree.

(ii) If $\Gamma = \mathbb{Z}$ and if each fundamental domain is connected to its neighbours by a single connecting edge (and its inverse), i.e., $|E(D, \widetilde{G})| = 2$. Define the magnetic potential α^t on G as $\alpha_e^t = t$ and $\alpha_{\bar{e}}^t = -t$ if $[e] \in [E(D, \widetilde{G})]$ and zero otherwise. Denote $\sigma\left(\Delta_{\alpha^t}^{\widetilde{G}}\right) := \{\lambda_i^t \mid i = 1, \ldots, n\}$ be the eigenvalues in ascending order and repeated according to their multiplicities, then following results in [EKW10] shows that

$$\sigma(\Delta^{\widetilde{G}}) = \bigcup_{i=1}^{|V(G)|} [\min\{\lambda_i^0, \lambda_i^\pi\}, \max\{\lambda_i^0, \lambda_i^\pi\}].$$

Let $\boldsymbol{G} = (G, 0, w)$ a magnetic weighted graph. We say that $\boldsymbol{G}$ has the *full spectrum property (FSP)* if $\Delta^{\boldsymbol{G}} = [0, 2\rho_\infty]$. In fact, $\boldsymbol{G}$ has *FSP* if and only if $\mathcal{S}^{\boldsymbol{G}} = \varnothing$. The next conjecture is stated in [HS99]. Let $\widetilde{G}$ be a maximal Abelian covering of G, if G has no vertex of degree 1 then $\widetilde{G}$ has *FSP*. Moreover, they propose the next problem: Characterise all finite graphs whose maximal Abelian covering do not has *FSP*. Next, we partially solve the conjecture and the problem.

The following result verifies Higuchi-Shirai's conjecture in [HS04b] for $\mathbb{Z}$-periodic trees.

Theorem 4.1.10. *Let $\widetilde{\mathbf{G}} = (\widetilde{G}, 0, \widetilde{w})$ be a $\mathbb{Z}$-periodic tree with standard or combinatorial weights and quotient graph $\mathbf{G} = (G, 0, w)$. Then the following conditions are equivalent:*

(i) $\widetilde{\mathbf{G}}$ *has the full spectrum property;*
(ii) $\mathcal{S}^{\widetilde{\mathbf{G}}} = \emptyset$;
(iii) $\widetilde{G}$ *is the lattice* $\mathbb{Z}$;
(iv) $\mathcal{MS}^{\mathbf{G}} = \emptyset$;
(v) G *is a cycle graph;*
(vi) G *has no vertex of degree* 1.

Proof. In this situation, $\widetilde{G} \to G$ is a maximal Abelian covering if and only if the Betti number $b(G) = 1$ if and only if $\widetilde{G}$ is a $\mathbb{Z}$-periodic tree. Since $\widetilde{G}$ is a tree and $\widetilde{G} \to G$ is a maximal Abelian covering, then we have $\sigma(\Delta^{\widetilde{\mathbf{G}}}) = [0, 2p_\infty] \setminus \mathcal{MS}^{\mathbf{G}}$. The result then follows by Corollary 4.1.6. □

Remark 4.1.11. In Example 4.2.2 we will confirm the previous theorem. Besides, if $b(G) \geq 2$ one can easily produce periodic graphs based, e.g., with Example 4.1.5 where do not have the full spectrum property.

We apply now the technique stated in Corollary 2.4.16 to Γ-periodic graphs.

Theorem 4.1.12. *Let $\widetilde{\mathbf{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ be a Γ-periodic magnetic weighted graph. Consider a fundamental domain $D = (D^V, D^E)$ and $G = \widetilde{G}/\Gamma$. The functions w and α on G are induced by $\widetilde{w}$ and $\widetilde{\alpha}$ respectively. Let*

$$E_0 := [E(D, \widetilde{G})]$$

be the image of the connectivity edges on the quotient and V_0 in the neighbourhood of E_0. Define by

$$\mathbf{G}^- := \mathbf{G} - E_0 \qquad \text{and} \qquad \mathbf{G}^+ := \mathbf{G} - V_0\,,$$

the corresponding edge and vertex virtualised graphs, respectively. Then

$$\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{\mathbf{G}}}) \subset \bigcup_{k=1}^{|V(\mathbf{G})|} \underbrace{[\lambda_k(\Delta_{\alpha^-}^{\mathbf{G}^-}), \lambda_k(\Delta_{\alpha^+}^{\mathbf{G}^+})]}_{=:J_k}$$

where the eigenvalues of $\sigma(\Delta_{\alpha^-}^{\mathbf{G}^-})$ and $\sigma(\Delta_{\alpha^+}^{\mathbf{G}^+})$ are as in Corollary 2.4.16, i.e., are written in ascending order and repeated according to their multiplicities.

Proof. By Theorem 3.4.2 we have

$$\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{\mathbf{G}}}) = \bigcup_{\beta \in \mathcal{A}_D} \sigma(\Delta_{\beta}^{\mathbf{G}}).$$

Now, by the bracketing technique of Corollary 2.4.16, we have for any potential with the lifting property $\beta \in \mathcal{A}_D$ (cf., Definition 3.4.1):

$$\lambda_k(\Delta^{G^-}_{\alpha^-}) \le \lambda_k(\Delta^{G}_{\beta}) \le \lambda_k(\Delta^{G}_{\alpha^+}) \quad \text{for all} \quad k = 1, \dots, |V(G)|\,.$$

Therefore, by Equation (2.4.3)

$$\sigma(\Delta^{\widetilde{G}}_{\widetilde{\alpha}}) = \bigcup_{\beta \in \mathcal{A}_D} \sigma(\Delta^{G}_{\alpha}) \subset \bigcup_{\beta \in \mathcal{A}_D} \bigcup_{k=1}^{|V(G)|} \left[\lambda_k(\Delta^{G^-}_{\beta^-}), \lambda_k(\Delta^{G^+}_{\beta^+})\right];$$

since β has the lifting property, Equation (3.4.1) implies that there exists $\chi \in \widehat{\Gamma}$ such that:

$$\mathrm{e}^{i\beta_{[e]}} = \chi\left(\mathrm{ind}_D(e)\right) e^{i\widetilde{\alpha}_{[e]}} \qquad \text{for all } e \in E.$$

But for all $e \in E \setminus E_0 = E \setminus [E(D,G)]$ the index is trivial, i.e., $\mathrm{ind}_D(e) = 1_\Gamma$ (see Remark 3.2.6). Thus by Γ-periodicity, we obtain that $\beta_e = \alpha_e$ for oriented edge $e \in E \setminus E_0$. Since α and β are magnetic potentials acting on $\boldsymbol{G}$, and $\boldsymbol{G}^- = \widetilde{\boldsymbol{G}} - E_0$ then $\alpha^- = \beta^-$. Similarly, for $\boldsymbol{G}^+ = \boldsymbol{G} - V_0$ with V_0 in the neighbourhood of E_0, we have that $\alpha^+ = \beta^+$. We obtain finally

$$\sigma(\Delta^{\widetilde{G}}_{\widetilde{\alpha}}) \subset \bigcup_{\beta \in \mathcal{A}_D} \bigcup_{k=1}^{|V(G)|} \underbrace{\left[\lambda_k(\Delta^{G^-}_{\alpha^-}), \lambda_k(\Delta^{G^+}_{\alpha^+})\right]}_{=:J_k}.$$

Note that the last union does not depend on any more of β, and this fact concludes the proof. $\square$

Note that the bracketing intervals J_k depends on the fundamental domain D. A right choice is one where the set of connecting edges is as small as possible, providing high contrast between the interior of the fundamental domain and its boundary. In this case, we have a good chance that the localising intervals J_k do not cover the full interval $[0, 2\rho_\infty]$. This choice is a discrete geometrical version of a "thin–thick" decomposition as described in [LP08a], where a fundamental domain of the metric and discrete graph has only a few connections to its complement.

The next theorem gives a simple geometric condition on a magnetic weighted graph $\boldsymbol{G}$ for the existence of gaps in the spectrum of the *DML* on the Γ-covering graph. We will specify which edges and vertices should be virtualised in $\boldsymbol{G}$ to guarantee the existence of spectral gaps. This result generalises Theorem 4.4 in [FLP18].

Corollary 4.1.13. *Let $\widetilde{\boldsymbol{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ be a Γ-periodic magnetic weighted graph. Denote by $\boldsymbol{G} = (G, \alpha, w)$ the quotient graph, where $G = \widetilde{G}/\Gamma$ with induced magnetic potential α and induced weights w, respectively.*

The spectrum of the DML *has spectral gaps, i.e., $\sigma(\Delta^{\widetilde{G}}_{\widetilde{\alpha}}) \neq [0, 2\rho_\infty]$, if the following condition holds: there exists a vertex $v_0 \in V(G)$ and a fundamental domain D such that the connecting* *edges* $[B(D,\widetilde{G})]$ *contain no loops,* $[B(D,\widetilde{G})] \subset E_{v_0}$ *and*

$$\delta := \rho(v_0) - \sum_{e \in [B(D,\widetilde{G})] \cap E^-_{v_0}} \frac{w_e}{w(\partial^+ e)} - \frac{w([B(D,\widetilde{G})] \cap E^-_{v_0})}{w(v_0)} - \lambda_1(\Delta^{G^-}_{\alpha^-}) > 0\,, \tag{4.1.11}$$

where $\rho(v_0) = w(E^-_{v_0}))/w(v_0)$ *is the relative weight at* v_0 *and* $\boldsymbol{G}^- = (G^-, w^-)$ *with* $G^- = G - [B(D,\widetilde{G})]$.

Proof. By Theorem 4.1.12, we obtain

$$\sigma(\Delta^{\widetilde{\boldsymbol{G}}}_{\widetilde{\alpha}}) \subset \bigcup_{k=1}^{|V(\boldsymbol{G})|} \underbrace{[\lambda_k(\Delta^{\boldsymbol{G}^-}_{\alpha^-}), \lambda_k(\Delta^{\boldsymbol{G}^+}_{\alpha^+})]}_{=:J_k}$$

where

$$\boldsymbol{G}^- := \boldsymbol{G} - E_0 \qquad \text{and} \qquad \boldsymbol{G}^+ := \boldsymbol{G} - V_0.$$

the corresponding edge and vertex virtualised graphs, respectively, with $E_0 := [E(D,\widetilde{G})]$ and $V_0 = \{v_0\}$, then by the same arguments of the condition δ in Theorem 4.1.3 we obtain the result. □

In particular, the next criterion is a necessary condition to find spectral gaps for the magnetic Laplacian on a periodic magnetic graph (with the standard or normalized weights). So, under the same hypothesis of the previous corollary, we have the same remark:

Remark 4.1.14.

(i) If the graph has the standard weights, the condition becomes:

$$\delta = 1 - \sum_{e \in [B(D,\widetilde{G})] \cap E^-_{v_0}} \frac{1}{\deg(\partial^+ e)} - \frac{|[B(D,\widetilde{G})] \cap E^-_{v_0}|}{\deg(v_0)} - \lambda_1(\Delta^{G^-}_{\alpha^-}) > 0\,, \tag{4.1.12}$$

where $|[B(D,\widetilde{G})] \cap E^-_{v_0}|$ denote the cardinality of the set $[B(D,\widetilde{G})] \cap E^-_{v_0}$.

(ii) If we have the combinatorial weights, the condition becomes simply:

$$\delta = \deg(v_0) - |[B(D,\widetilde{G})]| - \lambda_1(\Delta^{G^-}_{\alpha^-}) > 0\,. \tag{4.1.13}$$

4.2 Examples

In this final section, we consider some examples of covering graphs used as models of important chemical compounds, like the polyacetylene and the graphene nanoribbons. The bracketing technique of Theorems 3.4.2 and 4.1.12 are used to localise the spectrum bands and gaps of the infinite covering graphs under the action of a periodic magnetic potential $\widetilde{\alpha}$. In particular, we show the dependence of the spectral gaps on the periodic potential $\widetilde{\alpha}$.

Let $\widetilde{\mathbf{G}}$ be a periodic graph. For simplicity, we consider here planar periodic magnetic potentials $\widetilde{\alpha}$ with the property that the flux through all cycles on $\widetilde{\mathbf{G}}$ is constant and equal to s for some $s \in [0, 2\pi)$. Two magnetic potentials are cohomologous if and only if they induce the same flux through all the cycles on the graph (see Lemma 1.3.2). Then, any periodic $\widetilde{\alpha}$ function on the edges is identified with one unique value in $s \in \mathbb{T}$. We call $\widetilde{\alpha}$ as a *constant magnetic field* with value s. A similar analysis could be done for non-constant magnetic potentials (just taking, for example, a fundamental domain that includes two cycles with different magnetic flux in each of them).

Let $\widetilde{\mathbf{G}} = (\widetilde{G}, \widetilde{w}, \widetilde{\alpha})$ be a periodic weighted graph with $\widetilde{\alpha}$ a constant magnetic field. The graph $\widetilde{G}$ models polyacetylene in Subsection 4.2.4 as well as nanoribbons with different symmetries in Section 4.2.5. In order to study the spectrum $\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}})$, we will use the results in Chapter 3 to obtain bracketing intervals localising the spectrum and showing the existence of spectral gaps. In Subsection 4.2.1, we present some examples without magnetic potential, i.e. $\widetilde{\alpha} \sim 0$ and in Subsection 4.2.2 following the same idea consider the case of $\widetilde{\alpha}$ a constant magnetic potential.

4.2.1 Periodic graph without magnetic field

In this subsection, we include several applications of the methods developed before. Our first example confirms using our simple geometric method the results by Suzuki in [Suz13] on periodic graphs with pendants edges (Example 4.2.1). The other examples are more elaborate and include modelisation of *polypropylene* (Example 4.2.2) and *polyacetylene* molecules (Example 4.2.3). This last example can be understood as an intermediate covering of graphane and shows that the bracketing technique developed here extends to a more general situation than the $\mathbb{Z}$-periodic trees, i.e., to higher Betti numbers of the quotient graphs.

Example 4.2.1. *(Suzuki's example).* Consider the graph T_n consisting of the $\mathbb{Z}$-lattice and a pendant edge at every n-th vertex as decoration (see Figure 4.3) with standard weights as in [Suz13]. It is easy to see that the tree T_n is maximal Abelian covering graph of G_n, where G_n is just the cycle graph C_n decorated with an additional edge attached to some vertex of the cycle (for example, see Figure 4.2 for G_6) with the standard weights. The graph T_n has spectral gaps, i.e., $\mathcal{S}^{T_n} \neq \emptyset$, as Suzuki proves. Our analysis allows an alternative and short proof: namely, by Corollary 4.1.6 we know that $\mathcal{MS}^{G_n} \neq \emptyset$, since T_n is a covering graph of G_n, we conclude by Theorem 4.1.10 that the Laplacian on T_n has spectral gaps, i.e., T_n has not the full spectrum property.

Example 4.2.2. *(Polypropylene).* Consider the graph associated with a thermoplastic polymer, the *propylene* or *polypropylene*. This structure consists of a sequence of carbon atoms (white vertices) with hydrogen (black vertices) and the methyl group CH_3. We denote the periodic weighted graph of the propylene as $\widetilde{\mathbf{G}} = (\widetilde{G}, 0, \deg)$, see Figure 4.4A.

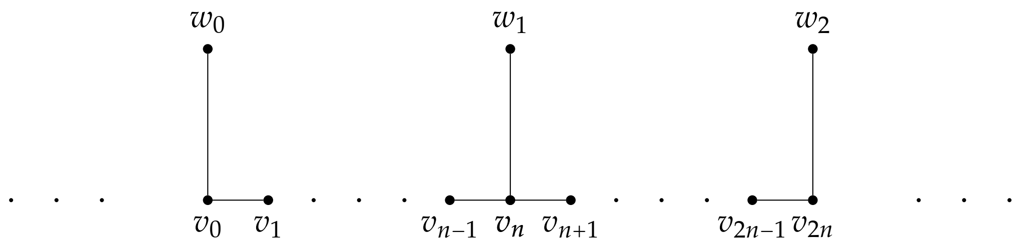


FIGURE 4.3: The graphs in this figure are trees denoted as T_n.

The infinite graph $\widetilde{G}$ is a covering graph of the bipartite graph denoted as G (see Figure 4.4B). Again, by Corollary 4.1.6 we get that the set of magnetic spectral gaps is not empty $\mathcal{MS}^G \neq 0$ and by Theorem 4.1.10 we conclude that the Laplacian on $\widetilde{\boldsymbol{G}}$ has spectral gaps. We show how to apply the technique developed in this dissertation.

First, consider the set of edges $E_0 = \{e_1, \overline{e_1}\}$. Then, we have that $V_0 = \{v_1\}$ is in the neighbourhood of E_0 (see Definition 4.1.2). Using the notation in Corollary 2.4.16 and Theorem 4.1.10 we get that $\sigma(\Delta^{\widetilde{\boldsymbol{G}}}) \subset J$, where J is a subset of $[0,2]$ (see Figure 4.4C). Because of G is bipartite, by Proposition 1.6.3 we get $\sigma(\Delta^{\widetilde{\boldsymbol{G}}}) \subset \kappa(J)$ and, therefore, the symmetry gives tighter localisation of the spectrum $\sigma(\Delta^{\widetilde{\boldsymbol{G}}}) \subset J \cap \kappa(J)$.

But, the set $V_0' = \{v_2\}$ is also a neighbourhood of the previous set E_0. Then, apply the same argument as before for E_0 and V_0' to obtain $J', \kappa(J')$. Again we get that $\sigma(\Delta^{\widetilde{\boldsymbol{G}}}) \subset J' \cap \kappa(J')$. We conclude that $\sigma(\Delta^{\widetilde{\boldsymbol{G}}}) \subset J \cap \kappa(J) \cap J' \cap \kappa(J')$. In fact, in Figure 4.4C, we see that our technique give an excellent estimation for the spectrum.

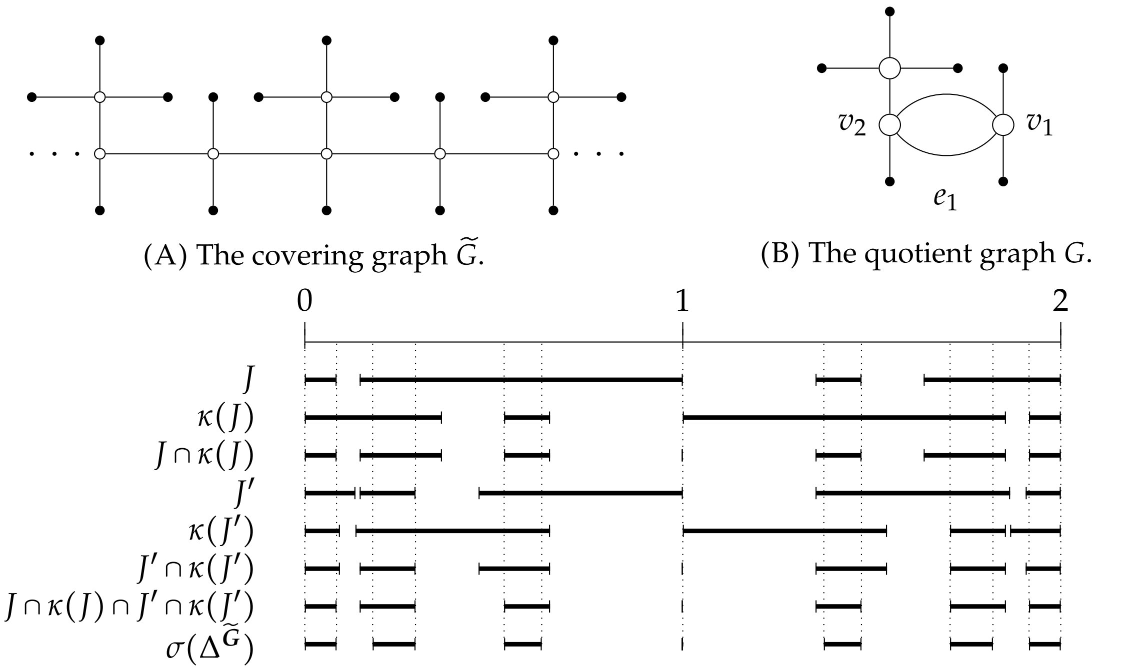
The previous examples show the existence of spectral gaps in periodic trees covering finite graphs with Betti number 1. In the next example, we show how to treat more complex periodic graphs.

Example 4.2.3. (*Polyacetylene*) Consider the *polyacetylene*, that consists of a chain of carbon atoms (white circles) with alternating single and double bonds between them, each with one hydrogen atoms (black vertex). We denote this magnetic weighted graph as $\widetilde{\boldsymbol{G}} = (\widetilde{G}, 0, \deg)$ and note that the graph $\widetilde{G}$ it is not a tree (cf., Figure 4.5A). The main question is compute $\sigma(\Delta^{\widetilde{\boldsymbol{G}}})$, and we use Theorem 3.4.2. The graph $\widetilde{G}$ is the covering graph from G (see Figure 4.5B) which is bipartite and has Betti number 2. In this case,

$$\sigma(\Delta^{\widetilde{\boldsymbol{G}}}) = \bigcup_{t \in [0,2\pi]} \sigma(\Delta^{G}_{\alpha^t})$$

where α^t is a magnetic potential supported only in $E_0 = \{e_1, \overline{e_1}\}$ with the property that $\alpha^t_{e_1} = t$ and $\alpha^t_{\overline{e_1}} = -t$.

As in the previous examples, since we are interested only in the magnetic potentials α supported on the set E_0, then just define $V_0 = \{v_1\}$ being in the neighbourhood of E_0. We can proceed as in the previous example to localise the spectrum within $J \cap \kappa(J)$ (see Figure 4.5). In fact, our method works almost perfectly in this case, since we detect



(A) The covering graph $\widetilde{G}$.

(B) The quotient graph G.

(C)

FIGURE 4.4: Spectral gaps of *polypropylene*, model by the magnetic weighted graph $\widetilde{\mathbf{G}} = (\widetilde{G}, 0, \deg)$. J is the spectral localisation of the pair $\mathbf{G} - E_0$ (where $E_0 = \{e_1, \overline{e_1}\}$) and $\mathbf{G} - \{v_1\}$, and bipartiteness gives $J \cap \kappa(J)$ as localisation set. Similarly, J' is the spectral localisation of the pair $\mathbf{G} - E_0$ and $\mathbf{G} - \{v_2\}$. Putting all this information together, we get the rather good spectral localisation $\sigma(\Delta^{\widetilde{\mathbf{G}}}) \subset J \cap \kappa(J) \cap J' \cap \kappa(J')$.

almost precisely the spectrum and also the spectral gap, i.e., we have the following equality

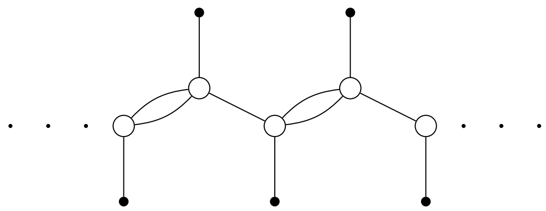
$$J \cap \kappa(J) \setminus \{1\} = \sigma(\Delta^{\widetilde{\mathbf{G}}}).$$

The graph $\widetilde{G}$ corresponds to an intermediate covering with respect to the maximal Abelian covering which, in this example, it is graphane. However, we cannot use Theorem 4.1.10, but we can apply the bracketing technique to detect the spectral magnetic gaps in G and hence spectral gaps in graphane. Just take $E_0 = \{e_1, e_2, \overline{e_1}, \overline{e_2}\}$ and $V_0 = \{v_1\}$ being in the neighbourhood of E_0, we define the bracketing intervals J and $\kappa(J)$ as before (see Figure 4.6). Again, our method works almost perfectly since $J \cap \kappa(J) \setminus \{1\} = \sigma(\Delta^{\widetilde{\mathbf{G}}})$.

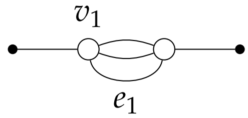
4.2.2 Periodic graph with periodic magnetic potential

For the first illustration of the existence of spectral gaps for covering graphs with periodic magnetic potential, we study the graph modelling polyacetylene.

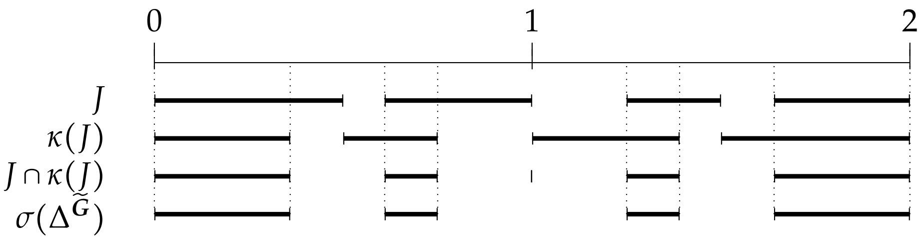
Example 4.2.4. (*Polyacetylene with magnetic potential.*)



(A) The covering graph $\widetilde{\mathbf{G}}$.



(B) The quotient graph G.

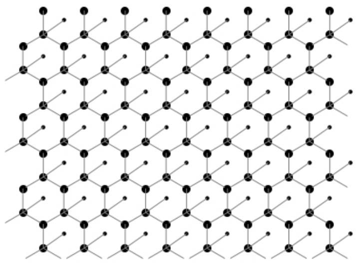


(C) Spectral bands.

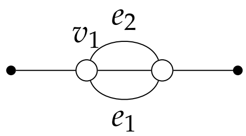
FIGURE 4.5: Spectral gaps of *polyacetylene*. In this example, the quotient graph has Betti number larger than 1. Here, J is the spectral localisation of the pair $\mathbf{G} - E_0$ where $E_0 = \{e_1, \overline{e_1}\}$ and $\mathbf{G} - \{v_1\}$, and bipartiteness gives again $J \cap \kappa(J)$ as localisation set. The spectral localisation J gives almost exactly the actual spectrum of $\widetilde{\mathbf{G}}$, except for the spectral value 1.

As we said in the previous example, his compound is an organic polymer that consists of a chain of carbon atoms (white circles) with alternating single and double bonds between them, each with one hydrogen atoms (black vertex). We denote this MW-graph as $\widetilde{\mathbf{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$, where $\widetilde{G}$ is the graph in Figure 4.7A. The polyacetylene belongs to the family of polymers, a chemical compound in long repeated chains modelled by covering graphs. The importance of the application of a magnetic potential on the polyacetylene is that the polymers have relevant electrical properties (see, e.g., [Chi12; Shi01] and references therein). In particular, the polyacetylene is a simple polymer with good electric conductance (cf., [EKN83]). In [FLP18] (as in the previous example) is studied the spectrum of the Laplacian in the infinite polyacetylene graph without any magnetic field. Applying the results of Section 3.4, we can now study the spectrum of the *DML* in the polyacetylene graph under the action of a periodic magnetic potential, in particular, the size and localisation of the spectral gaps. For the polyacetylene we will prove the following facts:

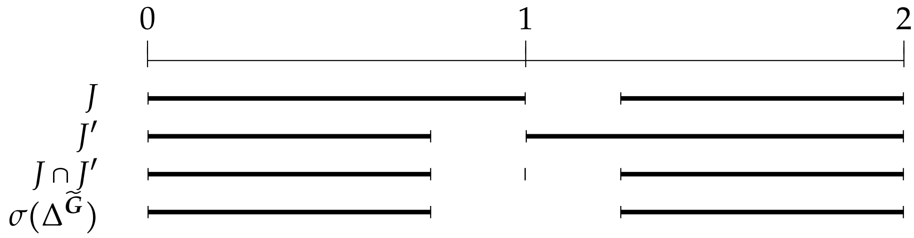
- *Fact 1.* Let w be the standard weights and $\widetilde{\alpha}$ a constant periodic magnetic potential. We show how to apply the bracketing technique to localise the spectrum for a specific value of the magnetic potential (equal to $s = \pi/2$) and then, how the bracketing intervals change as a function of $\widetilde{\alpha}$. We will show the existence of



(A) The Graphane $\widetilde{G}$.



(B) Quotient graph G.



(C) Spectral bands

FIGURE 4.6: Spectral gaps of *graphane*. This graph is again an example where the quotient graph has Betti number larger than 1. Here, J is the spectral localisation of the pair $\mathbf{G} - E_0$ where $E_0 = \{e_1, e_2, \overline{e_1}, \overline{e_2}\}$ and $\mathbf{G} - \{v_1\}$ giving an excellent result for the actual spectrum of $\mathbf{G}$ (except for the spectral value 1) again.

spectral gaps.

- *Fact 2.* Let w be the combinatorial weights and $\widetilde{\alpha}$ a periodic magnetic potential (not necessarily constant). Using the condition on δ in Equation (4.1.6), we show the existence of spectral gaps.
- *Fact 3.* Let w be the standard weights; we show the existence of periodic magnetic spectral gaps, i.e., a spectral gap which is stable under any perturbation of the constant periodic magnetic field.

Fact 1. We define a periodic magnetic potential $\widetilde{\alpha}$ acting as in Figure 4.7A, i.e., the potential acts only on the cycles defined by the double bonds. Observe that the action of any constant magnetic field on the polymer can be described by putting a suitable value s for the magnetic potential as in Figure 4.7A. To be concrete, we put first the value $s = \dfrac{\pi}{2}$ and want to specify the band/gap structure of the spectrum $\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}})$. The graph $\widetilde{G}$ in Figure 4.7A is the infinite covering of the finite graph G in Figure 4.7B. This graph is bipartite and has Betti number 2. In this case, if $\mathbf{G} = (G, \alpha, w)$ with w the standard weights, we have by Theorem 3.4.2 that

$$\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}) = \bigcup_{t\in[0,2\pi)} \sigma(\Delta_{\alpha^t}^{\boldsymbol{G}}),$$

where α^t is a magnetic potential acting on the quotient graph G with $\alpha^t(e_1) = t$, $\alpha^t(e_2) = s$, $\alpha^t(\overline{e_1}) = -t$, $\alpha^t(\overline{e_2}) = -s$ and zero in all the other edges. Define $E_0 := \{e_1, \overline{e_1}\}$ and $V_0 := \{v_1\}$, so that V_0 is in the neighbourhood of E_0 (see Definition 4.1.2). Then we construct $\boldsymbol{G}^+$ and $\boldsymbol{G}^-$ as before virtualising edges and vertices, i.e., $G^- := G - E_0$ and $G^+ := G - V_0$ as in Figure 4.7C. The induced weights w^- is defined as in Definition 2.4.8 and w^+ as in Definition 2.4.13. Using the notation of the Corollary 2.4.16 and 4.1.12, we get $\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}) \subset J \subset [0,2]$, where J is the union of the localising intervals J_k (see Figure 4.7d for the case of $s = \pi/2$). Since G is bipartite, we have the symmetry of spectrum under the function $\kappa(\lambda) = 2 - \lambda$ (cf., [LP08a], Proposition 2.3), hence we also have $\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}) \subset \kappa(J)$. Therefore, the intersection gives a finer localisation of the spectrum, i.e., we obtain finally $\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}) \subset J \cap \kappa(J)$. In this example, our method works almost perfectly, since we can determine almost precisely the spectrum:

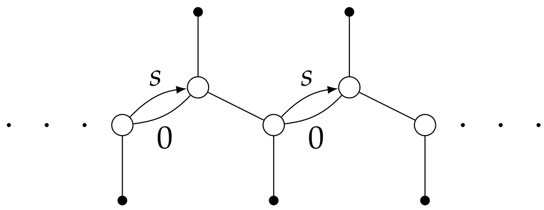
$$J \cap \kappa(J) \setminus \{1\} = \sigma\left(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}\right).$$

In conclusion, given a covering graph $\widetilde{G}$ with a periodic magnetic potential $\widetilde{\alpha}$ (see Figure 4.7 for $s = \pi/2$), we were able to localise $\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}})$ just by specifying the localisation of the spectrum is given by $J \cap \kappa(J)$ (and without computing explicitly the spectrum). Obviously, J depends on $\widetilde{\alpha}$ and therefore of the value of s. Therefore for each value of $\widetilde{\alpha}$ we can construct a bracketing $J(\widetilde{\alpha})$ of intervals for the spectrum of $\Delta_{\widetilde{\alpha}}^{\widetilde{G}}$ and, since in this case we have the reflection symmetry specified by κ and an additional interlacing property of $\boldsymbol{G}^-$ due to Cauchy's theorem, we are able to give a much finer localisation of the spectrum. In Figure 4.8 we plot the spectrum $\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}})$ of the *DML* as a function of the periodic magnetic potential $\widetilde{\alpha}$ varying within the interval $[0,2\pi]$. Here one can appreciate how the size of the gaps and their localisation within the interval $[0,2]$ changes as a function of the external magnetic field.

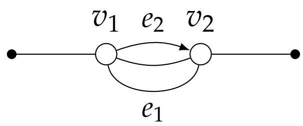
Fact 2. We have proved using the bracketing technique that the polyacetylene with standard weights has spectral gaps for any constant periodic magnetic potential acting on it. Now, if we consider the polyacetylene with combinatorial weight, we will prove more easily the existence of spectral gaps for all periodic magnetic potentials (not necessarily constant). Formally, let $\boldsymbol{G} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ be the periodic MW-graph where $\widetilde{G}$ is the polyacetylene (Figure 4.7A), $\widetilde{w}$ are the combinatorial weights and $\widetilde{\alpha}$ any periodic magnetic potential. Let $\boldsymbol{G}^-$ as in *Fact 1*, but now w^- are also the combinatorial weights. First, we observe that $\lambda_1(\Delta_{\alpha^-}^{G^-}) < 2$, then we calculate δ from condition in Eq. 4.1.13, i.e.,

$$\delta = \deg(v_1) - \|[B(D,\widetilde{G})]\| - \lambda_1(\Delta_{\alpha^-}^{G^-}) > 4 - 2 - 2 = 0,$$

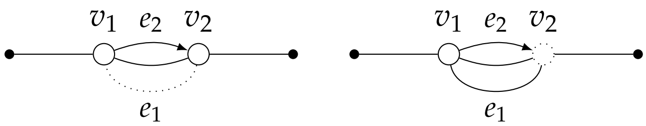
then by Corollary 4.1.13, we can assure the existence of spectral gaps. Observe we do this without computing explicitly any eigenvalue and only using the geometry of the graph.



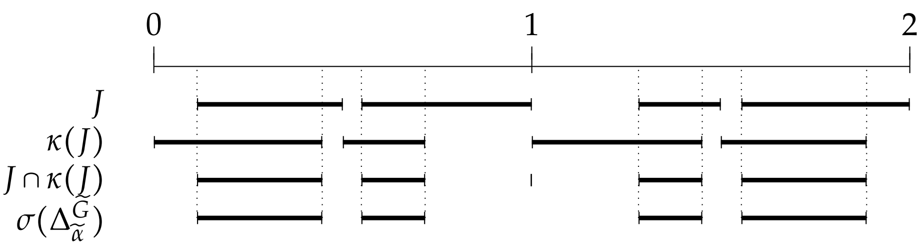
(A) Polyacetylene modelled by the covering graph $\widetilde{G}$.



(B) The quotient graph G.



(C) The graph G^- and the graph G^+.



(D) Spectral bands.

FIGURE 4.7: Spectral gaps of the *polyacetylene* graph for a constant magnetic potential $\widetilde{\alpha} = \pi/2$. Here, J is the spectral localisation for the pair $G - E_0$ where $E_0 = \{e_1, \overline{e_1}\}$ and $G - \{v_1\}$. Bipartiteness gives a finer localisation $J \cap \kappa(J)$. In this case, we obtain the spectrum almost exactly, except for the spectral value 1.

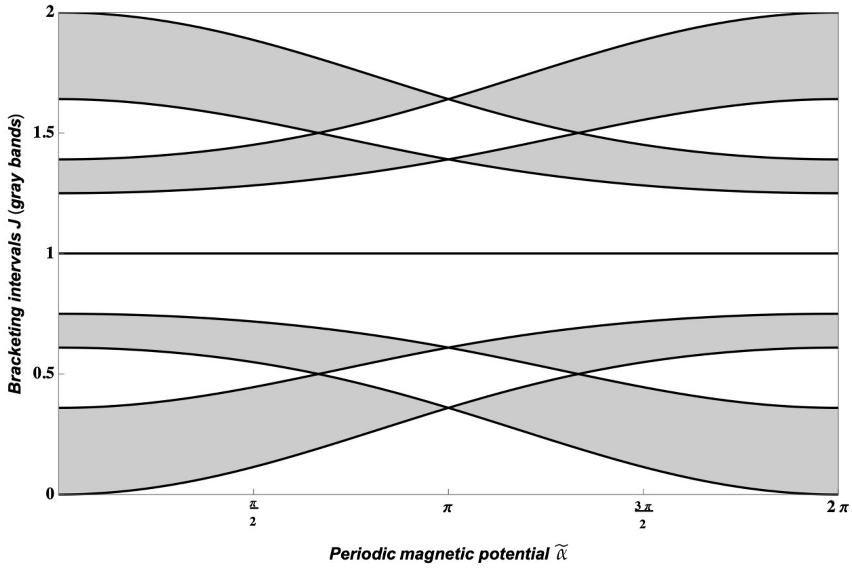


FIGURE 4.8: The horizontal axis represents the values of the magnetic potential $\widetilde{\alpha} \in [0, 2\pi)$ acting on the *polyacetylene* polymer with standard weights. For any fixed $\widetilde{\alpha}$ we obtain the intervals J given by the bracketing technique as we did in the case $\widetilde{\alpha} = \pi/2$ in Figure 4.7 (and also using the symmetry given by the bipartiteness). In the vertical axis, we represent the spectral bands and gaps for each constant value $\widetilde{\alpha}$.

Fact 3. Our method of virtualising suitable edges and vertices allows proceeding also alternatively. Define now $E_1 := \{e_1, e_2, \overline{e_1}, \overline{e_2}\}$ and $V_1 := \{v_1\}$ so that V_1 is a neighbourhood of E_1 (see Definition 4.1.2). We construct as usual the MW-graphs $\boldsymbol{G}_1^+$ and $\boldsymbol{G}_1^-$ setting $\boldsymbol{G}_1^+ = \boldsymbol{G} - E_1$ and $\boldsymbol{G}_1^- = \boldsymbol{G} - V_1$ as in Figure 4.9 and inducing the weights as in Definition 1.1.4 and 2.4.13 (observe that in this case $\boldsymbol{G}_1^+ = \boldsymbol{G}^+$). Using the notation of the Corollary 2.4.16 and Theorem 3.4.2, we observe now that the spectral localisation intervals do *not* depend on the periodic magnetic potential. In fact, using the same idea that before we obtain

$$\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}}) \subset [0, 3/4] \cup [5/4, 2] \quad \text{for all periodic constant magnetic potential} \quad \widetilde{\alpha},$$

in particular, $(3/4, 5/4)$ is a spectral gap which is stable under any perturbation by the magnetic field. Finally, we note that if the magnetic potential has a constant value equal to π, then the spectrum degenerates to four eigenvalues with infinity multiplicity, i.e., the gaps consist of the whole interval $[0, 2]$ except for the four eigenvalues. In this case, the polyacetylene becomes essentially an insulator under the influence of this particular value of the magnetic field.

Example 4.2.5. (*Graphene nanoribbons*)

In this example, we will apply our method to study the example of the graphene nanoribbons (GNRs), also known as nano-graphene ribbons or nano-graphite ribbons. These are strips of graphene with semi-conductive properties which are very promising

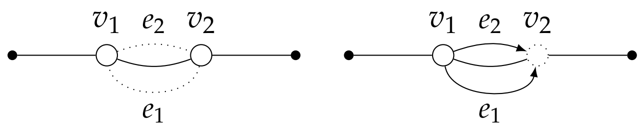


FIGURE 4.9: Using this graph $\boldsymbol{G}_1^-$ and $\boldsymbol{G}_1^+$, we can find spectral gaps in common for all periodic magnetic potential $\widetilde{\alpha}$ acting on the polyethylene, represented by the covering graph $\boldsymbol{G}$.

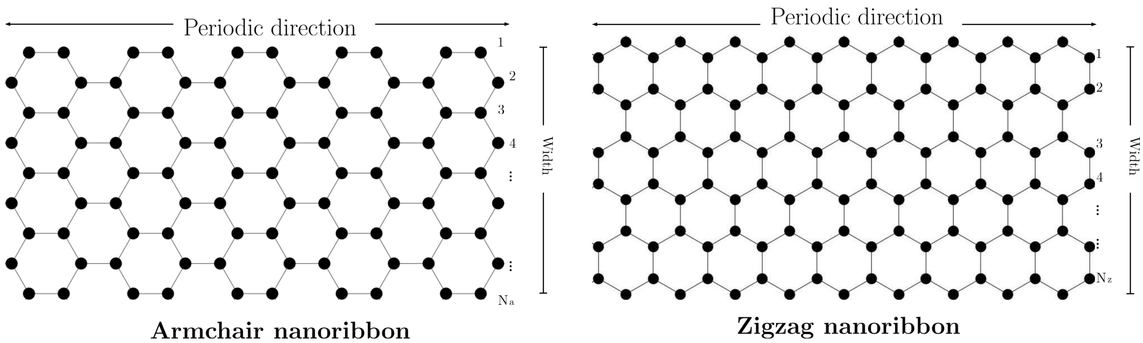


FIGURE 4.10: Two structures of the graphene nanoribbons: armchair and zigzag. These structures are covering graphs only in one direction.

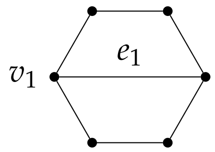
as nano-electronic devices (see, e.g., [SCB09]). One of the most interesting fields of research of the nanoribbons is the energy gaps as a function of their widths. We refer, for example [SCL06]. The GNRs repeat their geometry structure in two different ways and can be represented as $\mathbb{Z}$-covering graphs (see Figure 4.10).

(i) The first variant is called armchair nanoribbon with a width equal to N_a and denoted as N_a-aGNR (see Figure 4.10). Consider, for example, the case of a 3-aGNR which has a similar structure as the poly-para-phenylene (PPP), one of the most important conductive polymers. Let $\widetilde{\boldsymbol{G}} = (\widetilde{G}, \widetilde{\alpha}, \widetilde{w})$ the MW-graph with standard weights where $\widetilde{G}$ the $\mathbb{Z}$-covering graph representing the 3-aGNR and $\widetilde{\alpha}$ a constant (periodic) magnetic potential, the idea will be using the bracketing technique to localise $\sigma(\Delta_{\widetilde{\alpha}}^{\widetilde{G}})$ and we proceed as in the previous examples. Figure 4.11A is the finite quotient graph $\boldsymbol{G} = \widetilde{G}/\mathbb{Z}$. Define in this case $E_1 = \{e_1, \overline{e_1}\}$ and $V_1 = \{v_1\}$ so that V_1 is a neighbourhood of E_1 (see Definition4.1.2). We construct $\boldsymbol{G}_1^+$ and $\boldsymbol{G}_1^-$ as before: $\boldsymbol{G}_1^+ = \boldsymbol{G} - E_1$ and $\boldsymbol{G}_1^- = \boldsymbol{G} - V_1$ (cf., Figure 4.11B). The weights are induced as in Definitions 1.1.4 and 2.4.13. Using again the notation of the Corollary 2.4.16 and Theorem 3.4.2 we obtain now a spectral localisation J that depends on $\widetilde{\alpha}$. Finally, in Figure 4.11C, we plot the spectral bands and gaps specified by J for the different values of the magnetic field within the interval $[0, 2\pi]$. Observe that in this case, we do not have a spectral gap common to all values of $\widetilde{\alpha}$ (as we had for the polyacetylene).
A similar analysis could be done for any N_a-aGNR under the action of any periodic magnetic potential, and the bracketing technique will give good estimates of the intervals where the spectrum lies.
Also, observe that for the combinatorial weights, we can show the existence of

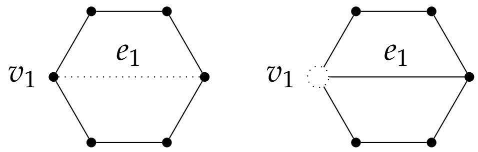
spectral gaps using the condition of Eq. 4.1.13 as in *Fact 2* in the polyacetylene example. We have in this case,

$$\delta = \deg(v_1) - |[B(D, \widetilde{G})]| - \lambda_1(\Delta_{\beta^-}^{G^-}) > 3 - 2 - 1 = 0.$$

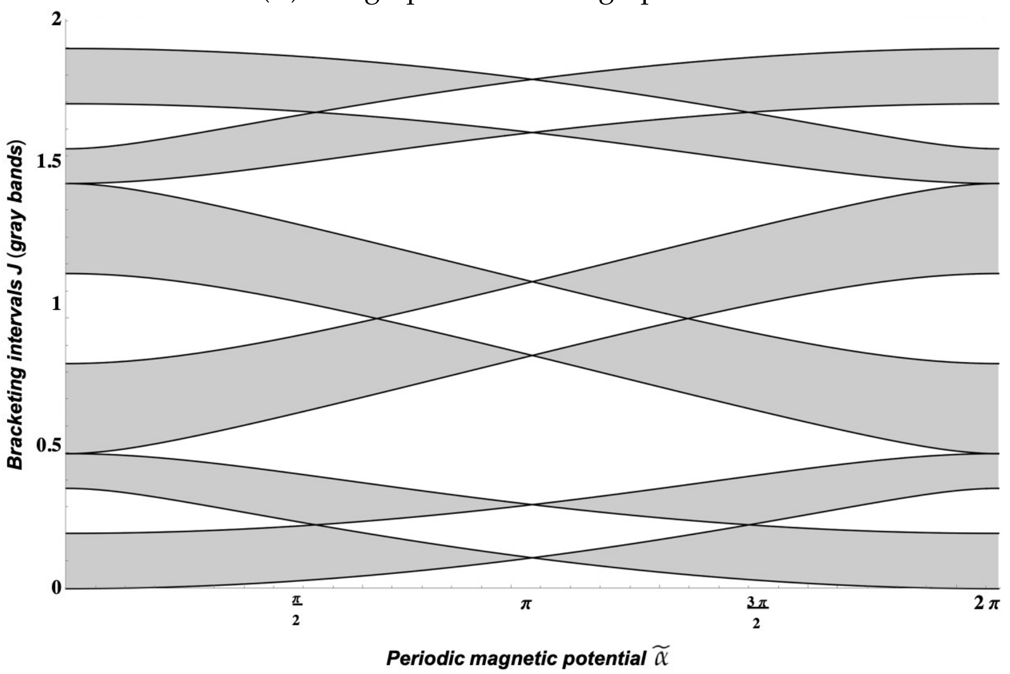
(ii) The second variant is the so-called zigzag nanoribbon with a width equal to N_z are denoted as N_z-zGNR (see Figure 4.10). Consider $\boldsymbol{G} = (G, \alpha, w)$ the MW-graph with standard weights and $\widetilde{G}$ is the graph given by the zigzag nanoribbons for a fixed N_z, and $\widetilde{\alpha} \sim 0$ acting on $\widetilde{G}$. In this case, our spectral localisation method does not specify spectral gaps (i.e., the spectral bands overlap). The reason is that for any width N_z the spectrum of the zigzag nanoribbons satisfies $\sigma(\Delta_0^{\widetilde{G}}) = [0, 2]$, i.e., in this case, there are no spectral gaps. This fact is also confirmed by our method.



(A) The quotient graph $\boldsymbol{G}$ of 3-aGRN.



(B) The graph $\boldsymbol{G}^-$ and the graph $\boldsymbol{G}^+$.



(C) Spectral bands and gaps as a function of the constant (periodic) magnetic potential $\widetilde{\alpha}$.

FIGURE 4.11: Spectral gaps of *3-aGNR* for a constant magnetic potential $\widetilde{\alpha} = s$. Here, J is the spectral localisation of the pair $\boldsymbol{G} - \{e_1, \overline{e_1}\}$ and $\boldsymbol{G} - \{v_1\}$, bipartiteness (and interlacing) gives again the bracketing J as localisation set.

5 Application II: Isospectral graphs

Since Weyl's seminal article in 1912 [Ivr16; Wey12] on the asymptotic distributions of eigenvalues of the Laplacian on a compact Riemannian manifold and, in particular, since Kac's celebrated article *Can you hear the shape of a drum?* [Kac66], the relation between the spectrum of the Laplacian and the geometric properties of the underlying space has been addressed from many different perspectives. The first example of two non-isomorphic compact Riemannian manifolds whose Laplacian operators have exactly the same eigenvalues was constructed by Milnor using 16-dimensions [Mil64]. The two-dimensional remained open until 1992 (cf. [GWW92]). For a survey on the variety of techniques used in the inverse spectral problems, we refer to [LR15]. In general, the construction of non-isomorphic structures (Riemannian manifolds, quantum graphs or discrete graphs) with isospectral Laplacians (or other natural operators) has been a very fruitful mathematical question with many applications. Recall that two linear operators with discrete spectrum are called *isospectral* (or *cospectral*), if their spectrum coincides, i.e., they have the same eigenvalues with the same multiplicity. One of the most widely used techniques is Sunada's method for constructing isospectral manifolds [Sun85]. Some construction for isospectral quantum graphs are presented in [BPB09]. Finally, for some application of the isospectrality, we refer [AYY13] and [Row91].

In this chapter, *isospectrality* refers to the spectrum of their discrete magnetic Laplacian of the corresponding *MW*-graphs. We will present a *geometric method* for the construction of isospectral graphs with normalized weights and a magnetic potential acting on it. More precisely, we find $\boldsymbol{G}_i = (G_i, \alpha_i, w_i)$ and $\boldsymbol{G}_j = (G_j, \alpha_j, w_j)$ two magnetic weighted graphs, such G_i and G_j are two non-isomorphic graphs, but theirs discrete magnetic Laplacians (with *normalized weights*) satisfy

$$\sigma\left(\Delta_{\alpha_i}^{G_i}\right) = \sigma\left(\Delta_{\alpha_j}^{G_j}\right) .$$

We will use the geometric and spectral preorders introduced in Sections 2.1 and 2.2 in the construction of the isospectral graphs. Moreover, an infinite number of isospectral pairs of graphs are labelled by different partitions of natural numbers. First, it will be necessary to construct families of *MW*-graphs with certain geometrical and spectral properties. Then, we chose two s-partitions of a natural number r. An s-partition of r is a way to write r as a sum of s positive integer, i.e., by decomposition r into two different sums with the same number of summands equal to s. We obtain two different s-partitions of the number r:

$$r = a_1 + \dots a_s = b_1 + \dots b_s \ ,$$

if at least a pair of a-summands is different from a pair of b-summands. In the previous chapters of the present dissertation, given a magnetic weighted graph (MW-graph for short) of order n, the spectrum of the discrete magnetic Laplacian was denoted by $\sigma(\Delta^G) = \{\lambda_1, \dots, \lambda_n\}$ where the eigenvalues are written in ascending order and repeated according to their multiplicities. In this chapter, we will not follow this convention. Instead, it will be more useful to write the spectrum as a *multiset* in order to control the effect of the geometric operations on the spectra of the corresponding graphs.

To finish this short motivation, let us also mention also why the choice of normalized weights, e.g., standard weights, is particularly interesting. In the next table taken from [BG11] (see also [HS04a]) the number of graphs with an isospectral mate are shown for different types of Laplacians: for the combinational Laplacian, the signless (combinatorial) Laplacian and for the normalized Laplacian. The underlying graphs are simple and have up to nine vertices.

No. vertices	No. graphs	Combinatorial	Signless	Normalized
1	1	0	0	0
2	2	0	0	0
3	4	0	0	0
4	11	0	2	2
5	34	0	4	4
6	156	4	16	14
7	1044	130	102	52
8	12346	1767	1201	201
9	274668	42595	19001	1092

Observe that as the order of the graph increases, the number of isospectral graphs for the normalized Laplacian is clearly lower than in the case of Laplacians with other weights. Many of the isospectral mates are found by computer programs that list the number of simple graphs with a fixed (and small) number of vertices and, then, determine the spectra of the corresponding Laplacians by hand. Given the huge complexity of graphs as the order increases it is clear that this strategy is limited. Few constructions are known for determining isospectral graphs for the normalized Laplacian. We present in this chapter a new geometrical construction leading to an infinite collection of families of graphs, where all the elements in each family are (finite) isospectral non-isomorphic graphs for the magnetic Laplacian with normalized weights. The construction is based on the the preorder of graphs introduced in Chapter 2. Moreover, the parametrization of the isospectral graphs in each family is given by a number theoretic notion: the different partitions of a natural number.

In this chapter, we will work with magnetic graphs with normalized weight (for example, the standard weights), because for the construction, it will be necessary the interlacing properties of the eigenvalues when we identify or glue some vertices, e.g., see the spectral interlacing in Corollary 2.4.6.

5.1 A motivating class of examples

We begin this chapter by defining the disjoint union of MW-graphs as follows: Consider $\boldsymbol{G}_1 = (G_1, \alpha_1, w_1)$ and $\boldsymbol{G}_2 = (G_2, \alpha_2, w_2)$ two magnetic weighted graphs, the *disjoint union* of the MW-graphs denoted as $\boldsymbol{G} = \boldsymbol{G}_1 \dot\cup \boldsymbol{G}_2$ is the magnetic weighted graph $\boldsymbol{G} = (G, \alpha, w)$ where $G = G_1 \dot\cup G_2$ is the disjoint union of graphs (defined in Subsection 1.1.2), the magnetic potential $\alpha\restriction_{E(G_i)} = \alpha_i$ and weights $w\restriction_{G_i} = w_i$ for $i = 1, 2$.

Now, we present a class of examples of non-isomorphic isospectral graphs that motivate the geometric construction formalised later. For simplicity, we will refer in this section to the standard Laplacians with magnetic field equal to zero, i.e., consider the next family of weighted magnetic graphs $\{\boldsymbol{G}_i\}_{i\in\mathbb{N}}$ where $\boldsymbol{G}_i = (G_i, 0, \deg)$ with G_i are rooted *diamond graphs* specified in Figure 5.1. The root (distinguished vertex) is coloured in green and will be needed for constructing the isospectral graphs.

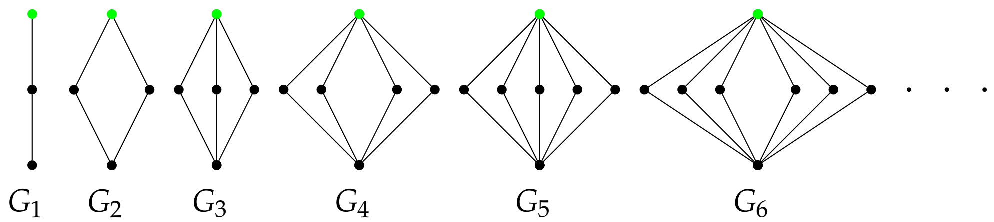


FIGURE 5.1: The family of diamond graphs G_i for $i \in \mathbb{N}$. Each graph G_i has a root vertex (in colour green).

Note that the family of graphs in Figure 5.1 has a high degree of symmetry, and this fact is reflected in the spectrum through eigenvalues with high multiplicity. The idea of the construction is to take this family of graphs as a frame which can be geometrically manipulated to produce new non-isomorphic graphs that preserve most of the eigenvalues of the initial frame. We will be able to control the spectrum of the new graphs thanks to the preorder relations studied in Chapter 2. The geometric operations will be described by different s-partitions of a natural number $r \in \mathbb{N}$.

To be concrete, let us begin by specifying two isospectral graphs out of the family of rooted diamonds given in Figure 5.1. Consider, for example, the following two different 2-partitions of the number 5: $A = [1, 4]$ and $B = [2, 3]$, i.e.,

$$5 = 1 + 4 = 2 + 3 .$$

Then, we construct the following magnetic graph associated with the first partition $\boldsymbol{G}(A)$ as follow: The first graph is constructed from the elements labelled by $[1, 4]$ in the family of diamond graphs in Figure 5.1 . Consider the MW-graph $\boldsymbol{G}_1 \dot{\cup} \boldsymbol{G}_4$ that is the disjoint union of the magnetic weighted graphs G_1 and G_4. Let $\sim_A$ be the equivalence relation on $V(G_1 \dot{\cup} G_4)$ that identifies (or glues) the set of two green root vertices of the graphs G_1 and G_4. Then, we define $\boldsymbol{G}(A) := (\boldsymbol{G}_1 \dot{\cup} \boldsymbol{G}_4)/\sim_A$, i.e., the MW-graph $\boldsymbol{G}(A)$ is made by glueing the roots of G_1 and G_4. Similarly, we can construct the second MW-graph $\boldsymbol{G}(B) := (\boldsymbol{G}_2 \dot{\cup} \boldsymbol{G}_3)/\sim_B$ where $\sim_B$ is the equivalence relation on $V(\boldsymbol{G}_2 \dot{\cup} \boldsymbol{G}_3)$ that identifies (or glues) the roots of G_2 and G_3. The graphs $\boldsymbol{G}(A)$ and $\boldsymbol{G}(B)$ are represented in Figure 5.2.

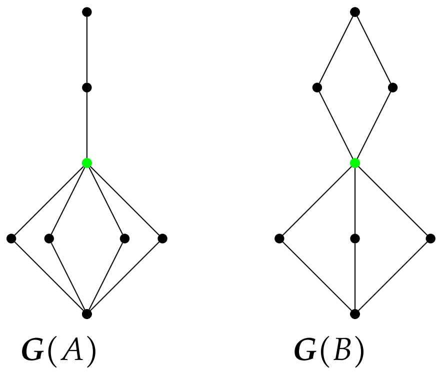


FIGURE 5.2: The graphs $\boldsymbol{G}(A)$ and $\boldsymbol{G}(B)$ are isospectral but not isomorphic magnetic weighted graphs.

An explicit computation of the eigenvalues of the corresponding Laplacian with standard weights and $\alpha = 0$ shows that both MW-graphs $\boldsymbol{G}(A)$ and $\boldsymbol{G}(B)$ are isospectral, concretely, their eigenvalues are the following:

$$\left[0, 1 - \frac{1}{\sqrt{2}}, 1^{(4)}, 1 + \frac{1}{\sqrt{2}}, 2\right].$$

Moreover, it is clear that they are not isomorphic, because $\boldsymbol{G}(A)$ has a pendant vertex while $\boldsymbol{G}(B)$ has no vertex of degree 1.

The important feature of the preceding example is the partition of a natural number that selects the diamonds that will be identified. In fact, there are many more isospectral graphs that can be constructed from the family of rooted diamonds $\{\boldsymbol{G}_i\}_{i \in \mathbb{N}}$. Given A a general *s-partition* of $r \in \mathbb{N}$, it will be convenient to define it as a *multiset* of natural numbers (that can be repeated) and with sum r (for a formal definition see Definition 5.2.1):

$$A = [a_1, a_2, \ldots, a_s] \quad \text{with} \quad \sum_{i=1}^{s} a_i = r.$$

The size of the partition A is the number s (which is its cardinality as a multiset) and we say that A is an s-partition of r. Note that $s \leq r$.

Given $s, r \in \mathbb{N}$ with $s \leq r$ and let A, B be two s-partition of the number r. Consider the graph $\dot{\bigcup}_{i \in A} \boldsymbol{G}_i$, i.e., the disjoint union of graphs labelled by the partition A. Let $\sim_A$ be the equivalence relation defined on $V(\dot{\bigcup\limits_{i\in A}} G_i)$ that identifies all the root (green) vertices of the graph into one vertex. Finally, define the MW-graph $\boldsymbol{G}(A) := (\dot{\bigcup\limits_{i\in A}} \boldsymbol{G}_i)/\sim_A$. Similarly, the graph $\boldsymbol{G}(B) = (\dot{\bigcup\limits_{i\in B}} \boldsymbol{G}_i)/\sim_B$ consists of the disjoint union of $\dot{\bigcup\limits_{i\in B}} G_i$, where the roots are glued together. We will show in the next section that $\boldsymbol{G}(A)$ and $\boldsymbol{G}(B)$ are isospectral.

Example 5.1.1. Consider the following 4-partitions of the number 8: $A_1 = [1,1,1,5]$, $A_2 = [1,1,2,4]$, $A_3 = [1,1,3,3]$, $A_4 = [1,2,2,3]$ and $A_5 = [2,2,2,2]$. For each partition A_i with $i = 1,2,\ldots,5$ construct the MW-graphs $\boldsymbol{G}(A_i)$ as previous, i.e.,

$$\boldsymbol{G}(A_i) := (\dot{\bigcup_{j\in A}} \boldsymbol{G}_j)/\sim_{A_i}$$

where each equivalence relation $\sim_{A_i}$ identifies the green roots of the graph $V(\dot{\bigcup\limits_{j\in A}} G_j)$ into one vertex.

In Figure 5.3 we present the five different graphs $\boldsymbol{G}(A_i)$, for $i = 1,\ldots,5$, where A_i correspond to 4-partitions of the number 8.

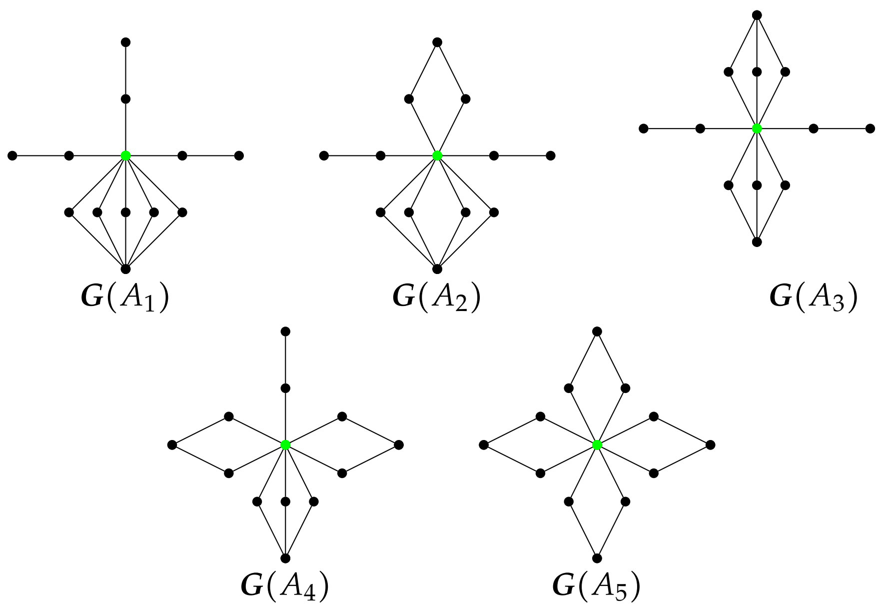


FIGURE 5.3: The graphs $\boldsymbol{G}(A_i)$ defined by the partition A_i, where $A_1 = [1,1,1,5]$, $A_2 = [1,1,2,4]$, $A_3 = [1,1,3,3]$, $A_4 = [1,2,2,3]$ and $A_5 = [2,2,2,2]$.

An explicit calculation of the eigenvalues of the Laplacian of $\boldsymbol{G}(A_i)$ shows that the graphs are isospectral for all $1 \le i \le 5$ and mutually non-isomorphic. More concrete, their eigenvalues are:

$$\left[0, \left(1 - \frac{1}{\sqrt{2}}\right)^{(3)}, 1^{(5)}, \left(1 + \frac{1}{\sqrt{2}}\right)^{(3)}, 2\right].$$

Finally, we need to show that the MW-graphs $\boldsymbol{G}(A_i)$ in Figure 5.3 are non-isomorphic graphs. We use its degree sequence.

Let G be a graph with n vertices and degrees $d_1 \leq d_2 \leq \cdots \leq d_n$, then the n-tuple $(d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G. Note that this sequence is unique, even if G has several vertex enumerations. The degree sequence is a graph invariant, so isomorphic graphs have the same degree sequence. Then, in the examples mentioned above the degree sequence of the graphs $\boldsymbol{G}(A_i)$ are the following:

Graph	Degree sequence
$\boldsymbol{G}(A_1)$	$(\mathbf{1},\mathbf{1},\mathbf{1},2,2,2,2,2,2,2,2,\mathbf{5},8)$
$\boldsymbol{G}(A_2)$	$(\mathbf{1},\mathbf{1},2,2,2,2,2,2,2,2,\mathbf{2},\mathbf{4},8)$
$\boldsymbol{G}(A_3)$	$(\mathbf{1},\mathbf{1},2,2,2,2,2,2,2,2,\mathbf{3},\mathbf{3},8)$
$\boldsymbol{G}(A_4)$	$(\mathbf{1},2,2,2,2,2,2,2,2,\mathbf{2},\mathbf{2},\mathbf{3},8)$
$\boldsymbol{G}(A_5)$	$(2,2,2,2,2,2,2,2,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},8)$

Each degree sequence is different, then the MW-graphs $\boldsymbol{G}(A_i)$ are non-isomorphic. Observe that each partition A_i is contained in its degree sequence (the bold numbers). Since the construction is based on different partitions of the same number, the resulting graphs must be non-isomorphic too.

5.2 Geometric construction of isospectral graphs and partitions of a natural number

To formalise the geometric method illustrated in the class of examples above and to prove our main theorem, first, we need to fix some notion. Given a countable family of graphs, two fundamental properties of this family on which the method is based are called Λ-*spectral* and Λ-*geometric* (see Definitions 5.2.5 and 5.2.10 below). Here $\Lambda \subset \mathbb{R}_+$ is a finite subset of non negative real numbers. Each element of the set Λ will appear as an eigenvalue with constant multiplicity in the different spectra associated with the Laplacians of the constructed graphs. The geometric property of the family of graphs is related to the geometric preorder $\sqsubseteq$ studied in Chapter 2.

We begin introducing the notion of a multiset and specify some elementary operations on them. It will be convenient to simplify the reasoning later to denote multisets in different ways.

Definition 5.2.1. A *multiset* is an ordered pair (A, m) where A is a set and $m \colon A \to \mathbb{N}$ a function on A. If $A = \{a_1, a_2, \ldots, a_s\}$, then the multiset is also denoted as

$$\begin{aligned}(A, m) &= [a_1^{m(a_1)}, a_2^{m(a_2)}, \ldots, a_s^{m(a_s)}] \\ &= [\underbrace{a_1, \ldots, a_1}_{m(a_1)}, \underbrace{a_2, \ldots, a_2}_{m(a_2)}, \ldots, \underbrace{a_s, \ldots, a_s}_{m(a_s)}] .\end{aligned}$$

The function m counts the number of occurrences of each element of the set A. The map m is called the *multiplicity* or *characteristic value*.

Let (A, m_A) and (B, m_B) be two multisets. We say that (A, m_A) is a *multisubset* of (B, m_B) if $A \subset B$ and $m_A(x) \leq m_B(x)$ for all $x \in A$, and we will denote this by $(A, m_A) \subset (B, m_B)$. If $(A, m_A) \subset (B, m_B)$ and $(B, m_B) \subset (A, m_A)$, then we say that the multisets are equal and denoted this by $(A, m_A) = (B, m_B)$.

The *sum of two multisets* is defined as $(A, m_A) \uplus (B, m_B) = (A \cup B, m_A \uplus m_B)$, where $m_A \uplus m_B := m_A \mathbf{1}_A + m_B \mathbf{1}_B$ and $\mathbf{1}_A$ is the *indicator function* for the set A, i.e., $\mathbf{1}_A(x) = 1$ if $x \in A$, and 0 otherwise.

The multiset (A, m_A) is called a *constant multiset* if all of its objects occur with the same multiplicity, i.e., there is an $i \in \mathbb{N}$ such that the multiplicity function $m_A \colon A \to \mathbb{N}$ is given by $m_A(x) = i$ for all $x \in A$. We denote these constant multisets simply as $A^{(i)}$. With this notation, a simple calculation shows that the sum of constant multisets gives us a new constant multiset, i.e., $A^{(i)} \uplus A^{(j)} = A^{(i+j)}$. We define $A^{(0)} := \varnothing$. Constant multisets will often appear as spectra of Laplacians associated with graphs resulting from geometric operations.

The cardinality of the multiset is the sum of the multiplicities of all its elements, i.e., given (A, m_A) its cardinality is $|(A, m_A)| = \sum_{x \in A} m_A(x)$. In particular, if the multiset is constant then $|A^{(i)}| = i|A|$ where $|A|$ is the cardinality of the set A. Moreover, if A is an s-partition of the number r, then the cardinality of the partition A as a multiset is denoted as the size of the partition: s.

Definition 5.2.2. An *s-partition* of a positive integer r is a multiset A of natural numbers with sum r, i.e.,

$$A = [a_1, a_2, \dots, a_s] \quad \text{such that} \quad \sum_{i \in 1}^{s} a_i = r \,,$$

The number s is named the *size of the partition*.

As mentioned above, it will be convenient for the proof of isospectrality property to denote the spectrum of the Laplacian also as a multiset.

Notation 5.2.3. Let $\mathbf{G} = (G, \alpha, w)$ be a magnetic weighted graph, in this chapter we denote the spectrum of the discrete magnetic Laplacian $\Delta^{\mathbf{G}}$ as the multiset $\sigma_m(\mathbf{G})$, where $\sigma(\mathbf{G})$ is the set of eigenvalues of $\Delta^{\mathbf{G}}$ and m the multiplicity of each eigenvalue, i.e., $m \colon \sigma(\mathbf{G}) \to \mathbb{N}$.

The following result will be important in the development of the method to construct the isospectral graphs.

Lemma 5.2.4. *Let $\mathbf{G} = (G, \alpha, \deg_G)$ and $\mathbf{G} = (G', \alpha', \deg_{G'})$ two finite magnetic weighted graph such that $G' = G/\!\sim$ for some equivalence relation $\sim$ on $V(G)$ and $\alpha = \alpha'$. If λ is an eigenvalue of the Laplacian on $\mathbf{G}$ with multiplicity k, then λ is an eigenvalue of the Laplacian on $\mathbf{G}'$ with multiplicity at least $k - s$, where $s = |G| - |G'|$ (with the convention that if $k < s$, the multiplicity is zero).*

Proof. Suppose that $|\boldsymbol{G}| = n$ and write the spectrum of the discrete magnetic Laplacian Δ_α^G of $\boldsymbol{G}$ as follow:

$$\sigma(\boldsymbol{G}) = \sigma(\Delta_\alpha^G) = (\lambda_1(\boldsymbol{G}), \lambda_2(\boldsymbol{G}), \dots, \lambda_n(\boldsymbol{G}))$$

where the eigenvalues are written in ascending order and repeated according to their multiplicities, in a similar way $|\boldsymbol{G}'| = n - s$ and we denote the spectrum of $\Delta_{\alpha'}^{G'}$ of $\boldsymbol{G}'$ as follow:

$$\sigma(\boldsymbol{G}) = \sigma(\Delta_{\alpha'}^{G'}) = \left(\lambda_1(\boldsymbol{G}'), \lambda_2(\boldsymbol{G}'), \dots, \lambda_{n-s}(\boldsymbol{G}')\right) .$$

Applying s-times the Corollary 2.4.6 (i), we obtain that

$$\boldsymbol{G} \overset{0}{\preccurlyeq} \boldsymbol{G}' \overset{s}{\preccurlyeq} \boldsymbol{G} . \tag{5.2.1}$$

But, the eigenvalue $\lambda \in \sigma(\boldsymbol{G})$ have multiplicity k, i.e., there exists $i \in \{1, 2, \dots, n\}$ such that $\lambda = \lambda_i(\boldsymbol{G}) = \lambda_{i+1}(\boldsymbol{G}) = \dots = \lambda_{i+k-1}(\boldsymbol{G})$ with $i + k - 1 \leq n$. Therefore, using Eq. (5.2.1), we obtain the inequalities

$$\lambda = \lambda_{i+j}(\boldsymbol{G}) \leq \lambda_{i+j}(\boldsymbol{G}') \leq \lambda_{i+j+s}(\boldsymbol{G}) = \lambda \quad \text{for all} \quad j \in \{0, 1, \dots, k - s - 1\}$$

hence $\lambda = \lambda_{i+j}(\boldsymbol{G}')$ for all $j \in \{0, 1, \dots, k - s - 1\}$, and we have proved that λ is an eigenvalue of the Laplacian on $\boldsymbol{G}'$ with multiplicity at least $k - s$. □

Let $\mathfrak{G} := \{ \boldsymbol{G}_i \,|\, i \in \mathbb{N} \}$ be a discrete family of magnetic graphs and $r \in \mathbb{N}$. Consider A an s-partition of r, we define the next magnetic weighted graph given as the disjoint union of the graphs labelled by the integers specifying the partition:

$$\mathfrak{G}(A) := \dot{\bigcup_{i \in A}} \boldsymbol{G}_i . \tag{5.2.2}$$

Moreover, if $\sim_A$ is an equivalence relation on the set of vertices $V(\mathfrak{G}(A))$, we define the MW-graph $\mathfrak{G}(A, \sim_A) := \mathfrak{G}(A)/\sim_A$ (see Subsection 2.4.2).

We introduce the first important property of a family of graphs to qualify as a frame for constructing isospectral graphs. This property says that the different members of the family have a common degree of symmetry; hence, the difference in the spectra of the Laplacians of distinct members of the family is reflected only in the multiplicity of a fixed set Λ.

Definition 5.2.5. Let $\mathfrak{G} := \{ \boldsymbol{G}_i \,|\, i \in \mathbb{N} \}$ be a countable family of magnetic graphs and $\Lambda \subset \mathbb{R}_+$ a finite set of non negative real numbers. The family $\mathfrak{G}$ is Λ-*spectral* if

$$\sigma_{m_i}(\boldsymbol{G}_i) = \sigma_{m_1}(\boldsymbol{G}_1) \uplus \Lambda^{(i-1)} \quad \text{for all} \quad i \in \mathbb{N} , \tag{5.2.3}$$

where the equality is understood as multisets.

Before continuing the analysis, let us check that Λ-spectrality is verified for two important infinite families of graphs. For simplicity, in the following two examples, we will set the magnetic potential $\alpha = 0$.

Example 5.2.6. Let $\mathfrak{G} = \{\boldsymbol{G}_i\}_{i\in\mathbb{N}}$ be a family of MW-graphs $\boldsymbol{G}_i = (G_i, 0, \deg)$ where G_i are the diamond graphs specified in Figure 5.1. In this case we have

$$\sigma_{m_1}(\boldsymbol{G}_1) = [0,1,2]\,, \quad \text{and}$$
$$\sigma_{m_i}(\boldsymbol{G}_i) = [0^{(1)}, 1^{(i)}, 2^{(1)}] = [0,1,2] \uplus [1^{(i-1)}]\,, \quad i = 2,3,\ldots$$

Defining the set $\Lambda := \{1\}$, we have

$$\sigma_{m_i}(\boldsymbol{G}_i) = \sigma_{m_1}(\boldsymbol{G}_1) \uplus \Lambda^{(i-1)} \quad \text{for all} \quad i \in \mathbb{N}\,.$$

In conclusion, $\mathfrak{G}$ is a Λ-spectral family of graphs.

Example 5.2.7. Consider $\mathfrak{G}' = \{\boldsymbol{G}'_i\}$ the family of MW-graphs, where $\boldsymbol{G}'_i = (G'_i, 0, \deg)$ and G'_i are the star graphs given in Figure 5.4. Let $i = 1,2,3,\ldots$, then for each star G_i, we will distinguish i roots vertices corresponding to the degree one vertices and colour them in red.

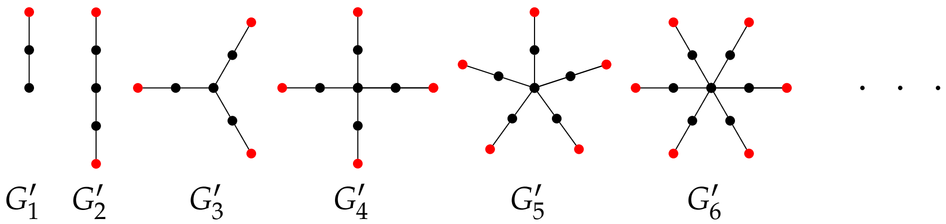


FIGURE 5.4: The family of MW-graphs $\mathfrak{G}' = \{\boldsymbol{G}'_i\}$, where $\boldsymbol{G}'_i = (G'_i, 0, \deg)$ and G'_i are the rooted family of star graphs in the figure.

It is straightforward to show that the spectrum of this family of MW-graphs are the following:

$$\sigma_{m_1}(\boldsymbol{G}'_1) = [0,1,2]\,, \quad \text{and}$$
$$\sigma_{m_i}(\boldsymbol{G}'_i) = \left[0, \left(1 - \frac{1}{\sqrt{2}}\right)^{(i-1)}, 1, \left(1 + \frac{1}{\sqrt{2}}\right)^{(i-1)}, 2\right]$$
$$= [0,1,2] \uplus \left[\left(1 - \frac{1}{\sqrt{2}}\right)^{(i-1)}, \left(1 + \frac{1}{\sqrt{2}}\right)^{(i-1)}\right], \qquad \text{for all} \quad i = 2,3,\ldots$$

Therefore, if we define the set $\Lambda := \left\{1 - \frac{1}{\sqrt{2}}, 1 + \frac{1}{\sqrt{2}}\right\}$, then

$$\sigma_{m_i}(\boldsymbol{G}'_i) = \sigma_{m_1}(\boldsymbol{G}'_1) \uplus \Lambda_1^{(i-1)} \quad \text{for all} \quad i \in \mathbb{N}$$

hence, the family $\mathfrak{G}'$ is Λ-spectral.

Consider A and B two s-partitions of r, defining the disjoint union of graphs as in Eq. (5.2.2) for each partition. The following result shows that if $\mathfrak{G}$ is Λ-spectral, then the graphs constructed are isospectral. This is the first step towards the proof of the main result.

Lemma 5.2.8. *Let $\mathfrak{G} := \{ \boldsymbol{G}_i \,|\, i \in \mathbb{N} \}$ be a discrete family of magnetic graphs and $\Lambda \subset \mathbb{R}_+$ a finite set. Consider $r \in \mathbb{N}$ and A and B two s-partitions of r.*

If $\mathfrak{G}$ is Λ-spectral *and define*

$$\mathfrak{G}(A) := \dot{\bigcup_{i \in A}} \boldsymbol{G}_i \,, \quad \mathfrak{G}(B) := \dot{\bigcup_{i \in B}} \boldsymbol{G}_i \,,$$

then the MW*-graphs $\mathfrak{G}(A)$ and $\mathfrak{G}(B)$ are isospectral.*

Proof. The family $\mathfrak{G}(A)$ is the disjoint union of some MW-graphs, and their corresponding Laplacians decompose as a direct sum of Laplacians of each $\boldsymbol{G}_i$ and, therefore

$$\begin{aligned}
\sigma_m(\mathfrak{G}(A)) = \sigma_m(\dot{\bigcup_{j \in A}} \boldsymbol{G}_j) &= \biguplus_{j \in A} \sigma_{m_j}\left(\boldsymbol{G}_j\right) \\
&= \biguplus_{j \in A} \left(\sigma_{m_1}(\boldsymbol{G}_1) \uplus \Lambda^{(i-1)}\right) \\
&= \left(\sigma_{m_1}(\boldsymbol{G}_1)\right)^{(s)} \uplus \Lambda^{(r-s)} \,, \qquad (5.2.4)
\end{aligned}$$

where for the last equation, we have used the elementary properties of multisets mentioned before. Now, since the last equation only depends on the s-partition, then we can repeat the computation for the MW-graph $\mathfrak{G}(B)$, and we obtain

$$\sigma_m(\mathfrak{G}(B)) = \biguplus_{j \in B} \left(\sigma_{m_1}(\boldsymbol{G}_1) \uplus \Lambda^{(i-1)}\right) = \left(\sigma_{m_1}(\boldsymbol{G}_1)\right)^{(s)} \uplus \Lambda^{(r-s)} \,.$$

Both equations show that both MW-graphs are isospectral. □

Remark 5.2.9. Note that the proof of the previous result, already allows counting the number of eigenvalues of magnetic Laplacian associated with the graph $\mathfrak{G}(A)$:

$$|\sigma_m(\mathfrak{G}(A))| = |\mathfrak{G}(A)| = s|\boldsymbol{G}_1| + (r-s)|\Lambda| \,. \qquad (5.2.5)$$

The second important notion for the construction of isospectral graphs is based on the geometric preorder $\sqsubseteq$ introduced in Definition 2.1.1 of Section 2.1.

Definition 5.2.10. Let $\mathfrak{G} = \{ \boldsymbol{G}_i \,|\, i \in \mathbb{N} \}$ be a countable family of magnetic graphs. We say that $\mathfrak{G}$ is *geometric* if there exists a family of magnetic weighted graphs $\mathfrak{G}' = \{ \boldsymbol{G}'_i \,|\, i \in \mathbb{N} \}$ with the following properties: for any $s, r \in \mathbb{N}$ with $s \le r$ and for any s-partition A of r, there is an equivalence relation $\approx_A$ on the vertex set $V(\boldsymbol{G}'_r)$ and an MW-homomorphism from $\mathfrak{G}(A) = \dot{\bigcup_{i \in A}}(\boldsymbol{G}_i)$ into the quotient graph, i.e., $\mathfrak{G}(A)$ is geometrically smaller than the quotient

$$\mathfrak{G}(A) \sqsubseteq \boldsymbol{G}'_r/{\approx_A}$$

with $|\boldsymbol{G}'_r| - |\mathfrak{G}(A)| = r - s$.

If, in addition, the family $\mathfrak{G}'$ is also Λ-*spectral* for some finite set $\Lambda \subset \mathbb{R}_+$, we say that $\mathfrak{G}$ is Λ-*geometric*.

Under the hypothesis of Definition 5.2.10, in particular,

$$\mathfrak{G}(A) \sqsubseteq \boldsymbol{G}'_r/\approx_A$$

and by Proposition 2.1.4 (iii) there exist $\sim_A$ an equivalence relation on $V(\mathfrak{G}(A))$ such that

$$\mathfrak{G}(A,\sim_A) := \mathfrak{G}(A)/\sim_A \cong \boldsymbol{G}'_r/\approx_A ,$$

and $|\mathfrak{G}(A)| - |\mathfrak{G}(A,\sim_A)| = s-1$.

We show next a class of graphs having the property of being Λ-geometric. Again, for simplicity, we will assume that the vector potential fulfils $\alpha = 0$.

Example 5.2.11. Let $\mathfrak{G} = \{\boldsymbol{G}_i\}$ be a family of MW-graphs $\boldsymbol{G}_i = (G_i, 0, \deg)$ where G_i are the rooted diamonds graphs given in Figure 5.1. We will show that $\mathfrak{G}$ is Λ-geometric. For prove it, we use the family of rooted star graphs $\mathfrak{G}' = \{\boldsymbol{G}'_i\}$ defined in Figure 5.4. Let $s, r \in \mathbb{N}$ with $s \le r$ and consider A any s-partition r. We will show that

$$\mathfrak{G}(A) \sqsubseteq \boldsymbol{G}'_r/\approx_A$$

for some $\approx_A$ in $V(\boldsymbol{G}'_r)$ with $|\boldsymbol{G}'_r| - |\mathfrak{G}(A)| = r - s$. Observe that the vertices of the stars $V(G'_r)$ contain r pendant vertices (with degree 1) which we have distinguished as roots and marked with red in Figure 5.4. Numerate the set the roots as $V_0 = \{v_1, v_2, \ldots, v_r\}$. Based on the partition $A = [a_1, a_2, \ldots, a_s]$ we construct a partition the set of roots V_0 into s disjoint sets

$$V_k := \{\, v \in V_0 \,|\, v = v_{a_{k-1}+1}, v_{a_{k-1}+2}, \ldots, v_{a_{k-1}+a_k} \,\} , \qquad \text{for all} \qquad 1 \le k \le s$$

with the convention that $a_0 = 0$. Let $\approx_A$ be the equivalence relation on $V(\boldsymbol{G}'_r)$ that glues all the vertices of the set V_k into a single one denoted as $[v_k]$. Since

$$\mathfrak{G}(A) \sqsubseteq \boldsymbol{G}'_r/\approx_A ,$$

we define the MW-graph homomorphism $\varphi\colon \mathfrak{G}(A) \to \boldsymbol{G}'_r/\approx_A$ that takes each green vertex of G_k into the vertex $[v_k]$ for all $1 \le k \le s$. Note that the quotient graph $\boldsymbol{G}'_r/\approx_A$ has order $|\boldsymbol{G}'_r| - |\mathfrak{G}(A)| = r - s$. Moreover, the Example 5.2.6 shows that $\mathfrak{G}'$ is Λ_2-spectral with $\Lambda_2 = \{1\}$, therefore $\mathfrak{G}$ is Λ_2-geometric. Finally, the equivalence relation $\sim_A$ is just the identification of the green vertices of the family of magnetic graphs in Figure 5.1.

We arrive finally to the main result in this chapter.

Theorem 5.2.12. *Let $\mathfrak{G} = \{\, \boldsymbol{G}_i \,|\, i \in \mathbb{N} \,\}$ be a countable family of magnetic graphs, $\Lambda_1, \Lambda_2 \subset \mathbb{R}_+$ be two disjoint sets satisfying $\Lambda_1 \subset \sigma(\boldsymbol{G}_1)$ and $|\Lambda_2| = |G_1| - 1$. Let $r \in \mathbb{N}$ and A, B are two s-partitions of r.*

If $\mathfrak{G}$ is Λ_1-spectral and Λ_2-geometric, then

$$\mathfrak{G}(A,\sim_A) \quad \textit{and} \quad \mathfrak{G}(B,\sim_B) \quad \textit{are isospectral.}$$

Proof. In this proof, we will count the number of eigenvalues always taking the multiplicities into account. We divide the proof into two steps that exploit the properties of being Λ_1-spectral and Λ_2-geometric.

i) Suppose that A, B are s-partitions of r and $\mathfrak{G}$ is Λ_1-spectral. Then by Eq. (5.2.4) we have

$$\begin{aligned}\sigma_m(\mathfrak{G}(A)) &= \left(\sigma_{m_1}(\boldsymbol{G}_1)\right)^{(s)} \uplus \Lambda_1^{(r-s)} \\ &= \left(\sigma_{m_1}(\boldsymbol{G}_1) \setminus \Lambda_1^{(1)}\right)^{(s)} \uplus \Lambda_1^{(s)} \uplus \Lambda_1^{(r-s)} \\ &= \left(\sigma_{m_1}(\boldsymbol{G}_1) \setminus \Lambda_1^{(1)}\right)^{(s)} \uplus \Lambda_1^{(r)} .\end{aligned}$$

In particular, $\sigma_m(\mathfrak{G}(A))$ has $s|G_1| + |\Lambda_1|(r-s)$ eigenvalues and the equivalence relation $\sim_A$ is such that $|\mathfrak{G}(A)| - |\mathfrak{G}(A)/\sim_A| = s-1$, then by $s-1$ iterative application of the Corollary 2.4.6 we obtain

$$\mathfrak{G}(A) \overset{0}{\lessapprox} \mathfrak{G}(A)/\sim_A \overset{s-1}{\lessapprox} \mathfrak{G}(A) .$$

Then, by Lemma 5.2.4, any eigenvalue λ in the spectrum of the magnetic Laplacian acting on the *MW*-graph $\mathfrak{G}(A)$ with multiplicity k, appears as an eigenvalue λ of the *DML* of the magnetic graph $\mathfrak{G}(A)/\sim_A$ with multiplicity $k-s+1$ (for the case $k \geq s-1$). Therefore, we obtain

$$\begin{aligned}\sigma_m(\mathfrak{G}(A,\sim_A)) &\supset \left(\sigma_{m_1}(\boldsymbol{G}_1) \setminus \Lambda_1^{(1)}\right)^{(s-(s-1))} \uplus \Lambda_1^{(r-(s-1))} \\ &= \left(\sigma_{m_1}(\boldsymbol{G}_1)\right) \uplus \Lambda_1^{(r-s)} .\end{aligned} \tag{5.2.6}$$

Moreover, we know the graph $\mathfrak{G}(A,\sim_A)$ has $|G_1| + (r-s)|\Lambda_1|$ eigenvalues.

ii) Since $\mathfrak{G}$ is also Λ_2-geometric, there exists a family $\mathfrak{G}'$ of MW-graphs with the properties given in Definition 5.2.10, i.e.,

$$\sigma_{m'_r}(\boldsymbol{G}'_r) = \sigma_{m'_1}(\boldsymbol{G}'_1) \uplus \Lambda_2^{(r-1)} ,$$

and, therefore, for the equivalence relation $\approx_A$, we have $|\boldsymbol{G}'_r| - |\boldsymbol{G}'_r/\approx_A| = r-s$. This implies

$$\boldsymbol{G}'_r \overset{0}{\lessapprox} \boldsymbol{G}'_r/\approx_A \overset{r-s}{\lessapprox} \boldsymbol{G}'_r$$

and, by Lemma 5.2.4, it follows that any eigenvalue with a multiplicity $r-1$ in $\boldsymbol{G}'_r$ has multiplicity at least $(r-1)-(r-s)$ in $\boldsymbol{G}'_r/\approx_A$. It follows that

$$\sigma_{m'_r}(\boldsymbol{G}'_r/\approx_A) \supset \Lambda_2^{(r-1-(r-s))} = \Lambda_2^{(s-1)} ,$$

and since $\mathfrak{G}(A)/\sim_A \cong \boldsymbol{G}'_r/\approx_A$, we finally obtain

$$\mathfrak{G}(A)/\sim_A \supset \Lambda_2^{(r-1-(r-s))} = \Lambda_2^{(s-1)} . \tag{5.2.7}$$

Taking into account the inclusions given in Eqs. (5.2.6) and (5.2.7) and since Λ_1 and Λ_2 are disjoint we obtain

$$\sigma_m(\mathfrak{G}(A,\sim_A)) \supset \left(\sigma_{m_1}(\boldsymbol{G}_1)\right) \uplus \Lambda_1^{(r-s)} \uplus \Lambda_2^{(s-1)} . \tag{5.2.8}$$

Hence we have identified $|G_1| + (r-s)|\Lambda_1| + (s-1)|\Lambda_2|$ eigenvalues in the spectrum of the DML associated with $\mathfrak{G}(A,\sim_A)$. By hypothesis $|\Lambda_2| = |G_1| - 1$ and, therefore, we know $|\boldsymbol{G}_1| + (r-s)|\Lambda_1| - (s-1)$ eigenvalues which are precisely the cardinality of $|\sigma_m(\mathfrak{G}(A),\sim_A)|$. This implies that the inclusion in Eq. (5.2.7) is actually an equality.

Finally, observe that the spectrum does not depend on the partition but just on the size s of the partition of r. Therefore we can repeat the process described above for the partition B, and deduce that

$$\mathfrak{G}(A,\sim_A) \quad \text{and} \quad \mathfrak{G}(B,\sim_B) \quad \text{are isospectral,}$$

which concludes the proof. □

The proof of the previous theorem also allows specifying the spectrum of the corresponding graphs explicitly.

Corollary 5.2.13. *Consider $\mathfrak{G}$ and $\Lambda_1, \Lambda_2 \subset \mathbb{R}_+$ with the hypothesis of the preceding theorem. For any pair of s-partitions A, B of the number r, we have*

$$\sigma_m(\mathfrak{G}(A,\sim_A)) = \sigma_m(\mathfrak{G}(B,\sim_B)) = \left(\sigma_{m_1}(\boldsymbol{G}_1)\right) \uplus \Lambda_1^{(r-s)} \uplus \Lambda_2^{(s-1)} .$$

We verify next that the examples constructed before using the rooted diamonds fulfil the conditions of the main theorem.

Example 5.2.14. Let $\mathfrak{G} = \{\boldsymbol{G}_i\}$ be the countable family of rooted diamond graphs without vector potential given in Figure 5.1. In Example 5.2.6, we have proved that $\mathfrak{G}$ is Λ_1-spectral with the set $\Lambda_1 := \{1\}$. Also, in Example 5.2.7 we prove that $\mathfrak{G} = \{\boldsymbol{G}_i\}$ is Λ_2-geometric defined by the set $\Lambda_2 := \left\{1 - \dfrac{1}{\sqrt{2}}, 1 + \dfrac{1}{\sqrt{2}}\right\}$.

If A and B are two s-partition of the number r and $\sim_A$ and $\sim_B$ is just the identification of the green vertices of the family $\mathfrak{G}(A)$ and $\mathfrak{G}(B)$ of magnetic graphs in Figure 5.1, then by Theorem 5.2.12, we conclude that $\mathfrak{G}(A,\sim_A)$ and $\mathfrak{G}(B,\sim_B)$ are isospectral. In particular, he MW-graphs $\boldsymbol{G}(A_i)$ given by the 4-partition of the number 8 showed in Figure 5.3 are isospectral.

In the following example, we show how an infinite number of families of the class $\mathscr{G}$ also fulfil the hypothesis of Theorem 5.2.12.

Example 5.2.15. Fix $n \in \mathbb{N}$, and consider the countable family of MW-graphs $\mathfrak{G}_n = \{\boldsymbol{G}_i\}$ of n-diamond graphs. The case $n = 2$ is in Figure 5.1 and the case $n = 3$ is in Figure 5.5. More precisely, consider $\boldsymbol{G}_i = (G_i, 0, \deg)$ and G_i is the n-diamond graphs, i.e., G_i is the graph obtained by the identification of all the pendant vertices of the (i,n)-star (see Subsection 1.1.1 and Figure 1.3) into one vertex, then we obtain families of n-diamond graphs. Then

$$\sigma_{m_1}(\boldsymbol{G}_1) = \left[1 - \cos\left(\frac{\pi k}{n-1}\right)\right]_{k=0}^{n-1} \quad \text{and}$$
$$\sigma_{m_i}(\boldsymbol{G}_i) = \sigma_{m_1}(\boldsymbol{G}_1) \uplus \left(\left[1 - \cos\left(\frac{\pi k}{n-1}\right)\right]_{k=1}^{n-2}\right)^{(i-1)} .$$

Therefore, if we define the set

$$\Lambda_n = \left\{1 - \cos\left(\frac{\pi k}{n-1}\right)\right\}_{k=1}^{n-2},$$

then

$$\sigma_{m_i}(\boldsymbol{G}_i) = \sigma_{m_1}(\boldsymbol{G}_1) \uplus \Lambda_n^{(i-1)} \quad \text{for all} \quad i \in \mathbb{N} .$$

In conclusion, and by Definition 5.2.5, we have showed that the family of MW-graphs $\mathfrak{G}_n$ is Λ_n-spectral.

Now, for the fixed $n \in \mathbb{N}$, consider $\mathfrak{G}'_n = \{\boldsymbol{G}'_i\}$ be a countable family of magnetic graphs, where $\boldsymbol{G}'_i = (G'_i, 0, \deg)$ and G_i is the (i,n)-star (see Subsection 1.1.1 and Figure 1.3), then:

$$\sigma_{m_1}(\boldsymbol{G}'_1) = \left[1 - \cos\left(\frac{\pi k}{2n-2}\right)\right]_{k=0}^{2n-2} \quad \text{and}$$
$$\sigma_{m_i}(\boldsymbol{G}'_i) = \left[1 - \cos\left(\frac{\pi k}{n-1}\right)\right]_{k=1}^{n-2} \uplus \left(\left[1 - \cos\left(\frac{\pi k}{n-1}\right)\right]_{k=1, k \text{ is odd}}^{2n-1}\right)^{(i-1)} .$$

Therefore, if we define

$$\Lambda_2 = \left\{1 - \cos\left(\frac{\pi k}{n-1}\right)\right\}_{k=1, k \text{ is odd}}^{2n-1} .$$

then, by Definition 5.2.10, we conclude that $\mathfrak{G}'_n$ is Λ_2-geometric

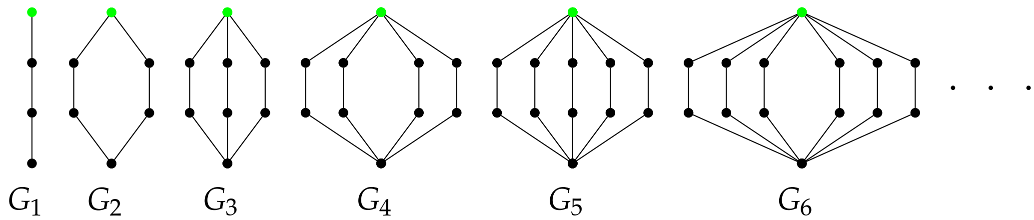


FIGURE 5.5: The family of diamond graphs G_i for $i \in \mathbb{N}$. Each graph G_i has a root vertex (in green).

As in Example 5.2.14, we can construct isospectral graphs because the family $\mathfrak{G}_n$ defined in this example fulfil the condition in Theorem 5.2.12 for each $n \in \mathbb{N}$. An example for isospectral graphs (mutually non-isomorphic) for $n = 3$ and for several partitions of the number 8 is showed in Figure 5.6.

To show that the MW-graphs $\boldsymbol{G}(A_i)$ in Figure 5.6 are non-isomorphic, we use their degree sequence presented in the following table:

Graph	Degree sequence
$\boldsymbol{G}(A_1)$	$(\mathbf{1},\mathbf{1},\mathbf{1},2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,\mathbf{5},8)$
$\boldsymbol{G}(A_2)$	$(\mathbf{1},\mathbf{1},2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,\mathbf{2},\mathbf{4},8)$
$\boldsymbol{G}(A_3)$	$(\mathbf{1},\mathbf{1},2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,\mathbf{3},\mathbf{3},8)$
$\boldsymbol{G}(A_4)$	$(\mathbf{1},2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,\mathbf{2},\mathbf{2},\mathbf{3},8)$
$\boldsymbol{G}(A_5)$	$(2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},8)$

Each degree sequence is different, then the MW-graphs $\boldsymbol{G}(A_i)$ are non-isomorphic. Observe that each partition A_i is contained in its degree sequence (the bold numbers).

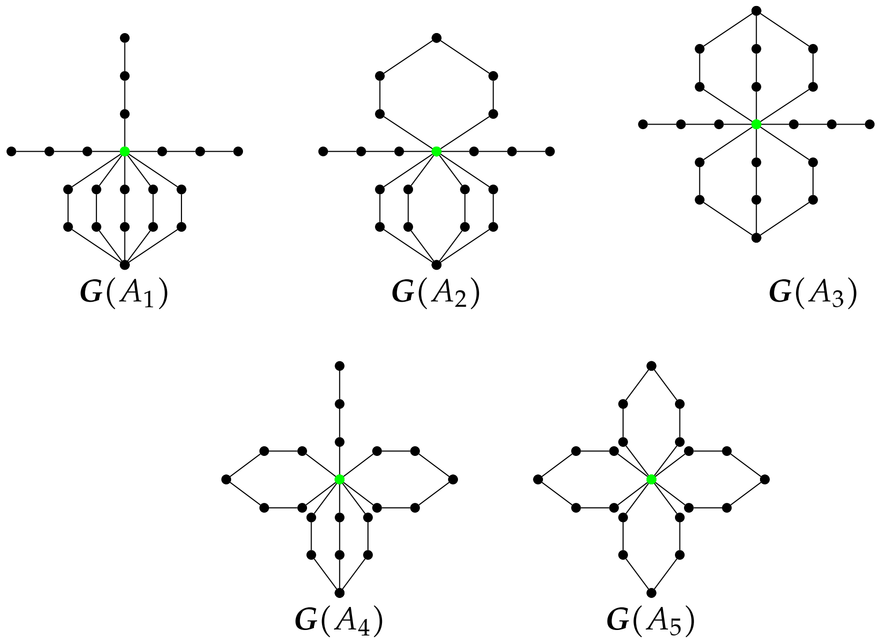


FIGURE 5.6: The graphs $\boldsymbol{G}(A_i)$ are isospectral for all partition A_i, where $A_1 = [1,1,1,5]$, $A_2 = [1,1,2,4]$, $A_3 = [1,1,3,3]$, $A_4 = [1,2,2,3]$ and $A_5 = [2,2,2,2]$.

5.3 Examples of isospectral graphs with magnetic potentials

For simplicity and to illustrate more clearly the geometric method we have considered examples with a zero magnetic potential acting on it. However, the principle described in the previous section can also be applied to graphs with a non-trivial magnetic potential. We present next a class of examples of non-isomorphic graphs with non trivial magnetic potential whose DMLs have the same spectrum. These examples show how universal the geometric procedure is.

Example 5.3.1. Fix $t \in [0,2\pi]$ and consider the countable family of magnetic weighted graphs $\mathfrak{G}_t = \{\boldsymbol{G}_i \mid i \in \mathbb{N}\} \subset \mathscr{G}_{\deg}$ (cf. Notation 1.4.2), where $\boldsymbol{G}_i = (G_i, \alpha_i^t, \deg_{G_i})$ is a magnetic graph defined by the graph G_i, this graph is a decorated diamond graph showed in Figure 5.7 and considered with the standard weights and the magnetic potential defined as $(\alpha_i^t)_e = t$ and $(\alpha_i^t)_{\overline{e}} = -t$ if e is a loop and 0 otherwise.

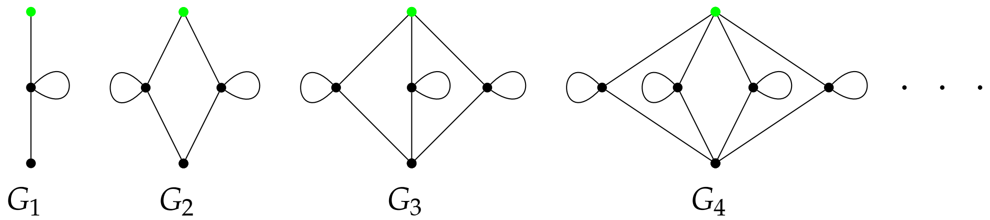


FIGURE 5.7: The family of decorated diamond graphs G_i for all $i \in \mathbb{N}$. Each graph G_i has a root vertex (in green).

It can be shown that the family $\mathfrak{G}_t$ of decorated diamond graphs is Λ-spectral where

$$\Lambda = \left\{1 - \frac{\cos(t)}{2}\right\},$$

and also the family $\mathfrak{G}_t$ is Λ'-geometrical for the set

$$\Lambda' = \left\{1 - \frac{\cos(t)}{4} - a, 1 - \frac{\cos(t)}{4} + a\right\}$$

with $a = \dfrac{\sqrt{\cos(2t) + 17}}{4\sqrt{2}}$. By Theorem 5.2.12 and proceeding as in Example 5.2.14, we can show that the two graphs in Figure 5.8 are isospectral for any magnetic potential α_i^t with $t \in [0, 2\pi]$ defined previously. Then, clearly non-isomorphic graphs, because $\boldsymbol{G}(A)$ has a pendant vertex and $\boldsymbol{G}(B)$ has not.

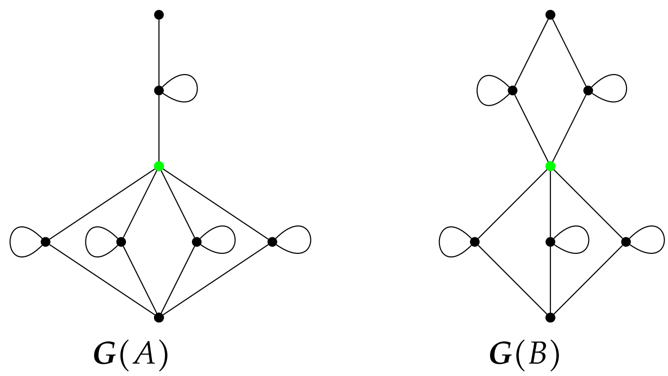


FIGURE 5.8: The graphs $\boldsymbol{G}(A)$ and $\boldsymbol{G}(B)$ are isospectral (non-isomorphic) graphs with non trivial magnetic potential.

Finally, in Figure 5.9, we show in the vertical axis the six (different) eigenvalues of the MW-graphs $\boldsymbol{G}(A)$ and $\boldsymbol{G}(B)$ for all the values $t \in [0, 2\pi]$ represented in the horizontal axis.

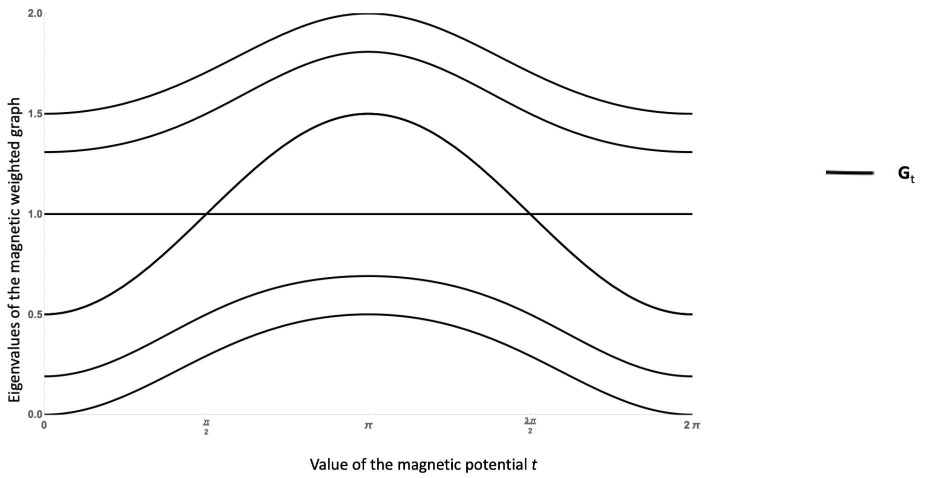


FIGURE 5.9: This figure shows the spectrum of the isospectral graphs for all the values $t \in [0, 2\pi]$.

6 Miscellaneous Applications

In his chapter, we present a large variety of applications of the different relations and preorder on the magnetic weighted graphs developed in Chapter 2. One of the most important applications is in chemical graph theory [Bal76; Tri92], where the graph theory is a useful tool because a graph is a mathematical object to represent a molecule (vertices) and the bonds between them (edges). One element of the chemical graph theory is the study of the *chemical index* (as the Estrada index or quasi-Wiener index), this is a number related to the chemical properties of the molecule, as the energy or boiling point, see, e.g., [Ayy+11; Aza15; Fis+02; GM96; Gut+09] and the reference therein.

In Section 6.1, we study some composite operation as edge contraction (Subsection 6.1.1) or delete a vertex (Subsection 6.1.2). For this, we use the results in Section 2.4, in particular, the spectrum of the magnetic Laplacian under two basic operation: delete an edge (Theorem 2.4.1) and contracting two vertices Theorem 2.4.5.

Also, we apply our results to study certain combinatorial aspects of graphs (Section 6.2), to prove how Cheeger's constant change under MW-homomorphisms (Subsection 6.2.1) and to study the stability of eigenvalues under perturbation of graphs with high multiplicity; Our results are also useful in order to show the monotony of indexes in chemical graph theory under elementary operation on the graphs (Section 6.3). These indexes (e.g., the magnetic quasi-Wiener index or the Estrada index) describe important physical and chemical properties of the molecules modelled by the graph.

6.1 Composite operations

6.1.1 Edge contraction

The modification of the graph called *contracting an edge* is just the composition of the two operations: deleting an edge e_0 (and its inverse $\overline{e_0}$), and contracting the adjacent vertices (note that the order of the operations does not matter). Formally, let G be a graph, an *edge contraction* of G is the graph G' where $G' = (G - e_0)/\{\partial^+ e_0, \partial^- e_0\} = G/\{\partial^+ e_0, \partial^- e_0\} - e_0$ for some edge $e_0 \in E(G)$ (see Subsection 2.4.1). We shortly write $G' = G/\{e_0\}$.

An example of a graph G is showed in Fig. 6.1A, and the contraction of the edge e_0 is in showed in Fig. 6.1B.

Let $\boldsymbol{G} = (G, \alpha, w)$ and $\boldsymbol{G}' = (G', \alpha', w')$ be two *MW*-graphs, where $G' = G/\{e_0\}$ for some $e_0 \in E(G)$ and $\alpha_e = \alpha'_e$ for all edge $e \in E(G - e_0)$. We say that $\boldsymbol{G}'$ is the edge e_0 contraction from $\boldsymbol{G}$ and we denote as $\boldsymbol{G}' = \boldsymbol{G}/\{e_0\}$. For the standard and combinatorial weights, we have the following corollary.

Corollary 6.1.1. *Let $\boldsymbol{G}$ and $\boldsymbol{G}'$ be two* MW*-graphs with $\boldsymbol{G}' = \boldsymbol{G}/\{e_0\}$.*

(i) If $\boldsymbol{G}, \boldsymbol{G}' \in \mathcal{G}_{\deg}$, then $\boldsymbol{G} \overset{1}{\preccurlyeq} \boldsymbol{G}' \overset{2}{\preccurlyeq} \boldsymbol{G}$. Moreover, if e_0 is a cut edge, then $\boldsymbol{G} \preccurlyeq \boldsymbol{G}' \overset{1}{\preccurlyeq} \boldsymbol{G}$

(ii) If $\boldsymbol{G}, \boldsymbol{G}' \in \mathcal{G}_{\mathbb{1}}$, then $\boldsymbol{G} \overset{1}{\preccurlyeq} \boldsymbol{G}' \overset{r+1}{\preccurlyeq} \boldsymbol{G}$ where $r = \min\{\partial^+ e_0, \partial^- e_0\}$. Moreover, if e_0 is a cut edge, then $\boldsymbol{G} \preccurlyeq \boldsymbol{G}'$.

Proof. Let $\boldsymbol{G} = (G, \alpha, w)$ and $\boldsymbol{G}' = (G', \alpha', w')$ be two *MW*-graphs where $G' = G/\{e_0\}$ for some $e_0 \in E(\boldsymbol{G})$ such that $\partial(e) = (v_1, v_2)$ and $\alpha_e = \alpha'_e$ for all edge in $E(G - e_0)$. We define some auxiliary *MW*-graphs related with $\boldsymbol{G} = (G, \alpha, w)$: $\boldsymbol{G}_0$, $\boldsymbol{G}_1$ and $\boldsymbol{G}_2$ giving by the same graph G and weights w, but that differed only by the magnetic potential acting on G, i.e., let $\boldsymbol{G}_0 = \boldsymbol{G}$, $\boldsymbol{G}_1 = (G, \alpha_1, w)$ and $\boldsymbol{G}_2 = (G, \alpha_2, w)$, where $(\alpha_1)_{e_0} = (\alpha_1)_{\overline{e_0}} = 0$, $(\alpha_2)_{e_0} = \pi$, $(\alpha_2)_{\overline{e_0}} = -\pi$ and $(\alpha_1)_e = (\alpha_2)_e = \alpha_e$ for all $e \neq e_0, \overline{e_0} \in E(G)$. If e_0 is a cut edge from the graph G, by Lemma 1.3.3 it follows that $\alpha \sim \alpha_1 \sim \alpha_2$ and hence $\sigma(\boldsymbol{G}_0) = \sigma(\boldsymbol{G}_1) = \sigma(\boldsymbol{G}_2)$. Define also the auxiliary *MW*-graphs $\boldsymbol{G}''_i = (G'', \alpha''_i, w'')$ for $i \in \{0, 1, 2\}$, determined by the graph $G''_i = G/\{v_1, v_2\}$, $w''_e = w_e$ for all edge $e \in E(G)$ and $\alpha''_i = \alpha_i$.

(i) Suppose that $\boldsymbol{G}, \boldsymbol{G}' \in \mathcal{G}_{\deg}$. Consider $\boldsymbol{G}''_i \in \mathcal{G}_{\deg}$ where $\boldsymbol{G}''_i = \boldsymbol{G}_i/\{\partial_- e_0, \partial_+ e_0\}$ for $i \in \{0, 1, 2\}$; then we conclude

$$\boldsymbol{G} \preccurlyeq \boldsymbol{G}''_i \overset{1}{\preccurlyeq} \boldsymbol{G} \qquad \text{for } i \in \{0, 1, 2\}\,, \tag{6.1.1}$$

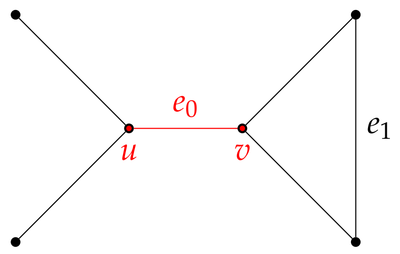
by Corollary 2.4.6 (i). Since $\boldsymbol{G}' = \boldsymbol{G}''_i - e_0$ for $i \in \{0, 1, 2\}$, we have by Corollary 2.4.2 (i)

$$\boldsymbol{G}''_i \overset{1}{\preccurlyeq} \boldsymbol{G}' \overset{1}{\preccurlyeq} \boldsymbol{G}''_i \qquad \text{for } i \in \{0, 1, 2\}\,. \tag{6.1.2}$$

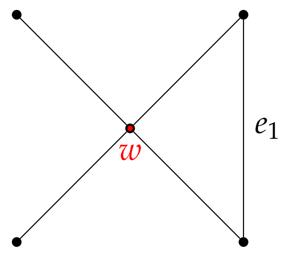
Moreover, Eq. (6.1.1) and Eq. (6.1.2) together with the transitivity in Lemma 2.2.3 (iii) then imply $\boldsymbol{G} \overset{1}{\preccurlyeq} \boldsymbol{G}' \overset{2}{\preccurlyeq} \boldsymbol{G}$.

If e_0 is a cut edge, we conclude $\boldsymbol{G}' \preccurlyeq \boldsymbol{G}''_1$ and $\boldsymbol{G}''_2 \preccurlyeq \boldsymbol{G}'$ from Corollary 2.4.2 (i). Together with Eq. (6.1.1) and by the transitivity in Lemma 2.2.3 (iii) we finally have $\boldsymbol{G} \preccurlyeq \boldsymbol{G}' \overset{1}{\preccurlyeq} \boldsymbol{G}$.

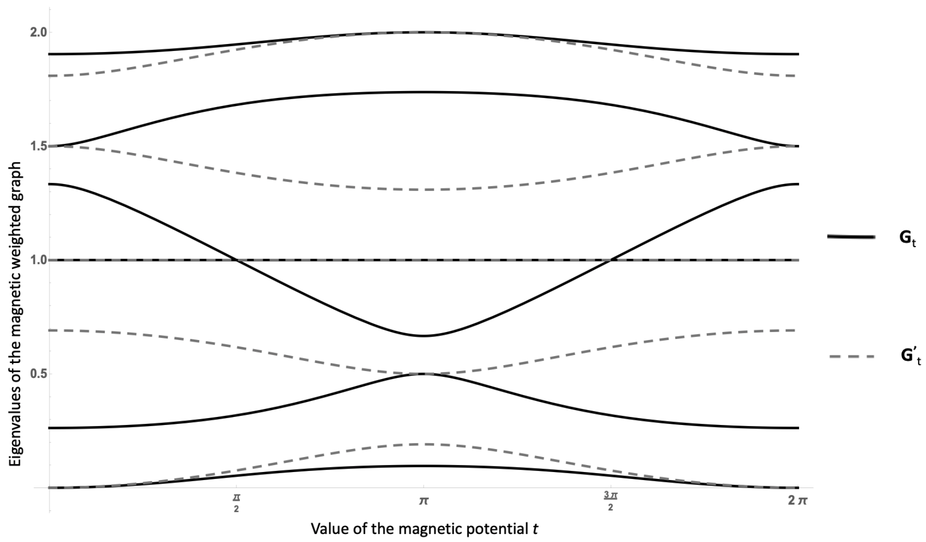
(ii) Suppose that $\boldsymbol{G}, \boldsymbol{G}' \in \mathcal{G}_{\mathbb{1}}$. Consider $\boldsymbol{G}''_i \in \mathcal{G}_{\mathbb{1}}$ with $\boldsymbol{G}''_i = \boldsymbol{G}_i/\{\partial_- e_0, \partial_+ e_0\}$ for $i = 0, 1$. By Corollary 2.4.6 (ii) it follows that $\boldsymbol{G} \preccurlyeq \boldsymbol{G}''_i \overset{r+1}{\preccurlyeq} \boldsymbol{G}$ for $i = 0, 1$ where $r = \min\{\partial^+ e_0, \partial^- e_0\}$. Since $\boldsymbol{G}' = \boldsymbol{G}''_i - e_0$ for $i \in \{0, 1, 2\}$, by Corollary 2.4.2 (ii) that $\boldsymbol{G}''_i \overset{1}{\preccurlyeq} \boldsymbol{G}' \preccurlyeq \boldsymbol{G}''_i$ for $i = 0, 1$. Finally by the transitivity in Lemma 2.2.3 (iii) we conclude $\boldsymbol{G} \overset{1}{\preccurlyeq} \boldsymbol{G}' \overset{r+1}{\preccurlyeq} \boldsymbol{G}$. If e_0 is a cut edge, similar to (i) we have $\boldsymbol{G} \preccurlyeq \boldsymbol{G}'$. □



(A) Graph G.



(B) Graph $G' = G/\{e_0\}$.



(C) The spectrum of G and G' with magnetic potential.

FIGURE 6.1: If we contract the edge e_0 of the graph G in Fig. 6.1A, we obtain the graph $G' = G/\{e_0\}$ as in Fig. 6.1B. Let $t \in [0, 2\pi]$ and $\boldsymbol{G}_t, \boldsymbol{G}'_t \in \mathscr{G}_{\text{deg}}$ the corresponding magnetic weighted graphs, then $\sigma(\boldsymbol{G}_t)$ (respectively, $\sigma(\boldsymbol{G}'_t)$) as solid (respectively, dashed) lines are plotted in Fig. 6.1C for all $t \in [0, 2\pi]$. Here, we have $\boldsymbol{G}_t \preccurlyeq \boldsymbol{G}'_t \overset{1}{\preccurlyeq} \boldsymbol{G}_t$, and one can see this classical interlacing by the fact that the solid and dashed lines do not intersect, and solid and dashed lines alternate. Note that the horizontal eigenvalue (independent of t) is an eigenvalue for both graphs.

In particular, if e_0 is a pendant edge, the relation in (ii) is $\boldsymbol{G} \overset{1}{\preccurlyeq} \boldsymbol{G}' \overset{2}{\preccurlyeq} \boldsymbol{G}$ because of $r = 1$. We show an example to illustrate the Corollary 6.1.1.

Example 6.1.2. For any $t \in [0, 2\pi]$, consider the magnetic weighted graph $\boldsymbol{G}_t = (G, \alpha^t, \mathbb{1})$. The graph G is in Figure 6.1A. The magnetic potential α^t is defined as follow: $\alpha^t_{e_1} = t$, $\alpha^t_{\overline{e_1}} = -t$ and zero in all the other edges. Thus, $\sigma(\boldsymbol{G}_t)$ consists of six eigenvalues that depend on the value of t. The spectrum $\sigma(\boldsymbol{G}_t)$ is plotted as a solid line in Figure 6.1C for all $t \in [0, 2\pi]$. If we consider $\boldsymbol{G}'_t = (G', \alpha^t_1, \mathbb{1})$ where $G' = G/\{e_0\}$ (see Figure 6.1B) and $\alpha^t_1 = \alpha^t \restriction_{E(G')}$. The spectrum $\sigma(\boldsymbol{G}'_t)$ consists of five eigenvalues (dashed lines in Figure 6.1C). Since e_0 is a cut edge, we see graphically the interlacing given by Corollary 6.1.1 (the solid and dashed line alternate); i.e. $\boldsymbol{G}_t \preccurlyeq \boldsymbol{G}'_t \overset{1}{\preccurlyeq} \boldsymbol{G}_t$ for any $t \in [0, 2\pi]$.

6.1.2 Delete a vertex

Let G be a graph and $v_0 \in V(G)$, the graph $G - v_0$ is obtained by *deleting the vertex* v_0 and together with all the edges adjacent to v_0. Let $\boldsymbol{G} = (G, \alpha, w)$ and $\boldsymbol{G}' = (G', \alpha', w')$ be two *MW*-graphs, where $G' = G - v_0$ for some $v_0 \in V(G)$ and $\alpha_e = \alpha'_e$ for all edge $e \in E(G')$. We say that $\boldsymbol{G}'$ is the vertex v_0 deletion from $\boldsymbol{G}$ and we denote as $\boldsymbol{G}' = \boldsymbol{G} - v_0$. For the standard and combinatorial weights, we have the following corollary.

Corollary 6.1.3. *Let $\boldsymbol{G}, \boldsymbol{G}'$ be two* MW*-graphs where $\boldsymbol{G}' = \boldsymbol{G} - v_0$. If $r = \deg(v_0)$, then*

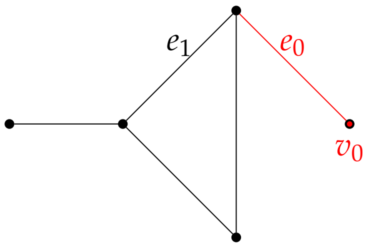
(i) Let $\boldsymbol{G}, \boldsymbol{G}' \in \mathscr{G}_{\deg}$, then $\boldsymbol{G} \overset{r-1}{\preccurlyeq} \boldsymbol{G}' \overset{r}{\preccurlyeq} \boldsymbol{G}$.

(ii) Let $\boldsymbol{G}, \boldsymbol{G}' \in \mathscr{G}_{\mathbb{1}}$, then $\boldsymbol{G} \overset{r-1}{\preccurlyeq} \boldsymbol{G}' \overset{1}{\preccurlyeq} \boldsymbol{G}$.

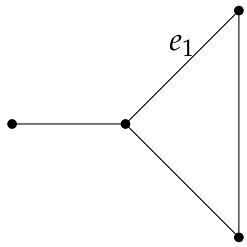
Proof. First, delete $r - 1$ edges of v_0 and apply Corollary 2.4.2, then v_0 is a pendant vertex, and delete v_0 is equivalent to contract the pendant edge, then apply Corollary 6.1.1. Finally, with the transitivity in Lemma 2.2.3 (iii) the result follows. □

In particular, if v_0 is a pendant vertex, the relation in (i) is $\boldsymbol{G} \preccurlyeq \boldsymbol{G}' \overset{1}{\preccurlyeq} \boldsymbol{G}$ because $r = 1$ and similarly the relation in (ii) is $\boldsymbol{G} \preccurlyeq \boldsymbol{G}' \overset{1}{\preccurlyeq} \boldsymbol{G}$. We show an example to illustrate the Corollary 6.1.3.

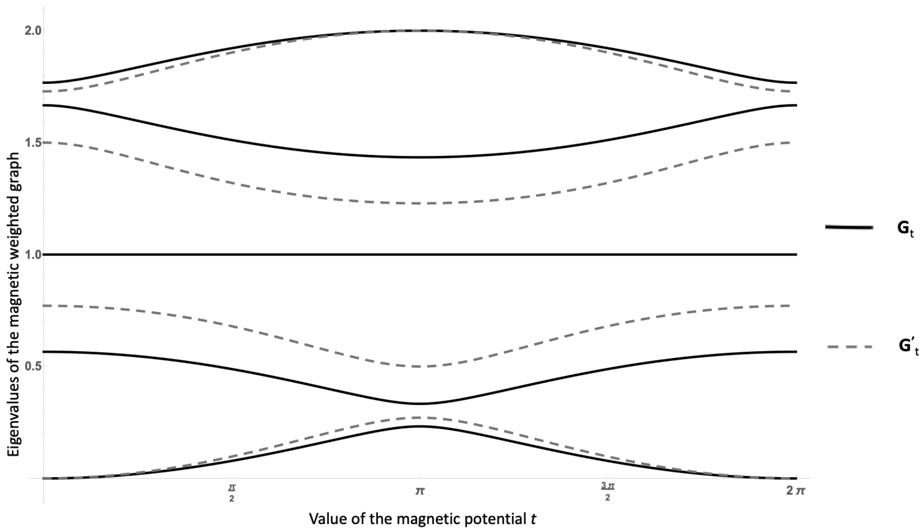
Example 6.1.4. For all $t \in [0, 2\pi]$, consider the magnetic weighted graph $\boldsymbol{G}_t = (G, \alpha^t, \mathbb{1})$. The graph G is in Figure 6.2A. The magnetic potential α^t is defined as follow: $\alpha^t_{e_1} = t$, $\alpha^t_{\overline{e_1}} = -t$ and zero in all the other edges. Thus, $\sigma(\boldsymbol{G}_t)$ consists of five eigenvalues that depend on the value of t. The spectrum $\sigma(\boldsymbol{G}_t)$ is plotted as a solid line in Figure 6.2C for all $t \in [0, 2\pi]$. If we consider $\boldsymbol{G}'_t = (G', \alpha^t_1, \mathbb{1})$ where $G' = G - v_0$ (see Figure 6.2B). and $\alpha^t_1 = \alpha^t \restriction_{E(G')}$. The spectrum $\sigma(\boldsymbol{G}'_t)$ consists of four eigenvalues (dashed lines in Figure 6.2C). Since v_0 is a pendant vertex, we see graphically the interlacing given by Corollary 6.1.3 (the solid and dashed line alternate); i.e. $\boldsymbol{G}_t \preccurlyeq \boldsymbol{G}'_t \overset{1}{\preccurlyeq} \boldsymbol{G}_t$ for any $t \in [0, 2\pi]$. This interlacing property for the combinatorial weights is only true for pendant vertex and not for vertex with degree greater than 1.



(A) The graph G.



(B) $G' = G - v_0$.



(C) The spectrum of G and G' with magnetic potential.

FIGURE 6.2: The graph G with v_0 a pendant vertex (Fig. 6.2A). If we delete the vertex v_0, we obtain the graph $G' = G - v_0$ in Fig. 6.2B. For any $t \in [0, 2\pi]$, consider the MW-graphs $\boldsymbol{G}_t, \boldsymbol{G}'_t$ defined by G (respectively, G'). In 6.2C, we plot $\sigma(\boldsymbol{G}_t)$ (respectively, $\sigma(\boldsymbol{G}'_t)$) in solid (respectively, dashed) line for all $t \in [0, 2\pi]$.

6.2 Spectral graph theory and combinatorics

(a) **(Spectral order of graphs)** We begin mentioning some natural interaction between the spectral preorder relations $\sqsubseteq$ (Section 2.1) and $\preccurlyeq$ (Section 2.2) and combinatorics. First, we apply the geometric perturbation and elementary operations on graphs established in Section 2.4 to present a new spectral order of MW-graphs. We illustrate this in the example of simple graphs up to order 6 and with combinatorial weights.
We have seen in Theorem 2.1.6 that for any fixed value $t \in [0, 2\pi]$ the family $\mathscr{G}_{\mathbb{1}}^t$ (see the notation established in 1.4.2) is partially ordered with respect to $\sqsubseteq$. In particular, the spectral relations below include the cases of the combinatorial Laplacian (if $t = 0$) and the signless Laplacian (if $t = \pi$). In Figure 6.3, we specify the spectral relations of a chain of simple graphs of order up to 6. Note first that $\boldsymbol{G}_i \sqsubseteq \boldsymbol{G}_{i+1}$ for $1 \leq i \leq 7$ is a consequence of Corollary 2.4.2 (ii) and the fact any two consecutive graphs differ by an edge. Moreover, $\boldsymbol{G}_8 \sqsubseteq \boldsymbol{G}_9$ is a consequence of Corollary 2.4.6 (ii) since the graph $\boldsymbol{G}_9$ is obtained from $\boldsymbol{G}_8$ by glueing the upper right vertex with the lower right vertex. Recall also that by Theorem 2.3.3 we directly obtain also the relation $\boldsymbol{G}_i \preccurlyeq \boldsymbol{G}_{i+1}$, $1 \leq i \leq 8$. Finally, note that the $\boldsymbol{G}_9 \sqsubseteq \boldsymbol{G}_{10}$ is false as a consequence of Lemma 2.1.3 since there can not be a homomorphism between $\boldsymbol{G}_9$ and $\boldsymbol{G}_{10}$ which is injective on the edges. Corollary 6.1.3 (ii) gives the relation $\boldsymbol{G}_9 \preccurlyeq \boldsymbol{G}_{10}$ both graphs differ by a pendant vertex.

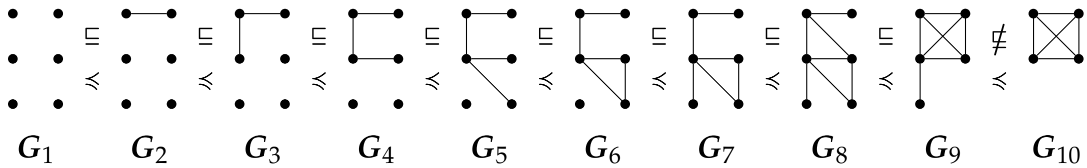


FIGURE 6.3: Example of the order in $\mathscr{G}_{\mathbb{1}}^t$.

(b) **(Minors)** A fundamental notion in combinatorics is that of a graph minor. Several fundamental results in this field are presented in terms of these (e.g. a characterization of the planarity of a graph). A graph H is called a *minor* of a given graph G if H is obtained from G by applying certain elementary operations. We can generalise this construction to MW-graphs and apply the results of the previous sections to give a spectral relation between a graph and its minor. We consider the following three elementary operations:

- Deleting an edge (Subsection 2.4.1),
- Contracting an edge (Subsection 6.1.1),
- Deleting pendant vertex (Subsection 6.1.2).

Let $\boldsymbol{G} \in \mathscr{G}$. If $\boldsymbol{G}' \in \mathscr{G}$ is obtained from $\boldsymbol{G}$ by successive application of the previous operations, then we say that $\boldsymbol{G}'$ is a *minor* of $\boldsymbol{G}$.

Corollary 6.2.1. *Let $\boldsymbol{G} \in \mathscr{G}$ and $\boldsymbol{G}'$ be a minor of $\boldsymbol{G}$ obtained by deleting p edges, contracting q edges and deleting s pendant vertices.*

(i) If $\boldsymbol{G}, \boldsymbol{G}' \in \mathscr{G}_{\deg}$, then $\boldsymbol{G} \overset{p+q}{\preccurlyeq} \boldsymbol{G}' \overset{p+2q+s}{\preccurlyeq} \boldsymbol{G}$.

(ii) If $\boldsymbol{G}, \boldsymbol{G}' \in \mathscr{G}_{\mathbb{1}}$*, then* $\boldsymbol{G} \overset{q}{\preccurlyeq} \boldsymbol{G}' \overset{p+q+r+s}{\preccurlyeq} \boldsymbol{G}$ *where* $r = \sum_{e \in E_0} \min\{\deg \partial^+ e_0, \deg \partial^- e_0\}$ *and* E_0 *is the set of* q *contracting edges.*

(c) **(Cliques and stability of eigenvalues)** Let $G = (V, E)$ be a graph. A d-clique of G is an induced subgraph $G[V_0]$, for some $V_0 \subset V$, isomorphic to the complete graph K_d of order d (see Definition 1.1.2 (ii)). For simplicity, we will denote the d-clique by K_d.

Let G be a graph with n vertices, m edges and k connected components, the first *Betti number* is defined as

$$b_1(G) := m - n + k. \tag{6.2.1}$$

In this item, we consider combinatorial weights and magnetic potential $\alpha = 0$. In the next theorem we will apply the geometric and spectral preorder relations given in Definitions 2.1.1 and 2.2.4 to identify the eigenvalue d in the spectrum of the Laplacian of the graph with a maximal d-clique and to provide a lower bound of its multiplicity.

Theorem 6.2.2. *Let* $\boldsymbol{G} = (G, 0, \mathbb{1})$ *be an* MW*-graph where* $G = (V, E)$ *is a connected graph having* n *vertices,* m *edges and a maximal* d*-clique* ($n \geq d \geq 1$) *and assume* $m \leq \dfrac{(d-1)(d+2)}{2}$*. Then* $d \in \sigma(\boldsymbol{G})$ *with multiplicity at least*

$$\frac{(d-1)(d+2)}{2} - m\,.$$

Proof. The strategy of the proof is to delete suitable edges on the complement of the maximal clique and control the spectral shifts s, t so that we finally obtain relations $\boldsymbol{G} \overset{s}{\preccurlyeq} \mathbf{K}_d \overset{t}{\preccurlyeq} \boldsymbol{G}$ where $\mathbf{K}_d = (K_d, 0, \mathbb{1})$. Then we can exploit the fact that for combinatorial weights the eigenvalue $d \in \sigma(\mathbf{K}_d)$ has high multiplicity, concretely multiplicity $d-1$.

The first Betti numbers of the graphs G and K_d are $b_1(G) := m - n + 1$ and $b_1(K_d) := \dfrac{d(d-1)}{2} - d + 1$ and denote its difference by

$$r := b_1(G) - b_1(K_d) = m - n - \frac{d(d-3)}{2}\,.$$

Denote by $\widetilde{E} := E(G) \setminus E(K_d)$ and let $\widehat{E}$ be a subset of r edges of $\widetilde{E}$ such that no cycles are present in the complement of the clique, i.e. $G - E(K_d) - \widehat{E}$ has no cycles. Construct first the *MW*-graphs $\boldsymbol{G}_1 = (G_1, 0, \mathbb{1})$ defined by the subgraph $G_1 = G - \widehat{E} = (V_1, E_1)$, i.e., $V_1 = V(G)$ and $E_1 = E(K_d) \cup \big(\widetilde{E} \setminus \widehat{E}\big)$. Applying iteratively Corollary 2.4.2 (ii) we obtain

$$\boldsymbol{G} \overset{r}{\preccurlyeq} \boldsymbol{G}_1 \preccurlyeq \boldsymbol{G}\,. \tag{6.2.2}$$

Note that the graph $G_1 - E(K_d)$ is a forest. Therefore, delete next all $n-d$ edges of this forest starting from the leaves and proceeding towards the d-clique K_d. (Note that it is important to control the spectral shift that one deletes only leaves in this process.) Then, applying Corollary 6.1.3 (ii) (observe that each leave is a pendant edge), we obtain

$$\boldsymbol{G}_1 \preccurlyeq \mathbf{K}_d \overset{n-d}{\preccurlyeq} \boldsymbol{G}_1\,.$$

Using the transitivity of the relation $\preccurlyeq$ as well as Eq. (6.2.2) we get finally the relations

$$\boldsymbol{G} \overset{r}{\preccurlyeq} \mathbf{K}_d \overset{n-d}{\preccurlyeq} \boldsymbol{G} \,. \tag{6.2.3}$$

We denote the spectra of the corresponding Laplacians as $\sigma(\boldsymbol{G}) = \{\lambda_1, \ldots, \lambda_n\}$ (again the spectrum is written in ascending order and repeated according to their multiplicities) and $\sigma(\mathbf{K}_d) = \{\mu_1, \ldots, \mu_d\}$, where for the complete graph of order d we have $\mu_1 = 0$ and $\mu_k = d$, $k = 2, \ldots, d$. The relations in Eq. (6.2.3) imply

$$\lambda_k \leq \mu_{k+r} \quad \text{for} \quad 1 \leq k \leq d - r \quad \text{and} \quad \mu_k \leq \lambda_{k+(n-d)} \quad \text{for} \quad 1 \leq k \leq d \,.$$

Note that the relations between the orders of the graphs and the spectral shift needed in Definition 2.2.4 are automatically satisfied in our case since $|E(K_d)| = \dfrac{d(d-1)}{2} \leq m$. Combining the preceding inequalities we obtain

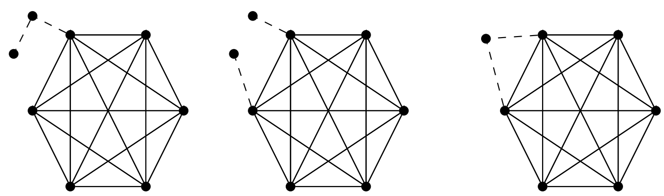
$$d = \mu_k \leq \lambda_{k+n-d} \leq \mu_{k+(n-d)+r} = d \quad \text{for} \quad 2 \leq k \leq 2d - n - r \,,$$

hence d is an eigenvalue of $\boldsymbol{G}$ with multiplicity given by

$$2d - n - r - 1 = \frac{d(d+1)}{2} - m - 1$$

which completes the proof. □

Example 6.2.3. We illustrate the preceding theorem with some examples having combinatorial weights, a vector potential cohomologous to zero ($\alpha = 0$) and a maximal 6-clique as shown in Figure 6.4. Concretely, the graphs G_1, G_2 and G_3 have $m = 17$ edges, $n = 7, 8$ vertices and a maximal 6-clique K_6. The three graphs have the eigenvalue $d = 6$ in its spectrum with multiplicity at least 3.



(A) G_1 (B) G_2 (C) G_3

FIGURE 6.4: An illustration of the Example 6.2.3 for $p = 6$. Let $\boldsymbol{G}_1$, $\boldsymbol{G}_2$ and $\boldsymbol{G}_3$ be MW-graphs (with combinatorial weight and no magnetic potential) defined by the graphs G_1, G_2 and G_3 respectively. The three graphs have $m = 17$ edges, $n = 8$ vertices and K_5 as an induced subgraph; therefore, the three subgraphs has the number 6 in its spectrum with multiplicity at least 3.

6.2.1 Cheeger constants and frustration index

The *Cheeger constant* (also know as *isoperimetric number*) is a quantitative measure of the connectedness of a graph, see, e.g. [Chu97]. Using the so-called *frustration index*, one can also define a Cheeger constant for *magnetic* Laplacians (see, e.g. [Lan+15] and references therein).

We now show that the preorder $\sqsubseteq$ (Section 2.1) in MW-graphs also gives simple inequalities for Cheeger constants. Here, we always denote the underlying graphs of $\boldsymbol{G}$ and $\boldsymbol{G}'$ by $G = (V, E)$ and $G' = (V', E')$.

We first define an ingredient necessary for the magnetic potential:

Definition 6.2.4 (Frustration index)**.** Let $\boldsymbol{G} = (G, \alpha, w)$ be an MW-graph and consider a function $\tau \colon V \to R$, where R is a subgroup of $\mathbb{R}/2\pi\mathbb{Z}$. We set

$$\iota(\boldsymbol{G}, \tau) := \|d_\alpha(\mathrm{e}^{\mathrm{i}\tau})\|_{\ell_1(E,w)} = \sum_{e\in E} w_e|\mathrm{e}^{\mathrm{i}\tau(\partial_+ e)} - \mathrm{e}^{-\mathrm{i}\alpha_e}\mathrm{e}^{\mathrm{i}\tau(\partial_- e)}|.$$

The *frustration index* of $\boldsymbol{G}$ is defined as

$$\iota(\boldsymbol{G}) := \inf_{\tau\in R^V} \iota(\boldsymbol{G}, \tau), \tag{6.2.4}$$

where R^V denotes the set of all maps $\tau \colon V \to R$.

Note that the infimum is actually a minimum. It is not hard to see that $\iota(\boldsymbol{G}) = 0$ if and only if $\alpha \sim 0$, i.e. if the magnetic potential is cohomologous to 0. An MW-graph homomorphism gives a natural inequality for the frustration indices:

Lemma 6.2.5. *Let $\pi \colon \boldsymbol{G} \to \boldsymbol{G}'$ be* MW*-graph homomorphism and let $\tau' \colon V' \to R$ a map, then*

$$\iota(\boldsymbol{G}, \tau' \circ \pi) \le \iota(\boldsymbol{G}', \tau') \qquad \text{and} \qquad \iota(\boldsymbol{G}) \le \iota(\boldsymbol{G}').$$

Proof. Note first that $d_\alpha(\mathrm{e}^{\mathrm{i}\tau'\circ\pi}) = (d_{\alpha'}(\mathrm{e}^{\mathrm{i}\tau'})) \circ \pi$ as π is a graph homomorphism and $\alpha' \circ \pi = \alpha$. Moreover, we have

$$\begin{aligned}
\iota(\boldsymbol{G}, \tau' \circ \pi) &= \sum_{e\in E} w_e \big|(d_\alpha(\mathrm{e}^{\mathrm{i}\tau'\circ\pi}))_e\big| = \sum_{e'\in E'} \sum_{e\in E, \pi(e)=e'} w_e \big|(d_{\alpha'}(\mathrm{e}^{\mathrm{i}\tau'}))_{e'}\big| \\
&= \sum_{e'\in E'} (\pi_* w)_{e'} \big|(d_{\alpha'}(\mathrm{e}^{\mathrm{i}\tau'}))_{e'}\big| \\
&\le \sum_{e'\in E'} w'_{e'} \big|d_{\alpha'}(\mathrm{e}^{\mathrm{i}\tau'})\big| = \iota(\boldsymbol{G}', \tau'),
\end{aligned}$$

as π is MW-graph homomorphism (and in particular, $(\pi_* w)_{e'} \le w'_{e'}$ for all $e' \in E'$). For the last inequality, note that the set R^V of maps $\tau \colon V \to R$ is larger than the subset $\{\, \tau' \circ \pi \,|\, \tau' \in R^{V'} \,\} \subset R^V$; hence we have

$$\iota(\boldsymbol{G}) \le \inf_{\tau'\in R^{V'}} \iota(\boldsymbol{G}, \tau' \circ \pi) \le \inf_{\tau'\in R^{V'}} \iota(\boldsymbol{G}', \tau') = \iota(\boldsymbol{G}'). \qquad \square$$

We denote by $\boldsymbol{G}[V_0]$ the induced subgraph $G[V_0]$ with vertex set $V_0 \subset V$, and edge set $E(V_0)$ (see Definition 1.1.2 (i)) together with the natural restrictions of w and α to V_0 respectively $E(V_0)$. A k-subpartition of V is given by k pairwise disjoint non-empty subsets $V_1, \dots, V_k$ of V; the set of all k-subpartitions $\Pi = \{V_1, \dots, V_k\}$ of V is denoted by $\Pi_k(V)$.

Definition 6.2.6. Let $\boldsymbol{G}$ be an MW-graph. For a subset $V_0 \subset V$, we set

$$h(\boldsymbol{G}, V_0) := \frac{\iota(\boldsymbol{G}[V_0]) + w(E(V_0, V_0^{\mathsf{c}}))}{w(V_0)}.$$

The *k-th* (also called *k-way) (magnetic weighted) Cheeger constant* $h_k(\boldsymbol{G})$ is defined as

$$h_k(\boldsymbol{G}) := \inf_{\Pi \in \Pi_k(V)} \sup_{V_0 \in \Pi} h(\boldsymbol{G}, V_0). \tag{6.2.5}$$

Note that the infimum and supremum are actually minimum and maximum. It is not hard to see that $h_k(\boldsymbol{G}) \le h_{k+1}(\boldsymbol{G})$. Moreover, for $k = 1$ resp. $k = 2$ we have

$$h_1(\boldsymbol{G}) = \min_{V_0 \subset V, V_0 \ne \varnothing} h(\boldsymbol{G}, V_0) \quad \text{resp.} \quad h_2(\boldsymbol{G}) = \min_{V_0 \subset V, V_0 \ne \varnothing, V_0 \ne V} \max\{h(\boldsymbol{G}, V_0), h(\boldsymbol{G}, V_0^{\mathsf{c}})\}$$

for the first and second Cheeger constant (the latter is usually called *the* Cheeger constant). If $\alpha \sim 0$ then the second (usual) Cheeger constant equals

$$h_2(\boldsymbol{G}) = \min_{V_0 \subset V, V_0 \ne \varnothing, V_0 \ne V} \frac{w(E(V_0, V_0^{\mathsf{c}}))}{\min\{w(V_0), w(V_0^{\mathsf{c}})\}}.$$

Lemma 6.2.7. *Let $\pi \colon \boldsymbol{G} \to \boldsymbol{G}'$ be an* MW*-graph homomorphism, then*

$$h(\boldsymbol{G}, \pi^{-1}(V_0')) \le h(\boldsymbol{G}', V_0')$$

for all $V_0' \subset V'$, $V_0' \ne \varnothing$.

Proof. If $\pi \colon \boldsymbol{G} \to \boldsymbol{G}'$ is an *MW*-graph homomorphism, then the restriction $\pi \colon \boldsymbol{G}[\pi^{-1}(V_0')] \to \boldsymbol{G}'[V_0']$ is defined as map (as $\pi(\pi^{-1}(V_0')) \subset V_0'$ and $\pi(E^G(\pi^{-1}(V_0'))) \subset E^{G'}(V_0')$ because the graph homomorphism preserves the orientation, and again *MW*-graph homomorphism. In particular, from Lemma 6.2.5, we conclude that

$$\iota(\boldsymbol{G}[\pi^{-1}(V_0')]) \le \iota(\boldsymbol{G}'[V_0']).$$

Next, we have $E^G(\pi^{-1}(V_0'), (\pi^{-1}(V_0'))^{\mathsf{c}}) = \pi^{-1}(E^{G'}(V_0', (V_0')^{\mathsf{c}}))$ again by π is a graph homomorphism and as $(\pi^{-1}(V_0'))^{\mathsf{c}} = \pi^{-1}((V_0')^{\mathsf{c}})$. In particular, we conclude

$$w\big(E^G(\pi^{-1}(V_0'), (\pi^{-1}(V_0'))^{\mathsf{c}})\big) = (\pi_* w)\big(E^{G'}(V_0', (V_0')^{\mathsf{c}})\big) \le w'\big(E^{G'}(V_0', (V_0')^{\mathsf{c}})\big)$$

as π is an *MW*-graph homomorphism. Similarly, we have

$$w\big(\pi^{-1}(V_0')\big) = (\pi_* w)(V_0') \ge w'(V_0'),$$

and the desired inequality follows. □

We are now able to prove the main result of this section:

Theorem 6.2.8. *Let $\pi\colon \boldsymbol{G} \to \boldsymbol{G}'$ be an* MW*-graph homomorphism between two* MW*-graphs $\boldsymbol{G}$ and $\boldsymbol{G}'$, then we have*

$$h_k(\boldsymbol{G}) \le h_k(\boldsymbol{G}')$$

for all $k \in \mathbb{N}$.

Proof. Let the minimum in $h_k(\boldsymbol{G}')$ be achieved at $\Pi' = \{V_1', \dots, V_k'\} \in \Pi_k(V')$, and the maximum at V_1', i.e. assume that $h_k(\boldsymbol{G}') = h(\boldsymbol{G}', V_1')$. As π is surjective on the vertices (see Lemma 2.1.3 (i)), $\Pi := \{\pi^{-1}(V_1'), \dots, \pi^{-1}(V_k')\}$ is again a k-subpartition (all sets are pairwise disjoint *and* non-empty by the surjectivity). Now we have

$$h_k(\boldsymbol{G}) \le \sup_{j=1,\dots,k} h(\boldsymbol{G}, \pi^{-1}(V_j')) \le \sup_{j=1,\dots,k} h(\boldsymbol{G}', (V_j')) = h(\boldsymbol{G}', V_1') = h_k(\boldsymbol{G}')$$

as $h_k(G)$ is the infimum over all k-subpartitions, and Π is such a k-partition of V (first inequality). The second inequality follows from Lemma 6.2.7, and the last equality from the choice of the partition Π' and V_1'. □

Remark 6.2.9. Note that we have proven in Theorem 2.3.3 the inequality $\lambda_k(\boldsymbol{G}) \le \lambda_k(\boldsymbol{G}')$ if there is an *MW*-graph homomorphism $\pi\colon \boldsymbol{G} \to \boldsymbol{G}'$. We have just proven in Theorem 6.2.8 that an *MW*-graph homomorphism also increases the k-th Cheeger constant, hence Theorem 6.2.8 is in accordance with the (magnetic weighted) Cheeger inequalities

$$\frac{1}{2}\lambda_k(\boldsymbol{G}) \le h_k(\boldsymbol{G}) \le Ck^3\sqrt{\rho_\infty \lambda_k(\boldsymbol{G})}$$

for all $k \in \{1, \dots, |G|\}$ proven in [Lan+15], where $C > 0$ is a universal constant (recall that ρ_∞ is the supremum of the relative weight, see (1.2.3)). If $k = 1$, then $C = 1$, and if $k = 2$ and if $\alpha \sim 0$, then one can choose $C = \sqrt{2}/4$.

Example 6.2.10. Let $\boldsymbol{G} = (G, \alpha, w)$ and $\boldsymbol{G}' = (G', w', \alpha')$ be two magnetic weighted graphs.

- **Combinatorial weight and removing edges:** If $E_0 \subset E(G)$ and $\boldsymbol{G}$, $\boldsymbol{G}' = \boldsymbol{G} - E_0 \in \mathscr{G}_{\mathbb{1}}$, then $h_k(\boldsymbol{G} - E_0) \le h(\boldsymbol{G})$. Heuristically, this means that removing edges decreases the connectivity.
- **Standard and combinatorial weight compared:** If $G = G'$, $w = \deg$ and $w' = \mathbb{1}$, then $h_k(\boldsymbol{G}) \le h_k(\boldsymbol{G}')$ (the combinatorial weight has higher Cheeger constants).
- **Standard weight and glueing vertices:** If $\sim$ is an equivalence relation on $V(G)$, and if $\boldsymbol{G}$, $\boldsymbol{G}' = \boldsymbol{G}/\!\sim\, \in \mathscr{G}_{\deg}$, then $h_k(\boldsymbol{G}) \le h_k(\boldsymbol{G}/\!\sim)$. Heuristically, this means that glueing vertices together increases the connectivity.

6.2.2 Algebraic connectivity and spanning trees

We collect some basic facts that also follow from our spectral preorder. theory.

- **Algebraic connectivity.** Let $\boldsymbol{G} = (G, 0, \mathbb{1})$, the *algebraic connectivity* is defined as $a(G) = \lambda_2(\boldsymbol{G})$. This number gives information about how well connected is the graph.

$$G \preccurlyeq G' \implies \alpha(G) \leq \alpha(G')$$

Naturally deleting an edge increases the connectivity and contracting vertex increase the connectivity.

- **Number of Spanning Trees.** Let $G = (G, 0, \mathbb{1})$, the *number of spanning trees* can be computed by

$$\tau(G) = \frac{1}{n} \prod_{i=2}^{n} \lambda_i(G).$$

Also, it is clear that $G \preccurlyeq G'$ implies $\tau(G) \leq \tau(G')$.

6.3 Chemical graph theory

Chemical graph theory is a branch of mathematics which uses graph theory to describe properties of chemical compounds. In this fields, one typically associates numbers (indices) to a finite graph modelling certain properties of the molecule. Many chemical indices are functions of the eigenvalues of a combinatorial Laplacian without magnetic potential. In particular, if the function is monotonous, then the spectral preorder introduced in Chapter 2 induces an order of the corresponding indices. Moreover, we have a natural generalisation to *magnetic indices* by allowing non-trivial magnetic potentials.

Let $\mathcal{F}\colon [0,\infty) \to \mathbb{R}$ be a function and let $G \in \mathscr{G}$ be a finite *MW*-graph. We define by

$$\mathcal{F}(G) := \sum_{k=1}^{|G|} \mathcal{F}(\lambda_k(G))$$

the $\mathcal{F}$*-index* of G, i.e. the index is the restriction of $\mathcal{F}$ to the eigenvalues of the *DML*. By the definition of $\preccurlyeq$ (cf. Definition 2.2.4), we have the following simple observations:

Proposition 6.3.1. *Let $G, G' \in \mathscr{G}$, with $G \preccurlyeq G'$ and $\mathcal{F}$ a monotonous function,*

(i) If $\mathcal{F}$ is a non-negative decreasing function, then $\mathcal{F}(G) \geq \mathcal{F}(G')$.
(ii) If $\mathcal{F}$ is increasing and if $|G| = |G'|$, then $\mathcal{F}(G) \leq \mathcal{F}(G')$.

Proof. From $G \preccurlyeq G'$ we conclude $|G| \geq |G|'$ and $\lambda_k(G) \leq \lambda_k(G')$ for $k = 1, \ldots, |G'|$, and hence

$$\mathcal{F}(G) = \sum_{k=1}^{|G|} \mathcal{F}(\lambda_k(G)) \geq \sum_{k=1}^{|G'|} \mathcal{F}(\lambda_k(G')) = \mathcal{F}(G)$$

The second statement is obvious. □

Remark. Note that the second statement is not true if $G \preccurlyeq G'$, but $|G| > |G'|$: for example let G and G' be the combinatorial path graph with 3 and 2 vertices, respectively. Then their spectra are $(0,1,3)$ and $(0,2)$, respectively, hence $G \overset{G'}{\preccurlyeq}$. But if we choose $\mathcal{F}(\lambda) = \lambda$, then $\mathcal{F}$ is increasing, but $\mathcal{F}(G) = 4 > 2 = \mathcal{F}(G')$.

Graphs considered in chemical graph theory use combinatorial weights and no magnetic potential; hence we restrict the following theorems only to this case, i.e. we consider only $\mathbf{G} \in \mathscr{G}_{\mathbb{1}}$. However, these results can be generalised to other graphs $\mathbf{G}, \mathbf{G}' \in \mathscr{G}$ if we have the relation $\mathbf{G} \preccurlyeq \mathbf{G}'$.

Theorem 6.3.2. *Let $\mathbf{G}, \mathbf{G}' \in \mathscr{G}_{\mathbb{1}}$ be finite graphs and let $\mathcal{F}_1$ (respectively, $\mathcal{F}_2$) be a monotonously decreasing (respectively, increasing) function.*

(i) Deleting an edge increases the index $\mathcal{F}_1$ and decreases the index $\mathcal{F}_2$, i.e. if $\mathbf{G}' = \mathbf{G} - e_0$ then $\mathcal{F}_1(\mathbf{G}) \leq \mathcal{F}_1(\mathbf{G}')$ and $\mathcal{F}_2(\mathbf{G}') \leq \mathcal{F}_2(\mathbf{G})$.
(ii) Contracting vertices decreases the index $\mathcal{F}_1$, i.e. if $\mathbf{G}' = \mathbf{G}/\{v_1, v_2\}$, then $\mathcal{F}_1(\mathbf{G}') \leq \mathcal{F}_1(\mathbf{G})$.
(iii) Contracting a bridge edge decreases the index $\mathcal{F}_1$, i.e. if $\mathbf{G}' = \mathbf{G}/\{e_0\}$ for some bridge edge e_0, then $\mathcal{F}_1(\mathbf{G}') \leq \mathcal{F}_1(\mathbf{G})$.
(iv) Deleting a pendant vertex decrease the index $\mathcal{F}_1$, i.e., if $\mathbf{G}' = \mathbf{G} - v_0$ for a pendant vertex v_0, then $\mathcal{F}_1(\mathbf{G}') \leq \mathcal{F}_1(\mathbf{G})$.

We now specify the function $\mathcal{F}$ and obtain special cases:

Corollary 6.3.3. *Let $\mathbf{G} = (G, \alpha, w)$ and $\mathbf{G}' = (G', \alpha', w')$ be any two* MW*-graph.*

- *If $\mathbf{G} \preccurlyeq \mathbf{G}'$ with $|\mathbf{G}| = |\mathbf{G}'|$, then $\mathrm{MLEL}(\mathbf{G}) \leq \mathrm{MLEL}(\mathbf{G}')$ and $\mathrm{MLEE}(\mathbf{G}) \leq \mathrm{MLEE}(\mathbf{G}')$.*
- *If $\mathbf{G} \preccurlyeq \mathbf{G}'$ where G and G' are connected with $\alpha \sim 0$ and $\alpha' \sim 0$ (or $\alpha \nsim 0$ and $\alpha' \nsim 0$) then $\mathrm{W}(\mathbf{G}) \geq \mathrm{W}(\mathbf{G}')$.*
- *If $\mathbf{G} \sqsubseteq \mathbf{G}'$, $w = \deg$, G and G' are connected with $\alpha \sim 0$ and if $\alpha' \sim 0$ (or $\alpha \nsim 0$ and $\alpha' \nsim 0$) then $\mathrm{K}^*(\mathbf{G}) \geq \mathrm{K}^*(\mathbf{G}')$.*

One of the more studied properties in the literature of these chemical indices is found bounds for these numbers (especially for combinatorial weights). With the spectral preorder given in this dissertation, we can find some bounds in an easier way.

Corollary 6.3.4. *Let $\mathbf{G} = (G, \alpha, w)$ be an* MW*-graph where G is a simple connected graph of order n, then:*

(i) If $\mathbf{G} \in \mathscr{G}_{\mathbb{1}}^{0}$, then $LEL(G) \leq (n-1)\sqrt{n}$, $\mathrm{LEE}(G) \leq 1 + (n-1)e^n$ and $W(G) \geq n-1$.
(ii) If $\mathbf{G} \in \mathscr{G}_{\mathbb{1}}^{\pi}$, then $\mathrm{IE}(G) \leq \sqrt{2n-2} + (n-1)\sqrt{n-2}$ and $\mathrm{SLEE}(G) \leq e^{(n-2)}(e^n + n - 1)$.
(iii) If $\mathbf{G} \in \mathscr{G}_{\deg}^{0}$, then $\mathrm{NLEE}(G) \leq 1 + (n-1)e^{n/(n+1)}$.

Proof. We only prove the first part of (i), as the proofs of the other assertions are similar. Let $\mathbf{K}_n = (K_n, 0, \mathbb{1})$ where K_n the complete graph with n vertices. From Theorem 2.4.1 (ii) we conclude $\mathbf{G} \preccurlyeq \mathbf{K}_n$. Moreover, by Corollary 6.3.3, we have $\mathrm{LEL}(\mathbf{G}) \leq \mathrm{LEL}(\mathbf{K}_n)$. Finally, one can see that $\mathrm{LEL}(\mathbf{K}_n) = \sum_{i=1}^{n} \sqrt{\lambda_i(\mathbf{K}_n)} = \sum_{i=2}^{n} \sqrt{n} = (n-1)\sqrt{n}$. $\square$

Generalisation of chemical index to magnetic index

Magnetic index name	**$\mathcal{F}$-index**	**Generalisation and references**
Magnetic Laplacian-energy-like invariant $\mathrm{MLEL}(\boldsymbol{G})$	$\mathcal{F}(\lambda) = \sqrt{\lambda}$	
• If $\boldsymbol{G} \in \mathscr{G}_{\mathbb{1}}^{0}$		$\mathrm{LEL}(G)$ Laplacian-energy-like invariant References [LL08],[WL12].
• If $\boldsymbol{G} \in \mathscr{G}_{\mathbb{1}}^{\pi}$		$\mathrm{IE}(G)$ Incidence energy References [Gut+09], [LHY11], [RL13].
• If $\boldsymbol{G} \in \mathscr{G}_{\mathrm{deg}}^{0}$		$\mathrm{LIE}(G)$ Laplacian incidence energy References [CFK10],[MMM19].
Magnetic Laplacian Estrada index $\mathrm{MLEE}(\boldsymbol{G})$	$\mathcal{F}(\lambda) = \mathrm{e}^{\lambda}$	
• If $\boldsymbol{G} \in \mathscr{G}_{\mathbb{1}}^{0}$		$\mathrm{LEE}(G)$ Laplacian Estrada index References [PGR07], [Sha11], [ZZL11].
• If $\boldsymbol{G} \in \mathscr{G}_{\mathbb{1}}^{\pi}$		$\mathrm{SLEE}(G)$ Signless Laplacian Estrada index References [Ayy+11], [Aza15].
• If $\boldsymbol{G} \in \mathscr{G}_{\mathrm{deg}}^{0}$		$\mathrm{NLEE}(G)$ Normalized Laplacian Estrada index References [CC17], [LGS14].
Magnetic Wiener index $\mathrm{W}(\boldsymbol{G})$	$\mathcal{F}(\lambda) = \begin{cases} \frac{a}{\lambda} & \lambda > 0 \\ 0 & \lambda = 0, \end{cases}$	
• If $\boldsymbol{G} \in \mathscr{G}_{\mathbb{1}}^{0}$, G is a tree and $a = \lvert G \rvert$.		$\mathrm{W}(G)$ Wiener index. References [DEG01], [Fis+02] .
• If $\boldsymbol{G} \in \mathscr{G}_{\mathbb{1}}^{0}$ and $a = \lvert G \rvert$.		$\mathrm{W}^{*}(G)$ Quasi-Wiener index or Kirchhoff index. References [GM96], [Yan14].
• If $\boldsymbol{G} \in \mathscr{G}_{\mathrm{deg}}^{0}$ and $a = \lvert E(G) \rvert$.		$\mathrm{K}^{*}(G)$ Normalised Kirchhoff index. References [GLL12], [HL15].

7 Conclusions and future work

In this final chapter, we give a summary of the main results of this dissertation. We also present some natural developments based on the results given in this thesis and suggest some open questions for the near future.

The main object of study is the relation between the spectrum of the discrete magnetic Laplacian on weighted graphs and several aspects of its underlying graph. In particular, we study how geometric perturbations on finite graphs are manifested at the level of the spectrum. Also, we treat a special kind of infinite graphs, that are known as *periodic graphs* or *covering graph* and we consider the magnetic Laplacian with periodic potential acting on it. Some of the concrete results and their applications are:

- We present two different preorders on the discrete graphs to study the spectrum of the magnetic Laplacian under some geometrical perturbations (Section 2.1). The first one is based on a geometric perturbation of the graph. The second one is related to the order of the eigenvalues of the Laplacian (which are real and non-negative).
- We prove that the spectrum of the Laplacian on the periodic graph can be reduced to the study of the spectrum of the magnetic Laplacian in the finite quotient graph (Theorem 3.4.2).
- We solve (partially) the Higuchi and Shirai's conjecture with Theorem 4.1.10.
- We developed a discrete bracketing technique in the finite quotient graph, and by some perturbation on it, we obtain a localisation of its spectrum (Theorem 4.1.12).
- We give a geometrical criterion for the existence and localisation of spectral gaps in the spectrum of the Laplacian on periodic graphs in Theorem 4.1.3.
- We develop a geometrical technique producing an infinite collection of families of graphs, where all the elements in each family are (finite) isospectral (weighted) graphs for the magnetic Laplacian. The parametrization of the isospectral graphs in each family is based on different partitions of a natural number (Theorem 5.2.12).
- We also find some interesting application of the geometrical and spectral preorder, for example, in combinatorics in Section 6.2 or Chemistry (Section 4.2 and Subsection 6.3).

In relation to the previous items, we present some ideas that we are going to study in the future.

(i) Address a complete answer to the Higuchi and Shirai's conjecture stated in [HS04b]. With Theorem 4.1.10, we solve and provide a complete characterisation of the periodic graphs which have spectral gaps and its quotient graph has Betti number 1. For the proof, we use only the virtualisation of vertices and edges. But, with more general operations (deleting edges or vertices, contracting vertices or contracting edges), we can extend our criterion for graphs with a more complex topology. A first step will be to solve the conjecture for periodic graphs with finite quotient Betti number equal to 2.

(ii) An important topic in Graph Theory are expander graphs [HLW06], in particular, Ramanujan graphs [LPS88]. The expanders graphs are sparse graphs with high connectivity properties, and the optimal expander graphs are called Ramanujan graphs. These graphs are very important with a lot of application in computer science and communications (see, e.g., [Lub12]). However, to prove the existence and, in particular, the explicit construction of Ramanujan graphs is a very hard problem. An important recent breakthrough has been given in the recent article [MSS15]. The authors use the signature of a graph to construct a proper 2-lifting. The signature of a graph is just the action of a magnetic potential that takes values on all the edges equal to π, i.e., a magnetic potential α is a signature if $\alpha_e = \alpha_{\bar{e}} = \pi$ for all edge. An ambitious idea is to give a construction of Ramanujan graphs using a general magnetic potential and the geometric perturbation.

(iii) In Chapter 5, we developed a geometric construction (Theorem 5.2.12) resulting in the construction of large classes of examples of non-isomorphic isospectral magnetic weighted graphs with standard weights. The proof is based on the vertex contraction operation. This operation gives a small perturbation of the spectrum, but only for the normalized weight (see Corollary 2.4.6 (i)). For the combinatorial weights, the vertex contraction gives, in general, a larger deviation of its eigenvalues (see Corollary 2.4.6 (ii)). Therefore, the construction of Theorem 5.2.12 does not work for the combinatorial weights. However, for combinatorial weights the operation of deleting edges gives a small perturbation of the spectrum of the graph (see Corollary 2.4.2 (ii)). We think that the construction of isospectral magnetic weighted graphs with combinatorial weights could be using the delete edge operation (instead of the vertex contraction).

(iv) One of the important ideas in the construction of isospectral graphs in Chapter 5 is the use of frames that have high symmetry. Therefore, the frames have eigenvalues with high multiplicity that will persist the geometric manipulations of the graphs. An alternative idea is to develop the combination of the high symmetry directly with the construction of eigenfunctions of the Laplacian. With this alternative point of view, one can address, in principle, the construction of isospectral graphs for more general weights (and not only for normalized, combinatorial or standard weights).

(v) The construction of isospectral graphs presented in this thesis refers to finite *MW*-graphs. But, with the techniques studied for covering graphs developed in Theorem 3.4.2, it seems plausible to find a family of isospectral graphs for any magnetic potential in the family $\mathcal{A}_D$. This fact would immediately lead to the construct of isospectral periodic graphs.

A Discrete Floquet Theory

The *Floquet Theory* is a tool that finds applications in several areas of mathematics that study periodic structures. For example, this theory is used in Differential Equations in the study of solutions of periodic linear differential operators [Kuc93] or in the analysis of spectral gaps of Laplacian on periodic Riemannian manifolds [LP07], etc. In recent years, this theory has attracted much interest, particularly concerning the study of periodic elliptic equations in photonic crystals. The photonic crystals consist of a dielectric medium in which electromagnetic waves of specific frequencies cannot propagate [Kuc01]. The application of this theory can even reach our ability to control sound using the Floquet topological insulators [FKA16].

In this appendix, we develop a discrete Floquet Theory for the periodic graphs. We will assume throughout this appendix that $G = (V, E)$ is a Γ-periodic graph with Γ an Abelian, finitely generated discrete group with a fixed fundamental domain $D = (D^V, D^E)$ as in Definition 3.2.5. The main idea in this appendix is to use the group action on $V(G)$ and a partial Fourier transformation to decompose the Hilbert space $\ell_2(V(G))$ and the periodic operators (the *DML*) into a direct integral of simpler components that can be analyzed more easily. This appendix is just an adaptation for the main results of the Floquet theory to our context: the discrete graphs. For more details and additional motivations, we refer to [LP07, Section 3] and references therein.

Consider the following unitary operators:

$$\begin{aligned} T&:\Gamma \to \mathcal{U}\left(\ell_2(V)\right), \qquad & (T_{\gamma_0} f)(v) &= f(\gamma_0^{-1} v) \\ R&:\Gamma \to \mathcal{U}\left(\ell_2(\Gamma)\right), \qquad & (R_{\gamma_0} \mathbf{a})_\gamma &= \mathbf{a}_{\gamma\gamma_0} \\ L&:\Gamma \to \mathcal{U}\left(\ell_2(\Gamma)\right), \qquad & (L_{\gamma_0} \mathbf{a})_\gamma &= \mathbf{a}_{\gamma_0^{-1}\gamma}, \end{aligned}$$

where $f \in \ell_2(V)$, $\gamma, \gamma_0 \in \Gamma$ and $\mathbf{a} = \left(a_\gamma\right)_{\gamma\in\Gamma} \in \ell_2(\Gamma)$. In fact, T represents the*translations* on the graph G while the map R/L is the right/left regular representation of Γ.

A *unitary character* or simply a *character* χ of a group Γ is a group homomorphism $\chi: \Gamma \to \mathbb{T}$, where $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$ is a group respect to the complex multiplication. Then, χ satisfies the following properties:

(i) If 1_Γ is the unit in Γ, then $\chi(1_\Gamma) = 1$.
(ii) For any elements $\gamma_1, \gamma_2 \in \Gamma$ we have $\chi(\gamma_1\gamma_2) = \chi(\gamma_1)\chi(\gamma_2)$. In particular $\chi(\gamma_1^{-1}) = \overline{\chi(\gamma_1)}$.

The group of all characters is known as the ***dual group*** of Γ and is denoted by $\widehat{\Gamma}$. As mention before, the idea is to decompose the space $\ell_2(V)$ into a direct integral of simpler components that are the equivariant functions. Given a character χ, we can define the space of *equivariant functions* as follow:

$$\ell_2^\chi = \ell_2^\chi(V) = \{g\colon V(G) \to \mathbb{C} \mid g(\gamma v) = \chi(\gamma)g(v) \text{ for all } v \in V(G) \text{ and } \gamma \in \Gamma\} /;.$$

The space ℓ_2^χ has the natural inner product defined as

$$\langle g_1, g_2 \rangle = \sum_{v \in \mathcal{D}^V} g_1(v)\overline{g_2(v)}m(v),$$

where the previous product is independent of the choice of the fundamental set. The principal result of this appendix is the following:

Theorem A.0.1. *Let $G = (V, E)$ be a Γ-periodic graph with fundamental domain $D = (D^V, D^E)$. There is a unitary transformation*

$$\Phi\colon \ell_2(V(G)) \to \int_{\widehat{\Gamma}} \ell_2^\chi d\chi$$

given by:

$$(\Phi(f))_\chi(v) = \sum_{\gamma \in \Gamma} \overline{\chi(\gamma)} f(\gamma v)$$

that satisfies the equation $\Phi \circ T_{\gamma_0} = \widehat{L_{\gamma_0}} \circ \Phi$ and $\Phi \circ T_{\gamma_0^{-1}} = \widehat{R_{\gamma_0}} \circ \Phi$, where $\widehat{R}_{\gamma_0} = FR_{\gamma_0}F^{-1}$, $\widehat{L_{\gamma_0}} = FL_{\gamma_0}F^{-1}$ and $F\colon \ell_2(\Gamma) \to L_2(\widehat{\Gamma})$ is the Fourier transformation.

To give the complete proof of the previous Theorem, we develop with details the discrete Floquet Theory.

A.0.1 The Fourier transformation

Roughly speaking, a discrete Floquet transformation is a partial Fourier transformation which is applied only on the group part. The *Fourier transformation* is the operator $F\colon \ell_2(\Gamma) \to L_2(\widehat{\Gamma})$, defined by

$$(F\mathbf{a})(\chi) = \sum_{\gamma \in \Gamma} \overline{\chi(\gamma)} a_\gamma \quad \text{with } \mathbf{a} = \left(a_\gamma\right)_{\gamma \in \Gamma} \in \ell_2(\Gamma).$$

For example, if $\left\{\delta_\gamma\right\}_{\gamma \in \Gamma}$ is the standard orthonormal basis of $\ell_2(\Gamma)$, then:

$$\left(F(\delta_{\gamma_0})\right)(\chi) = \sum_{\gamma \in \Gamma} \overline{\chi(\gamma)} \left(\delta_{\gamma_0}\right)_\gamma = \overline{\chi(\gamma_0)}.$$

It's easy to check that $R_{\gamma_0}\delta_\gamma = \delta_{\gamma\gamma_0^{-1}}$ and $L_{\gamma_0}\delta_\gamma = \delta_{\gamma_0\gamma}$. Finally, since the group is abelian, it is also immediate that $L_{\gamma_0} = R_{\gamma_0}^{-1}$.
The *inverse of the Fourier transformation* is the operator $F^{-1}\colon L_2(\widehat{\Gamma}) \to \ell_2(\Gamma)$, given by

$$\left(F^{-1}u\right)_\gamma = \int_{\widehat{\Gamma}} \chi(\gamma)u(\chi)d\chi \text{ with } u \in L_2(\widehat{\Gamma}).$$

We prove that the operator F^{-1} is the inverse of F. In one side, we have the following equality

$$\begin{aligned}\left(F^{-1}(F\mathbf{a})\right)_\gamma &= \int_{\widehat{\Gamma}} \chi(\gamma)(F\mathbf{a})(\chi)d\chi = \int_{\widehat{\Gamma}} \chi(\gamma) \sum_{\gamma'\in\Gamma} \overline{\chi(\gamma')}a_{\gamma'}d\chi \\ &= \sum_{\gamma'\in\Gamma}\left(\int_{\widehat{\Gamma}} \chi(\gamma)\overline{\chi(\gamma')}d\chi\right)a_{\gamma'} = \sum_{\gamma'\in\Gamma}\left(\delta_\gamma\right)_{\gamma'} a_{\gamma'} = a_\gamma.\end{aligned}$$

On the other side, we have

$$\begin{aligned}\left(F(F^{-1}u)\right)(\chi) &= \sum_{\gamma\in\Gamma}\overline{\chi(\gamma)}(F^{-1}u)_\gamma = \sum_{\gamma\in\Gamma}\overline{\chi(\gamma)}\int_{\widehat{\Gamma}} \chi'(\gamma)u(\chi')d\chi' \\ &= \int_{\widehat{\Gamma}} \sum_{\gamma\in\Gamma}\overline{\chi(\gamma)}\chi'(\gamma)u(\chi')d\chi' = \int_{\widehat{\Gamma}} \langle\chi,\chi'\rangle\, u(\chi')d\chi' \\ &= \int_{\widehat{\Gamma}} \delta_\chi(\chi')u(\chi')d\chi' = u(\chi).\end{aligned}$$

We conclude checking that F preserves the inner product, i.e.,

$$\begin{aligned}\langle F\mathbf{a}, F\mathbf{b}\rangle_{L_2(\widehat{\Gamma})} &= \int_{\widehat{\Gamma}} (F\mathbf{a})(\chi)\overline{(F\mathbf{b})(\chi)}d\chi = \int_{\widehat{\Gamma}} \sum_{\gamma'\in\Gamma}\overline{\chi(\gamma')}a_{\gamma'}\sum_{\gamma\in\Gamma}\chi(\gamma)\overline{b_\gamma}d\chi \\ &= \int_{\widehat{\Gamma}} \sum_{\gamma',\gamma\in\Gamma}\overline{\chi(\gamma')}a_{\gamma'}\chi(\gamma)\overline{b_\gamma}d\chi = \sum_{\gamma',\gamma\in\Gamma}\int_{\widehat{\Gamma}} a_{\gamma'}\overline{b_\gamma}\chi(\gamma)\overline{\chi(\gamma')}d\chi \\ &= \sum_{\gamma',\gamma\in\Gamma} a_{\gamma'}\overline{b_\gamma}\int_{\widehat{\Gamma}}\overline{\chi(\gamma')}\chi(\gamma)d\chi = \sum_{\gamma',\gamma\in\Gamma} a_{\gamma'}\overline{b_\gamma}(\delta_\gamma)_{\gamma'} \\ &= \sum_{\gamma\in\Gamma} a_\gamma\overline{b_\gamma} = \langle\mathbf{a},\mathbf{b}\rangle_{\ell_2(\Gamma)}.\end{aligned}$$

Altogether we have shown that the Fourier transformation F is a unitary operator.

We present the relation between the Fourier transformation and the right/left regular representation. We define the next transformation operator $\widehat{R_{\gamma_0}} := FR_{\gamma_0}F^{-1}$. Then, the next explicit calculation shows that the operator is just a multiplication on the right, i.e.,

$$
\begin{aligned}
\left(\widehat{R_{\gamma_0}}(u)\right)(\chi) &= \left(FR_{\gamma_0}F^{-1}(u)\right)(\chi) = \sum_{\gamma\in\Gamma}\overline{\chi(\gamma)}\left(R_{\gamma_0}F^{-1}u\right)_{\gamma} = \sum_{\gamma\in\Gamma}\overline{\chi(\gamma)}\left(F^{-1}u\right)_{\gamma\gamma_0} \\
&= \sum_{\gamma\in\Gamma}\overline{\chi(\gamma)}\int_{\widehat{\Gamma}}\chi'(\gamma\gamma_0)u(\chi')d\chi' = \int_{\widehat{\Gamma}}\chi'(\gamma_0)\sum_{\gamma\in\Gamma}\left(\overline{\chi(\gamma)}\chi'(\gamma)\right)u(\chi')d\chi' \\
&= \int_{\widehat{\Gamma}}\chi'(\gamma_0)\langle\chi,\chi'\rangle u(\chi')d\chi' = \chi(\gamma_0)u(\chi).
\end{aligned}
$$

In a similar way, if we define the next operator $\widehat{L_{\gamma_0}} := FL_{\gamma_0}F^{-1}$, then

$$
\begin{aligned}
\left(\widehat{L_{\gamma_0}}(u)\right)(\chi) &= \left(FL_{\gamma_0}F^{-1}(u)\right)(\chi) = \sum_{\gamma\in\Gamma}\overline{\chi(\gamma)}\left(L_{\gamma_0}F^{-1}u\right)_{\gamma} = \sum_{\gamma\in\Gamma}\overline{\chi(\gamma)}\left(F^{-1}u\right)_{\gamma_0^{-1}\gamma} \\
&= \sum_{\gamma\in\Gamma}\overline{\chi(\gamma)}\int_{\widehat{\Gamma}}\chi'(\gamma_0^{-1}\gamma)u(\chi')d\chi' = \int_{\widehat{\Gamma}}\chi'(\gamma_0^{-1})\sum_{\gamma\in\Gamma}\left(\overline{\chi(\gamma)}\chi'(\gamma)\right)u(\chi')d\chi' \\
&= \int_{\widehat{\Gamma}}\chi'(\gamma_0^{-1})\langle\chi,\chi'\rangle u(\chi')d\chi' = \chi(\gamma_0^{-1})u(\chi).
\end{aligned}
$$

Therefore $\widehat{R_{\gamma_0}}/\widehat{L_{\gamma_0}}$ is just a multiplication operator with $\chi(\gamma_0)/\chi(\gamma_0^{-1})$. Moreover, we will show that the inverse of $\widehat{R_{\gamma_0}}$ is $\widehat{L_{\gamma_0}}$, i.e.

$$
\left(\widehat{R_{\gamma_0}}\widehat{L_{\gamma_0}}(u)\right)(\chi) = \chi(\gamma_0)\left(\widehat{L_{\gamma_0}}(u)\right)(\chi) = \chi(\gamma_0)\chi(\gamma_0^{-1})u(\chi) = u(\chi),
$$

therefore $\widehat{R_{\gamma_0}}^{-1} = \widehat{L_{\gamma_0}}$.

A.0.2 Discrete Floquet theory on graphs.

In this section, we will make precise in which sense the Floquet Theory can be understood as a *partial Fourier transformation*. Since we are working with $G = (V, E)$ a Γ-periodic graph with Γ an Abelian, finitely generated discrete group with a fundamental domain $D = (D^V, D^E)$, the idea is just split the periodic graph into two parts: the fundamental domain and the group part. We will apply the Fourier transformation on the last one. We begin proving the following result:

Lemma A.0.2. *Let G a Γ-periodic graph with fundamental domain $D = (D^V, D^E)$, then*

$$
\ell_2(V) \cong \ell_2(\Gamma)\otimes\ell_2(D^V) \cong \int_{\widehat{\Gamma}}\ell_2(D^V)d\chi\,.
$$

Moreover, for the quotient $G_0 = G/\Gamma$, we also have $\ell_2(V(G_0)) \cong \ell_2^{\chi} \cong \ell_2(\mathcal{D})$.

Proof. We show the unitarily equivalence with several operators in the following steps.

- The first step is to split f into a sequence of γ-translates over the fundamental domain to show
$$\ell_2(V) \cong \ell_2(\Gamma) \otimes \ell_2(D^V).$$
We define the operator
$$U\colon \ell_2(V) \to \ell_2(\Gamma) \otimes \ell_2(\mathcal{D}) \quad \text{given by} \quad U(f) = \sum_{\gamma \in \Gamma} \delta_\gamma \otimes (T_\gamma f|_{\mathcal{D}}).$$
The operator U preserves the inner product:
$$\begin{aligned}\langle Uf, Ug\rangle_{\ell_2(\Gamma)\otimes\ell_2(\mathcal{D})} &= \left\langle \sum_{\gamma\in\Gamma} \delta_\gamma \otimes (T_\gamma f|_{\mathcal{D}}), \sum_{\gamma'\in\Gamma} \delta_{\gamma'} \otimes (T_{\gamma'} g|_{\mathcal{D}}) \right\rangle \\ &= \sum_{\gamma,\gamma'\in\Gamma} \left\langle \delta_\gamma, \delta_{\gamma'} \right\rangle \left\langle T_\gamma f|_{\mathcal{D}}, T_{\gamma'} g|_{\mathcal{D}} \right\rangle \\ &= \sum_{\gamma\in\Gamma} \left\langle T_\gamma f|_{\mathcal{D}}, T_\gamma g|_{\mathcal{D}} \right\rangle = \langle f, g\rangle_{\ell_2(V(G))}.\end{aligned}$$
Since U is onto, we obtain that U is unitary. In addition, we have the following diagram,
$$\begin{array}{ccc} \ell_2(V) & \xrightarrow{U} & \ell_2(\Gamma) \otimes \ell_2(\mathcal{D}) \\ \downarrow{\scriptstyle T_{\gamma_0}} & & \downarrow{\scriptstyle R_{\gamma_0}\otimes\mathbf{1}} \\ \ell_2(V) & \xrightarrow{U} & \ell_2(\Gamma) \otimes \ell_2(\mathcal{D}) \end{array}$$
commutes because the following equality holds
$$\begin{aligned}\left(U \circ T_{\gamma_0}\right)(f) = U\left(T_{\gamma_0} f\right) &= \sum_{\gamma\in\Gamma} \delta_\gamma \otimes (T_\gamma T_{\gamma_0} f|_{\mathcal{D}}) = \sum_{\gamma\in\Gamma} \delta_\gamma \otimes (T_{\gamma_0\gamma} f|_{\mathcal{D}}) \\ &= \sum_{\gamma'\in\Gamma} \delta_{\gamma_0^{-1}\gamma'} \otimes (T_{\gamma'} f|_{\mathcal{D}}) = R_{\gamma_0} \otimes \mathbf{1} \left(\sum_{\gamma'\in\Gamma} \delta_{\gamma'} \otimes (T_{\gamma'} f|_{\mathcal{D}}) \right) \\ &= R_{\gamma_0} \otimes \mathbf{1}(Uf) = (R_{\gamma_0} \otimes \mathbf{1} \circ U) f.\end{aligned}$$

- The second step is to show
$$\ell_2(\Gamma) \otimes \ell_2(\mathcal{D}) \cong L_2(\widehat{\Gamma}) \otimes \ell_2(\mathcal{D}).$$
This is clear by applying the Fourier transformation on the first factor. More formally, we define the unitary map
$$V\colon \ell_2(\Gamma) \otimes \ell_2(\mathcal{D}) \to L_2(\widehat{\Gamma}) \otimes \ell_2(\mathcal{D}) \quad \text{given by} \quad V(\mathbf{a} \otimes \varphi) = F\mathbf{a} \otimes \varphi.$$
We have the following commutative diagram
$$\begin{array}{ccc} \ell_2(\Gamma) \otimes \ell_2(\mathcal{D}) & \xrightarrow{V} & L_2(\widehat{\Gamma}) \otimes \ell_2(\mathcal{D}) \\ \downarrow{\scriptstyle R_\gamma\otimes\mathbf{1}} & & \downarrow{\scriptstyle \widehat{R}_\gamma\otimes\mathbf{1}} \\ \ell_2(\Gamma) \otimes \ell_2(\mathcal{D}) & \xrightarrow{V} & L_2(\widehat{\Gamma}) \otimes \ell_2(\mathcal{D}) \end{array}$$

- In the third step, we show

$$L_2(\widehat{\Gamma}) \otimes \ell_2(\mathcal{D}) \cong \int_{\widehat{\Gamma}} \ell_2(\mathcal{D}) d\chi.$$

Consider the unitary operator

$$W\colon L_2(\widehat{\Gamma}) \otimes \ell_2(\mathcal{D}) \to \int_{\widehat{\Gamma}} \ell_2(\mathcal{D}) d\chi \quad \text{given by} \quad W(b \otimes f) = (b(\chi) f)_\chi$$

Which, again, preserves the inner product:

$$\begin{aligned}
\langle W(b_1 \otimes f_1), W(b_2 \otimes f_2) \rangle &= \int_{\widehat{\Gamma}} \langle b_1(\chi) f_1, b_2(\chi) f_2 \rangle_{\ell_2(\mathcal{D})} \, d\chi \\
&= \int_{\widehat{\Gamma}} \sum_{v \in \mathcal{D}} \langle b_1(\chi), b_2(\chi) \rangle \, f_1(v) \overline{f_2(v)} m(v) d\chi \\
&= \sum_{v \in \mathcal{D}} f_1(v) \overline{f_2(v)} m(v) \int_{\widehat{\Gamma}} \langle b_1(\chi), b_2(\chi) \rangle \, d\chi \\
&= \langle f_1, f_2 \rangle \cdot \langle b_1, b_2 \rangle = \langle b_1 \otimes f_1, b_2 \otimes f_2 \rangle .
\end{aligned}$$

Since W is onto, we obtain again that W is unitary. In addition, we have the following diagram,

$$\begin{array}{ccc}
L_2(\widehat{\Gamma}) \otimes \ell_2(\mathcal{D}) & \xrightarrow{W} & \int_{\widehat{\Gamma}} \ell_2(\mathcal{D}) d\chi \\
\big\downarrow {\scriptstyle R_\gamma \otimes \mathbf{1}} & & \big\downarrow {\scriptstyle \chi(\gamma)\cdot} \\
L_2(\widehat{\Gamma}) \otimes \ell_2(\mathcal{D}) & \xrightarrow{W} & \int_{\widehat{\Gamma}} \ell_2(\mathcal{D}) d\chi
\end{array}$$

$$\left(W \circ \widehat{R}_\gamma \otimes \mathbf{1}\right)(b \otimes f) = W(\widehat{R}_\gamma b \otimes f) = \left(\widehat{R}_\gamma b(\chi) f\right)_\chi = (\chi(\gamma) b(\chi) f)_\chi .$$

- Now, for the last part, it is clear that $\ell_2(V(G_0)) \cong \ell_2(\mathcal{D})$ since $|V(G_0)| = |\mathcal{D}|$. Finally, we need to show $\ell_2(\mathcal{D}) \cong \ell_2^\chi$, for this just define

$$T\colon \ell_2(\mathcal{D}) \to \ell_2^\chi \quad \text{given by} \quad (Th)(\gamma v) = \chi(\gamma) h(v) \text{ for all } h \in \ell_2(\mathcal{D}).$$

T preserves the inner product since:

$$\langle Th_1, Th_2 \rangle = \sum_{v \in \mathcal{D}} h_1(v) \overline{h_2(v)} m(v) = \langle h_1, h_2 \rangle .$$

Since T is onto, we obtain that T is unitary.

□

Now, we can prove the principal result of this appendix.

Proof of Theorem A.0.1 First, we prove that $(\Phi(f))_\chi \in \ell_2^\chi$,

$$(\Phi(f))_\chi(\gamma_0 v) = \sum_{\gamma\in\Gamma} \overline{\chi(\gamma)} f(\gamma\gamma_0 v) = \chi(\gamma) \sum_{\gamma\in\Gamma} \overline{\chi(\gamma)\chi(\gamma_0)} f(\gamma\gamma_0 v)$$
$$= \chi(\gamma) \sum_{\gamma'\in\Gamma} \overline{\chi(\gamma')} f(\gamma' v) = \chi(\gamma)(\Phi(f))_\chi(v).$$

Now, in order to show that Φ is a unitary transformation, we used the transformation given in Lemma A.0.2, in fact, is enough to show that:

$$\Phi = W \circ V \circ U$$

Let $f \in \ell_2(V(G))$, then

$$W \circ V \circ U(f) = W \circ V\left(\sum_{\gamma\in\Gamma} \delta_\gamma \otimes (T_\gamma f|_{\mathcal{D}})\right) = W\left(\sum_{\gamma\in\Gamma} F(\delta_\gamma) \otimes (T_\gamma f|_{\mathcal{D}})\right)$$
$$= \left(\sum_{\gamma\in\Gamma} \overline{\chi(\gamma)}(T_\gamma f|_{\mathcal{D}})\right)_\chi = \left(\sum_{\gamma\in\Gamma} \overline{\chi(\gamma)} f(\gamma^{-1}\cdot)|_{\mathcal{D}}\right)_\chi = \Phi(f).$$

Then Φ is a unitary operator. Now, we prove that $\Phi \circ T_{\gamma_0} = \widehat{R}_{\gamma_0} \circ \Phi$. Since $\widehat{R_{\gamma_0}}/\widehat{L_{\gamma_0}}$ is just a multiplication operator with $\chi(\gamma_0)/\chi(\gamma_0^{-1})$. Then,

$$\left(\Phi \circ T_{\gamma_0}(f)\right)_\chi = \left(\Phi\left(f(\gamma_0^{-1}\cdot)\right)\right)_\chi = \chi(\gamma_0^{-1})(\Phi(f))_\chi = \left(\widehat{L_{\gamma_0}} \circ \Phi(f)\right)_\chi$$

In conclusion $\Phi \circ T_{\gamma_0} = \widehat{L_{\gamma_0}} \circ \Phi$ and in a similar way we can show $\Phi \circ T_{\gamma_0^{-1}} = \widehat{R_{\gamma_0}} \circ \Phi$. $\square$

B Program

In this Appendix, we present a simple routine to compute the eigenvalues of a finite magnetic weighted graph. The code is made for *Mathematica 12.0* software. The routine needs the input of the edges of the graph G (we allow loops and multiple edges), the weights w (in vertices and in edges) and the magnetic potential α. Using the previous information, it is constructed the matrix associated with the magnetic Laplacian as in the Eq. (1.5.4) (we use the orthonormal basis). The output of the code is a draw of the graph, the matrix associated to the Δ_α^G and its eigenvalues. Also, we present some routines for constructing some family of graphs and the spectrum of its magnetic Laplacian.

The code was very useful along the process of doing this dissertation. We did a lot of examples of computing the spectrum of the magnetic Laplacian on a graph (and geometrical perturbations). Such experiments were the motivation for some results of this thesis, for example, Theorem 4.1.10. Also, the properties prove in this thesis was checked by simple numerical examples (cf. the geometric perturbation in Section 2.4). Finally, the plots to draw the spectrum of the magnetic Laplacian in this work was done with this program (for example, Figure 0.2).

B.0.1 Code

The next program draws the graph, computes the magnetic Laplacian matrix and its spectrum. Because of the presence of the magnetic potential and to simplify the computation, we define an orientation of the graph (i.e., we replacing each edge by one if its possible arcs $\{e, \bar{e}\}$). The inputs of the program are the following:

- **Input:** G. We define an orientation on the graph, then we introduce the set of arcs and its vertices that joins, For example, the arc $\{1,2\}$ is the arc that joins the origin, the vertex 1 to the final vertex 2.
- **Input:** *Alpha*. Define the magnetic potential, i.e., if R any subgroup of $\mathbb{R}/2\pi\mathbb{Z}$ the *Alpha* is the map $\alpha\colon E \to R$.

- **Input:** wE. Define the weights on G, i.e., in the set of edges $w\colon E \to (0, \infty)$. If we put value equal to 1, all the edges take this value.
- **Input:** wV. Define the weights on the set of vertices $V(G)$, i.e., $w\colon V \to (0, \infty)$. To consider the standard weights is enough to put *std* and for the combinatorial weights put *comb*.

The code is the following.

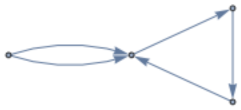
```
MagLap[G_, Alpha_, wE_, wV_] := (
Ver = DeleteDuplicates@Flatten@G;
n = Dimensions[Ver][[1]];(*number of vertices*)

L = ConstantArray[0, {n, n}];(*Define the Laplacian matrix as zero*)

m = Dimensions[G][[1]];(*number of edges*)

deg = Table[
Count[G, Ver[[i]], 2], {i, n}] ; (*degree vector of the vertices*)

VP = If[NumberQ[Alpha], ConstantArray[0, {m}], Alpha];(*If 0,
then \alpha\sim 0*)

mE = If[NumberQ[wE], ConstantArray[1, {m}],
wE];(*standart weight if wE=0 or wE=1*)

mV = Switch[wV, std, deg, comb, ConstantArray[1, {n}], _,
wV];(*standart weight if wV=deg*)
For [i = 1, i <= m, i++,
j = Position[Ver, G[[i, 1]]][[1]][[1]];
k = Position[Ver, G[[i, 2]]][[1]][[1]];
L[[j, k]] = -(mE[[i]])*
E^(-I*VP[[i]])/(Sqrt[mV[[j]]]*Sqrt[mV[[k]]]) + L[[j, k]];
L[[k, j]] = -(mE[[i]])*
E^(I*VP[[i]])/(Sqrt[mV[[j]]]*Sqrt[mV[[k]]]) + L[[k, j]];
L[[j, j]] = mE[[i]]/mV[[j]] + L[[j, j]] ;
L[[k, k]] = mE[[i]]/mV[[k]] + L[[k, k]]
]; (*compute the laplacian*)

Edges = Table[G[[i, 1]] -> G[[i, 2]], {i, 1, m}];
(*labels=Table[Subscript[e,Ver[[i]]],{i,m}];*)

Gra = Graph[Edges(*,VertexLabels\[Rule]Table[i\[Rule]Subscript[v,
Ver[[i]]],{i,n}],EdgeLabels\[Rule]Table[Edges[[
i]]\[Rule]Subscript[e,i],{i,m}]*)];(*define grpah draw*)
{Gra,
Simplify[L] // MatrixForm,
Sigma = Sort[FullSimplify[Reverse[Eigenvalues[L, Cubics -> True]]],
Greater]}(*output: graph,matrix and eigenvalues*)
)
```

We show in this Appendix some simple examples of how use the code. More information and elaborated examples are collected in the following link https://github.com/JohnFabila/Magnetic-Laplacian.

Example B.0.1. A graph with multiple edges is considered in this example, see Figure 2.1. The graph G is defined by its arcs, and we consider standard weights and zero magnetic potential. We obtain, a vector, where the first element contains the picture of the graph, the second element contains the matrix associated to the magnetic Laplacian and finally, the exact values of its eigenvalues are in the third element of the vector.

```
In[98]:= G = {{1, 2}, {1, 2}, {2, 3}, {3, 4}, {4, 2}};
         MagLap[G, 0, 1, std]
```

Out[99]= {



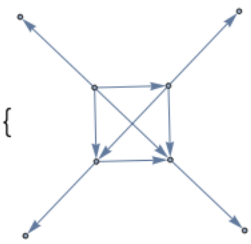
$$, \begin{pmatrix} 1 & -\frac{1}{\sqrt{2}} & 0 & 0 \\ -\frac{1}{\sqrt{2}} & 1 & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} \\ 0 & -\frac{1}{2\sqrt{2}} & 1 & -\frac{1}{2} \\ 0 & -\frac{1}{2\sqrt{2}} & -\frac{1}{2} & 1 \end{pmatrix}, \left\{\frac{1}{4}(5+\sqrt{5}), \frac{3}{2}, \frac{1}{4}(5-\sqrt{5}), 0\right\}\}$$

FIGURE 2.1: A simple example to show how works the program.

Example B.0.2. Consider the magnetic weighted graph $\mathbf{G}_n = (G, \alpha, w)$, where the graph G is making of decorating the complete graph K_n with a pendant edge on each vert of the graph, α is the zero magnetic potential and w is the combinatorial graph. A simple code is presented for computing the eigenvalues of the magnetic Laplacian of $\mathbf{G}_n$ for any n integer. The case $n = 4$ is illustrated in Figure 2.2:

```
In[103]:= n = 4; Aristas = Union[Subsets[Table[i, {i, 1, n}], {2}], Table[{i, i + n}, {i, 1, n}]]; MagLap[Aristas, 0, 1, comb]
```

{



$$, \begin{pmatrix} 4 & -1 & -1 & -1 & -1 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & 0 & -1 & 0 & 0 \\ -1 & -1 & 4 & -1 & 0 & 0 & -1 & 0 \\ -1 & -1 & -1 & 4 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 \end{pmatrix}, \{3+\sqrt{5}, 3+\sqrt{5}, 3+\sqrt{5}, 2, 3-\sqrt{5}, 3-\sqrt{5}, 3-\sqrt{5}, 0\}\}$$

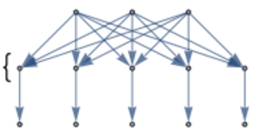
FIGURE 2.2: Example for the decorated complete graph.

Example B.0.3. Similar to the previous case, consider the magnetic weighted graph $\mathbf{G}_{n,m} = (G, \alpha, w)$, where the graph G is making of decorating the complete bipartite graph $K_{n,m}$ with n pendant edges attached on each of the n vertices that give the bipartition, α is the zero magnetic potential and w is the standard weights. We can compute the spectrum for the decorated complete bipartite graph with the next line of code, and the case of Figure 2.3 shows an example: for $n = 5$ and $m = 3$.

We conclude these examples, with the computation of the spectrum of the decorated diamond graphs Figure 5.7, this example shows how include loops in the graph.

Example B.0.4. Let $\mathbf{G}_n = (G_n, \alpha^t, \deg_{G_n})$ be a magnetic graph where G_n is a decorated diamond graph Figure 5.7 and magnetic potential $\alpha^t_e = t$, if e is a loop and 0 otherwise. For a fixed n integer, in Figure 2.4 we compute its eigenvalues of the magnetic Laplacian for the case $n = 4$.

```
(*Complete bipartite graph*)
n1 = 3;
n2 = 5;
n = i + j;
a1 = Union[Table[{k, n2 + k}, {k, n1 + 1, n1 + n2}], Table[{i, j}, {i, 1, n1}, {j, n1 + 1, n1 + n2}]];
Aristas = Partition[Flatten[a1], 2];
MagLap[Aristas, 0, 1, std]
```

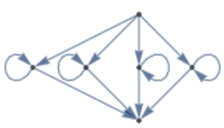
{ ,

$$\begin{pmatrix}
1 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\
-\frac{1}{2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\
0 & 0 & -\frac{1}{2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & -\frac{1}{2} & 0 & 0 & 0 & 0 & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\
0 & 0 & 0 & 0 & -\frac{1}{2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & -\frac{1}{2} & 0 & 0 & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\frac{1}{2} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 1 & 0 & 0 & 0 \\
-\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & 1 & 0 & 0 \\
-\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & 0 & 1 & 0 \\
-\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & -\frac{1}{2\sqrt{5}} & 0 & 0 & 0 & 1
\end{pmatrix}$$

$$, \left\{2, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, 1, 1, 1, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0\right\}\}$$

FIGURE 2.3: Example for the decorated complete bipartite graph.

```
In[10]:= s = 4; r = 2; A = ConstantArray[1, {2*s + s, 2}];
B = ConstantArray[0, 2*s + s];
For[i = 1, i ≤ s, i++,
  A[[i, All]] = {1, i + 1};
  A[[2*s + i, All]] = {i + 1, i + 1};
  B = ReplacePart[B, 2*s + i → t];
 ];
For[i = 1, i ≤ s, i++,
 A[[i + s, All]] = {i + 1, 2*s}
];
Cospectral[A, B, 1, std]
```

Out[13]= { ,

$$\begin{pmatrix}
1 & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & 0 \\
-\frac{1}{4} & 1-\frac{e^{-it}}{4}-\frac{e^{it}}{4} & 0 & 0 & 0 & -\frac{1}{4} \\
-\frac{1}{4} & 0 & 1-\frac{e^{-it}}{4}-\frac{e^{it}}{4} & 0 & 0 & -\frac{1}{4} \\
-\frac{1}{4} & 0 & 0 & 1-\frac{e^{-it}}{4}-\frac{e^{it}}{4} & 0 & -\frac{1}{4} \\
-\frac{1}{4} & 0 & 0 & 0 & 1-\frac{e^{-it}}{4}-\frac{e^{it}}{4} & -\frac{1}{4} \\
0 & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & 1
\end{pmatrix},$$

$$\left\{\frac{1}{8} e^{-it}\left(-1+8 e^{it}-e^{2it}+\sqrt{1+34 e^{2it}+e^{4it}}\right), -\frac{1}{8} e^{-it}\left(1-8 e^{it}+e^{2it}+\sqrt{1+34 e^{2it}+e^{4it}}\right), 1-\frac{\text{Cos}[t]}{2}, 1-\frac{\text{Cos}[t]}{2}, 1-\frac{\text{Cos}[t]}{2}, 1\right\}\}$$

FIGURE 2.4: Example for the decorated diamond graph.

List of Abbreviations

DML	**D**iscrete **M**agnetic **L**aplacian
FSP	**F**ull **S**pectrum **P**roperty
M-graph	**M**agnetic graph
MW-graph	**M**agnetic **W**eighted graph
W-graph	**W**eighted graph

Chemical indexes

LEE	**L**aplacian-**E**strada index
LEL	**L**aplacian-**E**nergy-**L**ike invariant
LIE	**L**aplacian-**I**ncidence-**E**nergy
MLEL	**M**agnetic **L**aplacian-**E**nergy-**L**ike invariant
MLEE	**M**agnetic **L**aplacian-**E**strada index
NLEE	**N**ormalized **L**aplacian **E**strada index
SLEE	**S**ignless **L**aplacian **E**strada index

List of Symbols

$\mathbb{N}$	Set of natural numbers
$\mathbb{N}_0$	Set of natural numbers with the 0
$\mathbb{Z}$	Additive group of integers
$\mathbb{Z}^n$	additive group of n-ple integers
$\mathbb{Z}_n(=\mathbb{Z}/n\mathbb{Z})$	Additive group of integers modulo n
$\lvert A\rvert$	cardinality of the set A
$A \times B$	Cartesian product of the sets A and B
$A \setminus B$	Difference of A and B
$A \subset B$	A is a subset of B
$deg_G(v)$	degree of the vertex v in the graph G
$E(G)$	set of edges of the graph G
E_v	set of edges adjacent to v
$f\colon A \to B$	A map of A into B
G	graph
$G \cong H$	isomorphic graphs
K_n	Complete graph on n vertices
$tr A$	Trace of the square matrix A
$V(G)$	set of vertices of the graph G
$w(A)$	weight of the set A
$w(v)$	weight of the vertex v
w_e	weight of the edge e
α	magnetic vector potential
$b_1(G)$	Betti number of graph G
d_α	(discrete) magnetic exterior derivative
$\partial = \partial_G$	incidence function of the graph G
$\partial^-(a)$	the initial vertex of the edge e
$\partial^+(a)$	the final vertex of the edge e
$\rho(v)$	the relative weight of the vertex v

List of Figures

References

[AHS78] J. Avron, I. Herbst, and B. Simon. Schrödinger operators with magnetic fields. I. General interactions. *Duke Math. J.* **45** (4) (1978), pp. 847–883.

[AL95] A. Ashtekar and J. Lewandowski. Differential geometry on the space of connections via graphs and projective limits. *J. Geom. Phys.* **17** (3) (1995), pp. 191–230.

[ARZ87] J. E. Avron, A. Raveh, and B. Zur. Quantum conductance in networks. *Phys. Rev. Lett.* **58** (20) (1987), pp. 2110–2113.

[AT14] F. M. Atay and H. Tunçel. On the spectrum of the normalized Laplacian for signed graphs: interlacing, contraction, and replication. *Linear Algebra Appl.* **442** (2014), pp. 165–177.

[Ayy+11] S. K. Ayyaswamy, S. Balachandran, Y. B. Venkatakrishnan, and I. Gutman. Signless Laplacian Estrada index. *MATCH Commun. Math. Comput. Chem.* **66** (3) (2011), pp. 785–794.

[AYY13] J. An, J.-K. Yu, and J. Yu. On the dimension datum of a subgroup and its application to isospectral manifolds. *J. Differential Geom.* **94** (1) (2013), pp. 59–85.

[Aza15] S. Azami. On Laplacian and signless Laplacian Estrada indices of graphs. *MATCH Commun. Math. Comput. Chem.* **74** (2) (2015), pp. 411–418.

[Bal76] A. T. Balaban, ed. *Chemical applications of graph theory*. Academic Press [Harcourt Brace Jovanovich, Publishers], London-New York, 1976.

[Bap10] R. B. Bapat. *Graphs and matrices*. Springer, London, 2010.

[Bar08] T. W. Barrett. *Topological foundations of electromagnetism*. World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2008.

[BC08] H.-J. Bandelt and V. Chepoi. Metric graph theory and geometry: a survey. *Surveys on discrete and computational geometry*. Amer. Math. Soc., Providence, RI, 2008, pp. 49–86.

[BE98] B. Bollobás and P. Erdős. Graphs of extremal weights. *Ars Combin.* **50** (1998), pp. 225–233.

[BG11] S. Butler and J. Grout. A construction of cospectral graphs for the normalized Laplacian. *Electron. J. Combin.* **18** (1) (2011), Paper 231, 20.

[BH12] A. E. Brouwer and W. H. Haemers. *Spectra of graphs*. Springer, New York, 2012.

[Bha07] R. Bhatia. *Perturbation bounds for matrix eigenvalues*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2007.

[Big93] N. Biggs. *Algebraic graph theory*. Second edition. Cambridge University Press, Cambridge, 1993.

[BK13] G. Berkolaiko and P. Kuchment. *Introduction to quantum graphs*. American Mathematical Society, Providence, RI, 2013.

[BM08] J. A. Bondy and U. S. R. Murty. *Graph theory*. Springer, New York, 2008.

[BPB09] R. Band, O. Parzanchevski, and G. Ben-Shach. The isospectral fruits of representation theory: quantum graphs and drums. *J. Phys. A* **42** (17) (2009), p. 175202.

[BS97] I. Benjamini and O. Schramm. Every graph with a positive Cheeger constant contains a tree with a positive Cheeger constant. *Geom. Funct. Anal.* **7** (3) (1997), pp. 403–419.

[But10] S. Butler. A note about cospectral graphs for the adjacency and normalized Laplacian matrices. *Linear Multilinear Algebra* **58** (3-4) (2010), pp. 387–390.

[CC17] G. P. Clemente and A. Cornaro. Novel bounds for the normalized Laplacian Estrada index and normalized Laplacian energy. *MATCH Commun. Math. Comput. Chem.* **77** (3) (2017), pp. 673–690.

[CDS95] D. M. Cvetković, M. Doob, and H. Sachs. *Spectra of graphs*. Third edition. Johann Ambrosius Barth, Heidelberg, 1995.

[CFK10] M. Cavers, S. Fallat, and S. Kirkland. On the normalized Laplacian energy and general Randić index R_{-1} of graphs. *Linear Algebra Appl.* **433** (1) (2010), pp. 172–190.

[Che+04] G. Chen, G. Davis, F. Hall, Z. Li, K. Patel, and M. Stewart. An interlacing result on normalized Laplacians. *SIAM J. Discrete Math.* **18** (2) (2004), pp. 353–361.

[Che70] J. Cheeger. A lower bound for the smallest eigenvalue of the Laplacian. *Problems in analysis (Papers dedicated to Salomon Bochner, 1969)*. 1970, pp. 195–199.

[Chi12] J. C. Chien. *Polyacetylene: chemistry, physics, and material science*. Elsevier, 2012.

[Chu97] F. R. K. Chung. *Spectral graph theory*. American Mathematical Society, Providence, RI, 1997.

[CR17] D. M. Cardoso and O. Rojo. Edge perturbation on graphs with clusters: adjacency, Laplacian and signless Laplacian eigenvalues. *Linear Algebra Appl.* **512** (2017), pp. 113–128.

[CS11] D. Cvetković and S. Simić. Graph spectra in computer science. *Linear Algebra Appl.* **434** (6) (2011), pp. 1545–1562.

[DD89] W. Dicks and M. J. Dunwoody. *Groups acting on graphs*. Cambridge University Press, Cambridge, 1989.

[DEG01] A. A. Dobrynin, R. Entringer, and I. Gutman. Wiener index of trees: theory and applications. *Acta Appl. Math.* **66** (3) (2001), pp. 211–249.

[Deo74] N. Deo. *Graph theory with applications to engineering and computer science*. Prentice-Hall, Inc., Englewood Cliffs, N.J., 1974.

[DH03] E. R. van Dam and W. H. Haemers. Which graphs are determined by their spectrum? *Linear Algebra Appl.* (2003), pp. 241–272.

[Die05] R. Diestel. *Graph theory*. Third edition. Springer-Verlag, Berlin, 2005.

[DKT08] M. Desbrun, E. Kanso, and Y. Tong. Discrete differential forms for computational modeling. *Discrete differential geometry*. Birkhäuser, Basel, 2008, pp. 287–324.

[DM06] J. Dodziuk and V. Mathai. Kato's inequality and asymptotic spectral properties for discrete magnetic Laplacians. *The ubiquitous heat kernel*. Amer. Math. Soc., Providence, RI, 2006, pp. 69–81.

[Eas73] M. S. P. Eastham. *The spectral theory of periodic differential equations*. Scottish Academic Press, Edinburgh; Hafner Press, New York, 1973.

[EKN83] F. Ebisawa, T. Kurokawa, and S. Nara. Electrical properties of polyacetylene polysiloxane interface. *Journal of applied physics* **54** (6) (1983), pp. 3255–3259.

[EKW10] P. Exner, P. Kuchment, and B. Winn. On the location of spectral edges in Z-periodic media. *J. Phys. A* **43** (47) (2010), pp. 474022, 8.

[Exn+08] P. Exner, J. P. Keating, P. Kuchment, T. Sunada, and A. Teplyaev, eds. *Analysis on graphs and its applications*. American Mathematical Society, Providence, RI, 2008.

[Fan+18] M. Fanuel, C. M. Alaıéz, Á. Fernández, and J. A. K. Suykens. Magnetic eigenmaps for the visualization of directed networks. *Appl. Comput. Harmon. Anal.* **44** (1) (2018), pp. 189–199.

[Fis+02] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Székely, and L. Volkmann. Wiener index versus maximum degree in trees. *Discrete Appl. Math.* **122** (1-3) (2002), pp. 127–137.

[FKA16] R. Fleury, A. B. Khanikaev, and A. Alù. Floquet topological insulators for sound. *Nature Communications*. Nature Publishing Group, 2016.

[FL19] J. S. Fabila-Carrasco and F. Lledó. Covering graphs, magnetic spectral gaps and applications to polymers and nanoribbons. *Symmetry* **11** (9) (2019), p. 1163.

[FLP18] J. S. Fabila-Carrasco, F. Lledó, and O. Post. Spectral gaps and discrete magnetic Laplacians. *Linear Algebra Appl.* **547** (2018), pp. 183–216.

[GLL12] X. Gao, Y. Luo, and W. Liu. Kirchhoff index in line, subdivision and total graphs of a regular graph. *Discrete Appl. Math.* **160** (4-5) (2012), pp. 560–565.

[GM08] S. Golénia and S. Moroianu. Spectral analysis of magnetic Laplacians on conformally cusp manifolds. *Ann. Henri Poincaré* **9** (1) (2008), pp. 131–179.

[GM82] C. D. Godsil and B. D. McKay. Constructing cospectral graphs. *Aequationes Math.* **25** (2-3) (1982), pp. 257–268.

[GM96] I. Gutman and B. Mohar. The quasi-Wiener and the Kirchhoff indices coincide. *Journal of Chemical Information and Computer Sciences* **36** (5) (1996), pp. 982–985.

[GP10] L. J. Grady and J. R. Polimeni. *Discrete calculus*. Springer-Verlag London, Ltd., London, 2010.

[GR01] C. Godsil and G. Royle. *Algebraic graph theory*. Springer-Verlag, New York, 2001.

[GT84] J. Garnett and E. Trubowitz. Gaps and bands of one-dimensional periodic Schrödinger operators. *Comment. Math. Helv.* **59** (2) (1984), pp. 258–312.

[GT87] J. Garnett and E. Trubowitz. Gaps and bands of one-dimensional periodic Schrödinger operators. II. *Comment. Math. Helv.* **62** (1) (1987), pp. 18–37.

[Guo07] J.-M. Guo. The Laplacian spectral radius of a graph under perturbation. *Comput. Math. Appl.* **54** (5) (2007), pp. 709–720.

[Gut+09] I. Gutman, D. Kiani, M. Mirzakhah, and B. Zhou. On incidence energy of a graph. *Linear Algebra Appl.* **431** (8) (2009), pp. 1223–1233.

[GWW92] C. Gordon, D. L. Webb, and S. Wolpert. One cannot hear the shape of a drum. *Bull. Amer. Math. Soc. (N.S.)* **27** (1) (1992), pp. 134–138.

[Hae+12] S. Haeseler, M. Keller, D. Lenz, and R. Wojciechowski. Laplacians on infinite graphs: Dirichlet and Neumann boundary conditions. *J. Spectr. Theory* **2** (4) (2012), pp. 397–432.

[Han+07] M. Y. Han, B. Ozyilmaz, Y. Zhang, and P. Kim. Energy band-gap engineering of graphene nanoribbons. *Physical review letters* **98** (20) (2007), p. 206805.

[Har55] P. G. Harper. Single band motion of conduction electrons in a uniform magnetic field. *Proceedings of the Physical Society. Section A* **68** (10) (1955), p. 874.

[HJ85] R. A. Horn and C. R. Johnson. *Matrix analysis*. Cambridge University Press, Cambridge, 1985.

[HL15] J. Huang and S. Li. On the normalised Laplacian spectrum, degree-Kirchhoff index and spanning trees of graphs. *Bull. Aust. Math. Soc.* **91** (3) (2015), pp. 353–367.

[HLW06] S. Hoory, N. Linial, and A. Wigderson. Expander graphs and their applications. *Bull. Amer. Math. Soc. (N.S.)* **43** (4) (2006), pp. 439–561.

[HN09] Y. Higuchi and Y. Nomura. Spectral structure of the Laplacian on a covering graph. *European J. Combin.* **30** (2) (2009), pp. 570–585.

[HP03] R. Hempel and O. Post. Spectral gaps for periodic elliptic operators with high contrast: an overview. *Progress in analysis, Vol. I, II (Berlin, 2001)*. World Sci. Publ., River Edge, NJ, 2003, pp. 577–587.

[HPS18] C. Hall, D. Puder, and W. F. Sawin. Ramanujan coverings of graphs. *Adv. Math.* **323** (2018), pp. 367–410.

[HRH02] P. D. Hoff, A. E. Raftery, and M. S. Handcock. Latent space approaches to social network analysis. *J. Amer. Statist. Assoc.* **97** (460) (2002), pp. 1090–1098.

[HS04a] W. H. Haemers and E. Spence. Enumeration of cospectral graphs. *European J. Combin.* **25** (2) (2004), pp. 199–211.

[HS04b] Y. Higuchi and T. Shirai. Some spectral and geometric properties for infinite graphs. *Discrete geometric analysis*. Amer. Math. Soc., Providence, RI, 2004, pp. 29–56.

[HS99] Y. Higuchi and T. Shirai. A remark on the spectrum of magnetic Laplacian on a graph. *Proceedings of the 10th Workshop on Topological Graph Theory (Yokohama, 1998)*. Vol. 47. Special Issue. 1999, pp. 129–141.

[Ivr16] V. Ivrii. 100 years of Weyl's law. *Bull. Math. Sci.* **6** (3) (2016), pp. 379–452.

[Jan+07] D. Janežič, A. Miličević, S. Nikolić, and N. Trinajstić. *Graph-theoretical matrices in chemistry*. University of Kragujevac, Faculty of Science, Kragujevac, 2007.

[Kac66] M. Kac. Can one hear the shape of a drum? *Amer. Math. Monthly* **73** (4, part II) (1966), pp. 1–23.

[KK02] P. Kuchment and L. Kunyansky. Differential operators on graphs and photonic crystals. 2-3. 2002, pp. 263–290.

[KOS89] T. Kobayashi, K. Ono, and T. Sunada. Periodic Schrödinger operators on a manifold. *Forum Math.* **1** (1) (1989), pp. 69–79.

[KS14] E. Korotyaev and N. Saburova. Schrödinger operators on periodic discrete graphs. *J. Math. Anal. Appl.* **420** (1) (2014), pp. 576–611.

[KS15] E. Korotyaev and N. Saburova. Spectral band localization for Schrödinger operators on discrete periodic graphs. *Proc. Amer. Math. Soc.* **143** (9) (2015), pp. 3951–3967.

[KS16] E. Korotyaev and N. Saburova. Effective masses for Laplacians on periodic graphs. *J. Math. Anal. Appl.* **436** (1) (2016), pp. 104–130.

[KS17a] E. Korotyaev and N. Saburova. Magnetic Schrödinger operators on periodic discrete graphs. *J. Funct. Anal.* **272** (4) (2017), pp. 1625–1660.

[KS17b] E. Korotyaev and N. Saburova. Schrödinger operators with guided potentials on periodic graphs. *Proc. Amer. Math. Soc.* **145** (11) (2017), pp. 4869–4883.

[Kuc01] P. Kuchment. The mathematics of photonic crystals. *Mathematical modeling in optical science*. SIAM, Philadelphia, PA, 2001, pp. 207–272.

[Kuc04] P. Kuchment. Quantum graphs. I. Some basic structures. *Waves Random Media* **14** (1) (2004), S107–S128.

[Kuc05] P. Kuchment. Quantum graphs. II. Some spectral properties of quantum and combinatorial graphs. *J. Phys. A* **38** (22) (2005), pp. 4887–4900.

[Kuc93] P. Kuchment. *Floquet theory for partial differential equations*. Birkhäuser Verlag, Basel, 1993.

[Lan+15] C. Lange, S. Liu, N. Peyerimhoff, and O. Post. Frustration index and Cheeger inequalities for discrete and continuous magnetic Laplacians. *Calc. Var. Partial Differential Equations* **54** (4) (2015), pp. 4165–4196.

[LGS14] J. Li, J.-M. Guo, and W. C. Shiu. The normalized Laplacian Estrada index of a graph. *Filomat* **28** (2) (2014), pp. 365–371.

[LHY11] B. Liu, Y. Huang, and Z. You. A survey on the Laplacian-energy-like invariant. *MATCH Commun. Math. Comput. Chem.* **66** (3) (2011), pp. 713–730.

[LL00] B. Liu and H.-J. Lai. *Matrices in combinatorics and graph theory*. Kluwer Academic Publishers, Dordrecht, 2000.

[LL08] J. Liu and B. Liu. A Laplacian-energy-like invariant of a graph. *MATCH Commun. Math. Comput. Chem.* **59** (2) (2008), pp. 355–372.

[LL93] E. H. Lieb and M. Loss. Fluxes, Laplacians, and Kasteleyn's theorem. *Duke Math. J.* **71** (2) (1993), pp. 337–363.

[LP07] F. Lledó and O. Post. Generating spectral gaps by geometry. *Prospects in mathematical physics*. Amer. Math. Soc., Providence, RI, 2007, pp. 159–169.

[LP08a] F. Lledó and O. Post. Eigenvalue bracketing for discrete and metric graphs. *J. Math. Anal. Appl.* **348** (2) (2008), pp. 806–833.

[LP08b] F. Lledó and O. Post. Existence of spectral gaps, covering manifolds and residually finite groups. *Rev. Math. Phys.* **20** (2) (2008), pp. 199–231.

[LPS88] A. Lubotzky, R. Phillips, and P. Sarnak. Ramanujan graphs. *Combinatorica* **8** (3) (1988), pp. 261–277.

[LR15] Z. Lu and J. Rowlett. The sound of symmetry. *Amer. Math. Monthly* **122** (9) (2015), pp. 815–835.

[Lub12] A. Lubotzky. Expander graphs in pure and applied mathematics. *Bull. Amer. Math. Soc. (N.S.)* **49** (1) (2012), pp. 113–162.

[Lub94] A. Lubotzky. *Discrete groups, expanding graphs and invariant measures*. Birkhäuser Verlag, Basel, 1994.

[Lux07] U. von Luxburg. A tutorial on spectral clustering. *Stat. Comput.* **17** (4) (2007), pp. 395–416.

[Maj13] S. Majid. Noncommutative Riemannian geometry on graphs. *J. Geom. Phys.* **69** (2013), pp. 74–93.

[Mar73] G. A. Margulis. Explicit constructions of expanders. *Problemy Peredači Informacii* **9** (4) (1973), pp. 71–80.

[Mer94] R. Merris. Laplacian matrices of graphs: a survey. *Linear Algebra Appl.* **197** (1994), pp. 143–176.

[Mer97] R. Merris. Large families of Laplacian isospectral graphs. *Linear and Multilinear Algebra* **43** (1-3) (1997), pp. 201–205.

[Mil64] J. Milnor. Eigenvalues of the Laplace operator on certain manifolds. *Proc. Nat. Acad. Sci. U.S.A.* **51** (1964), p. 542.

[MMM19] E. I. Milovanović, M. M. Matejić, and I. Ž. Milovanović. On the normalized Laplacian spectral radius, Laplacian incidence energy and Kemeny's constant. *Linear Algebra Appl.* **582** (2019), pp. 181–196.

[MOA11] A. W. Marshall, I. Olkin, and B. C. Arnold. *Inequalities: theory of majorization and its applications*. Second edition. Springer, New York, 2011.

[Moh82] B. Mohar. The spectrum of an infinite graph. *Linear Algebra Appl.* **48** (1982), pp. 245–256.

[Moh91] B. Mohar. The Laplacian spectrum of graphs. *Graph theory, combinatorics, and applications. Vol. 2 (Kalamazoo, MI, 1988)*. Wiley, New York, 1991, pp. 871–898.

[MSS15] A. W. Marcus, D. A. Spielman, and N. Srivastava. Interlacing families I: Bipartite Ramanujan graphs of all degrees. *Ann. of Math. (2)* **182** (1) (2015), pp. 307–325.

[MW89] B. Mohar and W. Woess. A survey on spectra of infinite graphs. *Bull. London Math. Soc.* **21** (3) (1989), pp. 209–234.

[MY02] V. Mathai and S. Yates. Approximating spectral invariants of Harper operators on graphs. *J. Funct. Anal.* **188** (1) (2002), pp. 111–136.

[MY99] V. Mathai and S. G. Yates. Discrete Morse theory and extended L^2 homology. *J. Funct. Anal.* **168** (1) (1999), pp. 84–110.

[Ols71] M. P. Olson. The selfadjoint operators of a von Neumann algebra form a conditionally complete lattice. *Proc. Amer. Math. Soc.* **28** (1971), pp. 537–544.

[PGR07] J. A. de la Peña, I. Gutman, and J. Rada. Estimating the Estrada index. *Linear Algebra Appl.* **427** (1) (2007), pp. 70–76.

[Pos03] O. Post. Periodic manifolds with spectral gaps. *J. Differential Equations* **187** (1) (2003), pp. 23–45.

[Pos12] O. Post. *Spectral analysis on graph-like spaces*. Springer, Heidelberg, 2012.

[PR00] T. Pisanski and M. Randić. Bridges between geometry and graph theory. *Geometry at work*. Math. Assoc. America, Washington, DC, 2000, pp. 174–194.

[RL13] O. Rojo and E. Lenes. A sharp upper bound on the incidence energy of graphs in terms of connectivity. *Linear Algebra Appl.* **438** (3) (2013), pp. 1485–1493.

[Ros97] S. Rosenberg. *The Laplacian on a Riemannian manifold*. Cambridge University Press, Cambridge, 1997.

[Row91] P. Rowlinson. Graph angles and isospectral molecules. *Univ. Beograd. Publ. Elektrotehn. Fak. Ser. Mat.* **2** (1991), pp. 61–66.

[SA00] J. H. Schenker and M. Aizenman. The creation of spectral gaps by graph decoration. *Lett. Math. Phys.* **53** (3) (2000), pp. 253–262.

[SCB09] H. Santos, L. Chico, and L. Brey. Carbon nanoelectronics: unzipping tubes into graphene ribbons. *Physical review letters* **103** (8) (2009), p. 086801.

[SCL06] Y.-W. Son, M. L. Cohen, and S. G. Louie. Energy gaps in graphene nanoribbons. *Physical review letters* **97** (21) (2006), p. 216803.

[Sha11] Y. Shang. Perturbation results for the Estrada index in weighted networks. *J. Phys. A* **44** (7) (2011), pp. 075003, 8.

[Shi01] H. Shirakawa. The discovery of polyacetylene film: the dawning of an era of conducting polymers (Nobel lecture). *Angewandte Chemie International Edition* **40** (14) (2001), pp. 2574–2580.

[Shu94] M. A. Shubin. Discrete magnetic Laplacian. *Comm. Math. Phys.* **164** (2) (1994), pp. 259–275.

[Sin06] A. Singer. From graph to manifold Laplacian: the convergence rate. *Appl. Comput. Harmon. Anal.* **21** (1) (2006), pp. 128–134.

[Skr85] M. M. Skriganov. The spectrum band structure of the three-dimensional Schrödinger operator with periodic potential. *Invent. Math.* **80** (1) (1985), pp. 107–121.

[SN10] A. Smith and S. Nie. Semiconductor nanocrystals: Structure, properties, and band gap engineering. Acc. *Chem. Res.* **43** (Jan. 2010), pp. 190–200.

[Spi12] D. Spielman. Spectral graph theory. *Combinatorial scientific computing*. CRC Press, Boca Raton, FL, 2012, pp. 495–524.

[ST93] J. H. Schmerl and W. T. Trotter. Critically indecomposable partially ordered sets, graphs, tournaments and other binary relational structures. *Discrete Math.* **113** (1-3) (1993), pp. 191–205.

[Sun08] T. Sunada. Discrete geometric analysis. *Analysis on graphs and its applications*. Amer. Math. Soc., Providence, RI, 2008, pp. 51–83.

[Sun13] T. Sunada. *Topological crystallography*. Springer, Tokyo, 2013.

[Sun85] T. Sunada. Riemannian coverings and isospectral manifolds. *Ann. of Math. (2)* **121** (1) (1985), pp. 169–186.

[Sun94] T. Sunada. A discrete analogue of periodic magnetic Schrödinger operators. *Geometry of the spectrum (Seattle, WA, 1993)*. Amer. Math. Soc., Providence, RI, 1994, pp. 283–299.

[Suz13] A. Suzuki. Spectrum of the Laplacian on a covering graph with pendant edges I: The one-dimensional lattice and beyond. *Linear Algebra Appl.* **439** (11) (2013), pp. 3464–3489.

[Tan98] J. Tan. On isospectral graphs. *Interdiscip. Inform. Sci.* **4** (2) (1998), pp. 117–124.

[TM76] W. T. Trotter Jr. and J. I. Moore Jr. Characterization problems for graphs, partially ordered sets, lattices, and families of sets. *Discrete Math.* **16** (4) (1976), pp. 361–381.

[Tri92] N. Trinajstić. *Chemical graph theory*. Second edition. CRC Press, Boca Raton, FL, 1992.

[Wey12] H. Weyl. Das asymptotische Verteilungsgesetz der Eigenwerte linearer partieller Differentialgleichungen (mit einer Anwendung auf die Theorie der Hohlraumstrahlung). *Math. Ann.* **71** (4) (1912), pp. 441–479.

[WF12] Y. Wang and Y.-Z. Fan. The least eigenvalue of signless Laplacian of graphs under perturbation. *Linear Algebra Appl.* **436** (7) (2012), pp. 2084–2092.

[WL12] W. Wang and Y. Luo. On Laplacian-energy-like invariant of a graph. *Linear Algebra Appl.* **437** (2) (2012), pp. 713–721.

[Yan14] Y. Yang. The Kirchhoff index of subdivisions of graphs. *Discrete Appl. Math.* **171** (2014), pp. 153–157.

[Zel92] E. Zelmanov. *Nil rings and periodic groups*. Korean Mathematical Society, Seoul, 1992.

[ZG11] Z. Zhang and W. Guo. Energy-gap modulation of BN ribbons by transverse electric fields: First-principles calculations. *Physical Review B* **77** (Jan. 2011), p. 075403.

[ZZL11] J. Zhang, B. Zhou, and J. Li. On Estrada index of trees. *Linear Algebra Appl.* **434** (1) (2011), pp. 215–223.

Alphabetical Index