DEGENERACIES IN THE EIGENVALUE SPECTRUM OF QUANTUM GRAPHS

A Dissertation

by

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ABSTRACT

In this dissertation, we analyze the spectrum of the Laplace operator on graphs. In particular, we are interested in generic eigenpairs.

We consider a wide range of vertex conditions on vertices of a quantum graph. Furthermore, we also investigate the eigenfunctions, showing that generically they do not vanish on vertices, unless this is unavoidable due to presence of looping edges. In the proof, the simplicity of eigenvalues and non-vanishing of eigenvalues are tightly interconnected; each property is assisting in the proof of the other (the proof is done by induction). The proof is geometric in nature and uses local modications of the graph to reduce it to previously considered cases. We also consider an application of the result to the study of the secular manifold of a graph, showing that for large classes of graphs, the set of smooth points of the manifold has exactly two connected components.

The spectrum of a symmetric quantum graph is also considered. We aim to give explicit and computation-oriented formulas for extracting the part of a Schrödinger operator on a graph which corresponds to a particular irreducible representation of the graph's symmetry. Starting with a representation of the symmetry by its action on the space of directed bonds of the graph, we find a basis which block-diagonalizes both the representation and the bond scattering matrix of the graph. The latter leads to a factorization of the secular determinant into factors that correspond to irreducible representation of the symmetry group.

DEDICATION

To my family

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1. INTRODUCTION

In discrete mathematics, a graph is a set of vertices (also called *nodes*) which are connected by edges, which may be directed or undirected. In applications, they can be used to model many types of relations and processes in physical, biological, social and information systems. A communication network in computer science, a local connection between interacting parts of a physics system, and the functional connection between brain areas in computational neuroscience, can all be described by graphs. In some applications, an edge is merely a symbolic link signifying a connection between two vertices. In the graphs that we study, the edges are physical one-dimensional objects, characterized by their lengths. Furthermore, a family of operators will be defined on the graph and the spectra of such operators will be studied. This chapter provides an overview of a selection of applications and current topics of interest of research on graphs. For more applications, see [22].

1.1 Quantum graphs

In mathematics and physics, a *quantum graph* is a metric graph together with a differential operator acting on functions defined on the edges and satisfying some matching conditions at the vertices. Quantum graphs have been used as a simpler setting to study complicated phenomena. Linus Pauling was the first person to use quantum graphs as models of free electrons in organic molecules [27] in the 1930s, where the molecules were modelled as vertices connected by paths with electrons obeying a one-dimensional Schrödinger equation with some potential. In [78], Ruedenberg and Scherr considered the free-electron network model for conjugated molecules and derived joint conditions (for branching points) and boundary conditions (for free endpoints).

In quantum chaos, a branch of physics studying the manifestation of classically chaotic motion in the quantum mechanics, quantum graphs have been used as model systems since the pioneering work of Kottos and Smilansky [60]. They showed that quantum graphs provided a simple model displaying most of the phenomena encountered in quantum chaos in closed systems. Later in [62], they turned quantum graphs into a scattering system and showed that they displayed all the features which characterize quantum scattering systems with an underlying classical chaotic dynamics. They also derived exact expressions for the scattering matrix and an exact trace formula (already known to mathematicians, see below), and they used them to investigate the origin of the connection between Random Matrix Theory and the underlying classical chaotic dynamics. From there, all aspects of quantum chaos have been covered: spectral statistics [18, 24, 26, 42, 59], wavefunction statistics [14, 19], and chaotic scattering [62]. To give some examples, in [18], Berkolaiko and Keating investigated the two-point spectral statisics for star graphs in the limit as the number of edges tends to infinity and used combinatorial techniques to evaluate both the diagonal (same orbit) and off-diagonal (different orbit) contributions; in [80], Schanz and Smilansky considered the Schrödinger operator on graphs and studied the spectral statistics of a unitary operator which represented the quantum evolution; such an operator is the quantum analogue of the classical evolution operator of the corresponding classical dynamics on the same graph; in [63], Kottos and Smilansky proposed and investigated a system that is convenient to study the generic behavior of chaotic scattering systems and their semiclassical description, and so on. For more details about quantum chaos, interested read should consult [52].

Another area of physics where quantum graphs models featured recently is Anderson localization. In 1958, Anderson discussed the behavior of electrons in a crystal with impurities [3]. He was the first person to suggest the possibility of electron

localization inside a semiconductor under certain conditions. Since then, Anderson localization has been used as a general wave phenomenon that arises in different areas. In [91], Wiersma *et al.* reported direct experimental evidence for Anderson localization of light in optical experiments performed on very strongly scattering semiconductor powders. Anderson localization has been observed in microwaves by Dalichaouch *et al.* in [30], in which they reported measurements of the electric-field energy density for microwave radiation localized in essentially two-dimensional space and detected regions of high energy density representing the signature of localized modes. Anderson localization has also been used for sound waves. Weaver, in [90], studied Anderson localization of ultrasound. On graphs, in [51], Hislop and Post proved that certain random models associated with radial, tree-like, rooted quantum graphs exhibit Anderson localization at all energies. They also proved Anderson localization for the random necklace model. Aslo on graphs, in [1], Aizenman *et al.* considered the Laplacian on a rooted metric tree with random edge lengths and showed the stability of the absolutely continuous spectrum for weak disorder. In [57], the spectral properties of the Laplacian on a class of quantum graphs with random metric structure were studied by Klopp and Pankrashkin. They showed that, under certain technical assumptions, the bottom of the spectrum is pure point with exponentially decaying eigenfunctions. Another important class of quantum graphs is given by $\mathbb{Z}^d$-lattices. Exner, Helm, and Stollmann studied the situation on a cubic-lattice quantum graph where each edge carried a random potential and showed the Anderson localization near the bottom of the spectrum [36].

Quantum graphs have been used to model thin structures. Smilansky and Solomyak studied a model system transiting from a network of channels with finite width to the corresponding graph consisting of infinitely thin wires in [84]. In [46], Grieser explained some common ideas and methods used in different areas where thin tubes

occur. He also explained some recent results, mainly from mathematical physics and spectral geometry. Exner and Post considered a family of compact manifolds which shrinks with respect to an appropriate parameter to a graph in [37]. Rubinstein and Schatzmann considered thin superconducting rings of arbitrary smooth shape in [76]. They also had basic estimates and convergence of the Laplacian spectrum in [77]. The interested reader should also see the review [64] by Kuchment, where a brief survey on graph models for wave propagation in thin structures was presented.

Recently, quantum graphs are used in studying nanostructures. Amovilli, Leys, and March, in [2], explained how a quantum network could be used as simple model to calculate complex band structures and provided applications to graphene, boron nitride, and polyacetylene chains. Although physical properties of carbon nanotubes were examined by Saito, G. Dresselhaus, and MS Dresselhaus in [79], carbon nanotubes have also been analyzed using quantum graphs by Kuchment and Post [66] and by Do and Kuchment [33]. Later, Iantchenko and Korotyaev considered the zigzag half-nanotubes in a uniform magnetic field which was described by the magnetic Schrödinger operator with a periodic potential plus a finitely supported perturbation and described all eigenvalues in [53].

The first mathematical approach to the study of the Laplacian on a metric graph is due to Roth in 1984, who derived a trace formula for the spectrum of the Laplacian [75]. The Laplace operator or Laplacian is a differential operator given by the divergence of the gradient of a function on Euclidean space. Such an operator is named after the French mathematician Pierre-Simon de Laplace, who first applied the operator to the study of celestial mechanics [67]. He also formulated Laplace equation, whose solutions, called "Harmonic functions", have found innumerable applications in mathematics and physics. The operator occurs in differential equations that describe many physical phenomena: electric potentials, the diffusion equation

for heat, wave propagation, quantum mechanics, and so on. Studying operators of Schrödinger type, i.e. the Laplace operator with electric potential, on metric graphs is a growing subfield of mathematical physics.

When talking about an operator, one often mentions its eigenvalues. If applying an operator to a function works the same as a constant being multiplied by that function, we say that the constant is an *eigenvalue* of the operator and that function is the corresponding *eigenfunction*. The spectrum of a linear operator A in H consists of all complex number λ such that the operator $A - \lambda I_H$ does not have a bounded inverse. For precise definitions and results concerning quantum graphs and their spectra, we refer the reader to a paper by Kuchment [65].

Diffusion problems on topological networks (one-dimensional networks) has been introduced by Lumer in 1980, see [69]. Later, following the work of Roth, Nicaise established different estimates of the eigenvalues of the Laplacian on a finite topological network in [70] and von Below deduced a characteristic equation for the spectrum of an eigenvalue problem on c^2-networks in [89]. Gerasimenko and Pavlov showed that for a compact graph with semibounded potentials the spectrum of the nonstandard Schrödinger operator was discrete and analyzed the Schrödinger equation on non-compact graphs in [41]. Kostrykin and Schrader [58] classified all vertex matching conditions giving rise to a self-adjoint Laplace operator on a metric graph. Another classification was found by Harmer [49], who used an explicit parameterisation of the Lagrange Grassmannian in terms of unitary matrices. Yet another parametrization of all self-adjoint vertex conditions was suggested in [65] and improved in [40]. The authors of [29] discovered a new form of boundary conditions, called the $PQRS$-form, and gave a natural scheme to design generalized low and high pass quantum filters.

Quantum graphs have been actively used to study properties of dispersion relation of periodic structures. In physics, dispersion relation is the relationship be-

tween oscillation frequency and wave vector. It occurs when pure plane waves of different wavelengths have different propagation velocities. Properties of dispersion relation on periodic graphs are studied by many mathematicians. In [66], Kuchment and Post provided a simple explicit derivation of the dispersion relations for Schrödinger operators on the graphene structure. Do and Kuchment studied the dispersion relations and spectra of invariant Schrödinger operators on a graphyne structure (lithographite) and provided a description of different parts of the spectrum, band-gap structure, and Dirac points in [34]. In her recent work, Do further described the dispersion relations and spectra of periodic Schrödinger operators on a graphyne nanotube structure in [33]. In [50], Harrison *et al.* discussed the frequently arising question on the spectral structure of periodic operators. The authors answered the question, *do the edges of the spectrum occur at the set of "corner" high symmetry points*, in the negative, providing some counter examples. It was also shown that the situation of spectral edges appeared at high symmetry points was stable under small perturbations in some cases.

Existence of gaps in the spectra of operators of mathematical physics plays important role in many areas, as it may be applied to constructions of thin branching structures. Based on the process of graph decoration, i.e., gluing to each vertex of the original graph a copy of a compact "decoration graph", Schenker and Aizenman presented a mechanism for the creation of gaps in the spectra of self-adjoint operators defined over a Hilbert space of functions on a graph in [82]. Similarly, Ong created spectral gaps by replacing each vertex of a graph with a finite graph in his thesis [71]. In [35], authors further presented some results on creating and manipulating spectral gaps for a quantum graph by inserting appropriate internal structures into its vertices.

Quantum graphs have been especially fruitful models for studying the properties

of zeros of the eigenfunctions. Some recent results include bounds on the number of nodal domains, specific formulae for some classes of graphs, variational characterizations, and inverse problems are developed. *Nodal domains* are connected domains of a metric graph on which a function has a constant sign, or equivalently, the connected components that remain after removing the set of points on which the eigenfunction is zero. An extension of Sturm Oscillation Theorem to quantum tree graph was obtained by Pokornyi and Pryadiev [73, 74] and by Schapotschnikow [81], who showed that the n-th eigenfunction on a tree has exactly n nodal domains. The upper bound on the number of nodal domains in $\mathbb{R}^d$ was adapted to metric graphs by Gnutzmann, Weber and Smilansky [43]. In [15], Berkolaiko studied Schrödinger operators on general graphs and found a lower bound for the number of nodal domains of the n-th eigenfunction. In [7], Band *et al.* provided a new interpretation for the nodal deficiency in the case of quantum graphs: it equals the Morse index of an energy functional on a suitably defined space of graph partitions. This discovery was extended to nodal domains of Laplacian on manifolds by Berkolaiko, Kuchment, and Smilansky [23]. In [25], Berkolaiko and Weyand proved an analogue of the magnetic nodal theorem on quantum graphs (see [16]), namely, the number of zeros of the n-th eigenfunction of the Schrödinger operator on a quantum graph is related to the stability of the n-th eigenvalue under perturbation of the operator by magnetic potential. Using this theorem, Band proved that if the n-th eigenfunction of a graph has $n-1$ zeros, then the graph is a tree in [4]. This is the converse theorem of the Sturn's oscillation theorem on trees of [73, 74, 81]. It should be noted that all these results are valid under the assumptions that the eigenvalue is simple and the eigenfunction does not vanish on vertices, see Section 1.2.

1.2 Simple eigenvalues

If the multiplicity of an eigenvalue is one, we say the eigenvalue is *simple*, otherwise it is called *degenerate*. One of the fundamental questions of the spectral theory is that of presence in the spectrum of degenerate (or repeated) eigenvalues. Uhlenbeck, in [87], established generic simplicity of eigenvalues of the Laplace-Beltrami operator on compact manifolds, with respect to the set of all possible metrics on the manifold. Some generic properties of eigenfunctions were also established. For a more general result, see [88]. Since then, various extensions and generalizations of this result have been proven for different circumstances. In [47], Guillemin, Legendre, and Sena-Dias used the first variational formula to reprove an important result of Uhlenbeck's and imposed a question regarding the simple spectrum of a generic Kähler metric.

On graphs, the question of simplicity of eigenvalues was considered by Friedlander in [39], who proved that the eigenvalues are simple generically with respect to the perturbation of the edge lengths of the graph with Neumann conditions. The proof is based on perturbation theory. In [38], Friedlander considered the extremal properties of the eigenvalues of a graph with Neumann conditions. An outline of a shorter proof, under the same conditions, was released by Colin de Verdière [32]. In Section 3, we further generalize the result to a wider range of vertex conditions, namely the δ-type conditions on vertices of the graph. We also investigate the eigenfunctions, showing that generically they did not vanish on vertices, unless this was unavoidable due to presence of looping edges. Both of these results are important in applications, in particular all recent results on the number of zeros of graph eigenfunctions assume both the simplicity of eigenvalues and non-vanishing of eigenfunctions on vertices as a precondition [4, 8, 10, 11, 15, 25].

1.3 Representations, symmetries, and degenerate eigenvalues

A representation is a (linear) action of a group on a vector space. The representation theory of finite groups is a subject started in the late eighteen hundreds. The pioneers in the subject were G. Frobenius, I. Schur, and W. Burnside. Representation theory plays an important role in the classification of finite simple groups. For example, it applies to Burnside's pq-Theorem, where p, q are prime numbers, which states that a non-abelian group of order $p^a q^b$ cannot be simple. It is also a fundamental tool with applications to many areas of mathematics and statisics. Applications of representation theory to graph theory can be found in [31]. Some applications toward the computation of eigenvalues of Cayley graphs are given in [85].

Representations arise naturally in many branches of both mathematics and physics. One of the chief applications of representation theory is to exploit symmetry of a quantum system to facilitate computation of its spectrum. In addition, studying the representations of a group can give information about the group itself. For example, if G is a finite group, then the structure of this group algebra, which is the set of all linear combinations of finitely many elements of G with coefficients in a field, can be described in terms of the irreducible representations of G. For more details on how the representation theory relates to quantum mechanics, see [92].

It is well known that an operator possessing a large group of symmetries has degeneracies in the spectrum. Every eigenspace forms a representation for the group of symmetry. Usually (but not always) there are eigenspaces corresponding to all irreducible representations. If the irreducible representation has dimension bigger than two, the corresponding eigenvalue must be degenerate. If an eigenspace give rise to a reducible representations, such degeneracy is called *accidental*. It is a common physical conjecture that accidental degeneracies do not happen in a typical system.

In constrast, later in this dissertation, we will show that there will be persistent accidental degeneracy in the spectrum of symmetric graphs. It can be confirmed that the same eigenvalues come from different representations.

A related question is that of existence of isospectral graphs. Ever since 1966 Marc Kac asked his famous question: "Can one hear the shape of a drum?" [55], physicists and mathematicians have approached this problem from different aspects. Another way to interpret the question is to ask if the Laplacian on every planar domain with Dirichlet boundary conditions is uniquely determined by its spectrum. Attempts were made to reconstruct the shape of an object from its spectrum and to find different objects that are isospectral, i.e., have the same spectrum. In 1985, Sunada described a method for constructing isospectral Riemannian manifolds [86]. In 1992, based on Sunada's theorem, Gordon, Webb and Wolpert presented the first pair of isospectral two-dimensional planar domains [44, 45]. A set of seventeen isospectral families of planar domains, both Neumann and Dirichlet isospectral, was obtained later by Buser *et al.* [28]. Jakobson *et al.* and Levitin *et al.* found sets of four planar domains that are mutually isospectral by mixing the Neumann and Dirichlet boundary conditions [54, 68]. Gutkin and Smilansky answered Kac's question in the positive for generic quantum graphs with rationally independent edge lengths [48]. Based on representation theory arguments, Band, Parzanchevski, and Ben-Shach presented a method which generalized Sunada's method and enabled one to construct isospectral objects, such as quantum graphs and drums in [12, 72]. Representations can also be used to study the spectrum of a symmetric graph. In [6], authors aim to give explicit and computation-oriented formulas for extracting the part of a Schrödinger operator on a graph which corresponds to a particular representation of the graph's symmetry. The foundations of this work are laid out in Section 4 of this thesis.

1.4 Outline

In this dissertation, we discuss the degeneracies in the eigenvalue spectrum of quantum graphs. First we introduce some definitions that will be used throughout the dissertation and the concept of operators and functions acting on graphs in Section 2. We also provide some basic examples. In Section 3, we present results regarding the generic properties of the eigenvalues and eigenfunctions of a graph under a modification of the lengths of edges. In Section 4, we consider symmetric graphs and investigate the factorization of their secular determinant and its connection with the irreducible representations of the graph of symmetries. Finally in Section 5, we give a summary and talk about future work.

2. PRELIMINARIES: OPERATORS ON GRAPHS

We start by introducing some common graph notions and notation used throughout the dissertation.

2.1 Definitions

Definition 2.1.1. A *graph* Γ consists of a finite set of *vertices* (or *nodes*) $V = \{v_i\}$ and a set $E = \{e_j\}$ of *edges* connecting the vertices. We allow multiple edges and loops (edges connecting a vertex to itself). The *degree* d_v of a vertex v is the number of edges incident to it. A loop contributes twice to the degree of its vertex. Two vertices u and v are *adjacent* if there is at least one edge directly connecting them.

Remark 2.1.2. Below shows that one can turn a quantum graph with loops and multiple edges into an equivalent graph without those.

Definition 2.1.3. A *path* is a sequence $\{x_1, x_2, \ldots, x_n\}$ such that

$$(x_1, x_2), (x_2, x_3), \ldots, (x_{n-1}, x_n)$$

are edges of the graph and the x_i's are distinct. A *cycle* is a path on a graph that begins and ends at the same vertex.

Definition 2.1.4. A *tree* is a graph which is connected and has no cycles.

Definition 2.1.5. The graph Γ is said to be a *metric graph* if each of its edges e is assigned a positive length $l_e \in (0, \infty]$.

We will use x or x_e to denote the coordinate on the edge e. The coordinate starts from one end-vertex of the edge, which is chosen arbitrarily.

Definition 2.1.6. A metric graph is *infinite* if it has infinitely many vertices. Otherwise the graph will be called *finite*. A metric graph is *compact* if the graph is finite and each edge has finite length.

Definition 2.1.7. The space $L_2(\Gamma)$ on Γ consists of functions that are measurable and square integrable on each edge e and such that

$$\|f\|^2_{L_2(\Gamma)} \coloneqq \sum_{e\in E} \|f\|^2_{L_2(e)} < \infty.$$

The *inner product* of two functions on a metric graph Γ is defined by

$$\langle f, g\rangle = \sum_{e\in E} \int_e f(x)\overline{g(x)}dx.$$

The *Sobolev space* $H^1(\Gamma)$ consists of all continuous functions of Γ that belong to $H^1(e)$ for each edge e and such that

$$\|f\|^2_{H^1(\Gamma)} \coloneqq \sum_{e\in E} \|f\|^2_{H^1(e)} < \infty.$$

We denote by $\widetilde{H}^k(\Gamma)$ the space

$$\widetilde{H}^k(\Gamma) \coloneqq \bigoplus_{e\in E} H^k(e),$$

which consists of the functions f on Γ that on each edge e belong to the Sobolev space $H^k(e)$ and such that

$$\|f\|^2_{\widetilde{H}^k} \coloneqq \sum_{e\in E} \|f\|^2_{H^k(e)} < \infty.$$

Definition 2.1.8. An operator H with domain D is *self-adjoint* if $\langle Hf, g\rangle = \langle f, Hg\rangle$

for all functions $f, g \in D$ and the domain of the adjoint H^* is also equal to D.

Definition 2.1.9. A *quantum graph* is a metric graph equipped with a self-adjoint differential operator (usually of Schrödinger type) defined on the edges and with matching conditions specified at the vertices.

In this dissertation, we will study the Laplace operator H defined by

$$H : f \mapsto -\frac{d^2 f}{dx^2}, \tag{2.1.1}$$

acting on the functions that belong to the Sobolev $H^2(e)$ space on each edge e and satisfying the δ-type boundary conditions with coefficients α_v at the vertices of the graph, i.e.,

$$\begin{cases} f(x) \text{ is continuous at } v \\ \sum\limits_{e \in E_v} \dfrac{df}{dx_e}(v) = \alpha_v f(v) \end{cases}, \tag{2.1.2}$$

where for each vertex v, the parameter α_v is a fixed real number. Here the sum is taken over the set E_v of all edges e incident to the vertex v and the derivatives are assumed to be taken in the directions away from the vertex. We will frequently encounter the special case when $\alpha_v = 0$, which is known as the *Neumann (or Kirchhoff) condition*.

Remark 2.1.10. Neumann condition (equation (2.1.2) with $\alpha_v = 0$) at a vertex of degree 2 is equivalent to f being continuously differentiable at v. Therefore, a graph with a Neumann vertex of degree 2 is equivalent to a graph which has no vertex at this location, just a continuous edge. We will often use this fact in reverse, choosing a point on an edge and declaring it to be a vertex of degree 2 with Neumann condition. We will call such a vertex a *trivial vertex*. Introduction of such trivial vertices can turn a graph with multiple edges and loops into a graph without such. This is

convenient for numerical computations where multiple edges can cause unnecessary complications. We will sometimes use the notation (u, v) to denote the edge from the vertex u to the vertex v, implicitly assuming that all multiple edges have been converted by the introduction of vertices of degree two.

Definition 2.1.11. A point $\lambda \in \mathbb{C}$ is said to be an *eigenvalue* of H, if the kernel of the operator $H - \lambda I$ is non-trivial. The elements of this kernel are said to be the *eigenfunctions* corresponding to the eigenvalue λ. The *spectrum* of H consists of all complex $\lambda \in \mathbb{C}$ such that the operator $H - \lambda I$ does not have a bounded inverse.

Definition 2.1.12. Two linear operators are called *isospectral* if they have the same spectrum.

Definition 2.1.13. The eigenpair (λ, f) is called *generic* if the eigenvalue λ is simple and the corresponding eigenfunction f is different than zero on every vertex. Such λ and f in a generic pair are also called *generic*. A quantum graph is *generic* if all of its eigenpairs are generic.

The graphs we consider are undirected. However, it is physically relevant to talk about waves propogating on an edge in a certain direction. This motivates the following definition.

Definition 2.1.14. A *bond* is an edge of a graph together with an assigned direction. The *reversal* b of the bond b is the same edge with the opposite direction. Each edge thus gives rise to two bonds. The *incoming bonds* at a vertex v is the set of bonds such that the direction is pointing into the vertex while the *outgoing bonds* is the set of bonds such that the direction is pointing away from the vertex.

Definition 2.1.15. A *complete graph* K_n with n vertices is a simple undirected graph in which every pair of distinct vertices is connected by a unique edge.

Definition 2.1.16. Let $\lambda = k^2$. Consider the $2|E|$-dimensional complex space, with dimensions indexed by bonds. The *bond scattering matrix* S is defined to be

$$S_{b',b} = \begin{cases} 2/d - 1 & \text{if } b' = \bar{b} \\ 2/d & \text{if } b' \text{ follows } b \text{ and } b' \neq \bar{b} \\ 0 & \text{otherwise} \end{cases}$$

while the matrix $D(k)$ is diagonal with entries

$$D(k)_{b,b} = e^{ikL_b},$$

where L_b the length of the edge b. The edge b' follows b if the end-vertex of b is the start vertex of b'. The *scattering matrix* $S(k)$ for a graph, assuming no multiple edges or loops, with Neumann vertex conditions is

$$S(k) \coloneqq SD(k).$$

The *secular determinant* is the determinant of $S(k)$, i.e.

$$\Sigma(k) = \det\left(\mathbb{I} - S(k)\right).$$

Theorem 2.1.17 ([22])**.** *Consider the eigenvalue problem* $-\dfrac{d^2 f}{dx^2} = \lambda f$ *on a graph with vertex conditions (2.1.2). Then* $\lambda = k^2$ *is an eigenvalue if and only if* k *is a root of the secular equation*

$$\Sigma(k) = 0.$$

2.2 Examples

The eigenvalue problem we will be considering in this dissertation is

$$Hf \coloneqq -f'' = \lambda f = k^2 f, \tag{2.2.1}$$

where for convenience we substituted $\lambda = k^2$, together with the boundary condition (2.1.2). This is a second order linear equation with constant coefficients which for $k > 0$ is readily solved by

$$f(x) = C_1 \cos(kx) + C_2 \sin(kx). \tag{2.2.2}$$

We give some examples here.

Example 2.2.1 (A trivial graph — an interval)**.** An interval $[0, L]$ is the simplest example of a graph; it has two vertices (the endpoints of the interval) and one edge. The continuity condition is empty at every vertex since there is only one edge. We impose Neumann conditions at both vertices, i.e.

$$\begin{cases} f'(0) = 0 \\ -f'(L) = 0 \end{cases}.$$

The minus sign appeared because we agreed to direct the derivatives into the edge.

Consider the eigenvalue problem (2.2.1). Applying the first vertex condition $f'(0) = 0$ to (2.2.2), we get $C_2 = 0$ and $f(x) = C_1 \cos\left(\sqrt{\lambda}x\right)$. The second vertex condition becomes $C_1\sqrt{\lambda}\sin\left(\sqrt{\lambda}L\right) = 0$, which imposes a condition on k. We thus get the *eigenvalues*

$$\lambda = (k\pi/L)^2$$

with the corresponding eigenfunctions

$$f(x) = \cos(k\pi x/L)$$

defined up to an overall constant multiplier (as befits eigenvectors and eigenfunctions).

There is one other eigenvalue in the spectrum that we missed: $\lambda = 0$ with the eigenfunction $f(x) \equiv 1$.

Example 2.2.2 (A star graph with Neumann conditions at endpoints)**.** Consider now a first non-trivial example: a star graph with 3 edges meeting at a central vertex, see Figure 2.1.

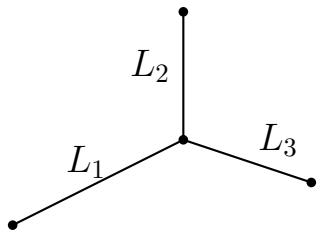

Figure 2.1: A star graph with three edges.

Consider the eigenvalue problem (2.2.1) again. Let f_i be the eigenfunction lies on edge L_i for $i = 1, 2, 3$. Applying Neumann conditions $f_i'(0) = 0$ to equation (2.2.2) at the end vertices, we get

$$f_i(x) = A_i \cos(kx), \quad i = 1, 2, 3$$

for some constants A_1, A_2 and A_3. Note that two conditions are imposed at the

central vertex, namely, Neumann condition and continuity condition, i.e.

$$\begin{cases} -f_1'(L_1) - f_2'(L_2) - f_3'(L_3) = 0 \\ f_1(L_1) = f_2(L_2) = f_3(L_3) \end{cases},$$

which implies that

$$\begin{cases} A_1 \cos(kL_1) = A_2 \cos(kL_2) = A_3 \cos(kL_3) \\ A_1 \sin(kL_1) + A_2 \sin(kL_2) + A_3 \sin(kL_3) = 0 \end{cases}. \tag{2.2.3}$$

Dividing the first equation in (2.2.3) by the second cancels the unknown constants, resulting in

$$\tan(kL_1) + \tan(kL_2) + \tan(kL_3) = 0. \tag{2.2.4}$$

Squares of the roots k of this equation (which cannot be solved explicitly except when all L's are equal) are the eigenvalues of the star graph. If $L := L_1 = L_2 = L_3$, then (2.2.4) implies that $3\sin(kL) = 0$. The eigenvalues are multiple with multiplicity 2, and they are

$$\lambda = (k\pi/L)^2 .$$

If L_i's are rationally independent of each other, then the eigenvalues are simple.

Example 2.2.3 (lasso (lollipop) graph)**.** Assume that on the graph Γ, see Figure 2.2, the Dirichlet condition is assigned at vertex v_1 and the Neumann condition is assigned at vertex v_2. Let l_1, l_2 be lengths of the corresponding edges and f be the eigenfunction. Note that we can always add a vertex v_3 anywhere on the circle with Neumann condition without affecting the conditions for the eigenfunctions on Γ.

First, we may compute $S, D(k)$, and the secular determinant according to the

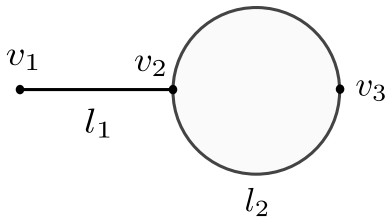

Figure 2.2: A graph with non-Neumann vertex conditions.

definitions.

$$S = \begin{pmatrix} 0 & -1/3 & 2/3 & 2/3 \\ 1 & 0 & 0 & 0 \\ 0 & 2/3 & 2/3 & -1/3 \\ 0 & 2/3 & -1/3 & 2/3 \end{pmatrix},$$

$$D(k) = \begin{pmatrix} e^{ikl_1} & 0 & 0 & 0 \\ 0 & e^{ikl_1} & 0 & 0 \\ 0 & 0 & e^{ikl_2} & 0 \\ 0 & 0 & 0 & e^{ikl_2} \end{pmatrix},$$

and

$$\Sigma(k) = \frac{1}{3}\left(e^{ikl_2} - 1\right)\left(3e^{ik(2l_1+l_2)} - e^{i2kl_1} + e^{ikl_2} - 3\right). \tag{2.2.5}$$

Second, let us consider the eigenvalue problem (2.2.1) again. Since Γ has reflection symmetry, for every eigenfunction f of Γ, f is either odd or even.

Case 1: f is odd, i.e. $f(R_x) = -f(x)$ for each point x on the graph. Since R preserves the points on edge (v_1, v_2),

$$f_1(x) = 0$$

on the edge. This means that the eigenfunction lies only on the circle, say $f_2(x)$. By continuity, $f_1(v_2) = f_2(0) = 0$. Then equation (2.2.2) with Dirichlet condition at v_2 becomes

$$f_2(x) = C_2 \sin\left(\sqrt{\lambda}x\right).$$

At vertex v_3, we know that $-f_2(v_3) = f_2(R_{v_3}) = f_2(v_3)$, which implies that $f_2(v_3) = f_2(l/2) = 0$. Then for $k \in \mathbb{N}$

$$\sqrt{\lambda} = 2k\pi/l_2. \tag{2.2.6}$$

Case 2: f is even, i.e. $f(R_x) = f(x)$ for each point x on the graph. For edge (v_1, v_2), if we set $x = 0$ at v_1, then the Dirichlet condition at v_1 implies that the solution to equation (2.2.1) becomes

$$f_1(x) = A \sin\left(\sqrt{\lambda}x\right)$$

for some constant A. Smiliar argument shows that $f'(l/2) = 0$. If we set $x = 0$ at v_3 on the circle, then the solution to equation (2.2.1) is

$$f_2(x) = B \cos\left(\sqrt{\lambda}x\right)$$

for some constant B. Note that these two eigenfunctions f_1, f_2 lie on edge (v_1, v_2) and on the circle respectively. From the Neumann condition at v_2 and continuity condition at v_2, we have

$$\begin{cases} A\cos\left(\sqrt{\lambda}l_1\right) - 2B\sin\left(\sqrt{\lambda}l_2/2\right) = 0 \\ A\sin\left(\sqrt{\lambda}l_1\right) = B\cos\left(\sqrt{\lambda}l_2/2\right) \end{cases}.$$

This implies that

$$2\sin\left(\sqrt{\lambda}l_1\right)\sin\left(\sqrt{\lambda}l_2/2\right)-\cos\left(\sqrt{\lambda}l_1\right)\cos\left(\sqrt{\lambda}l_2/2\right)=0. \tag{2.2.7}$$

We claim that the eigenvalues of equations (2.2.6) and (2.2.7) will be disjoint, after changing the lengths of edges. Indeed, substitute (2.2.6) into equation (2.2.7), we see that

$$-\cos\left(2k\pi l_1/l_2\right)\cos\left(k\pi\right)=0,$$

which implies that $\cos\left(2k\pi l_1/l_2\right)=0$. If we choose l_1, l_2 to be rationally independent, then the latter condition is never satisfied.

Example 2.2.4 (Quotient graphs of the complete graph K_4)**.** Consider the complete graph K_4 with Neumann conditions on each vertex, see the left of Figure 2.3, where $1,2,3,4$ are vertices and a, b are corresponding edge lengths.

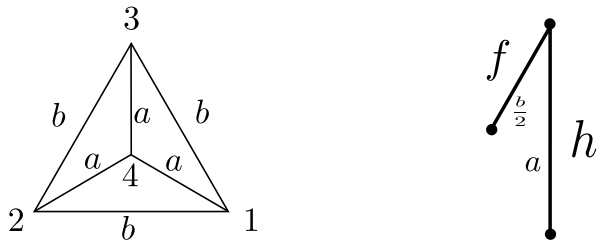

Figure 2.3: The complete graph K_4 and a quotient graph.

By definition, the secular determinant can be computed as

$$\begin{aligned}\Sigma(k)=&\frac{1}{27}\cdot\left(3e^{ik(2a+b)}-e^{i2ak}+e^{ibk}-3\right)\cdot\left(e^{ibk}-1\right)\\&\cdot\left(3e^{i2(a+b)k}+2e^{ik(2a+b)}+e^{i2ak}-e^{i2bk}-2e^{ibk}-3\right)^2.\end{aligned} \tag{2.2.8}$$

Here, we describe another way to obtain the factorizations of the secular determinant. Consider the subgraph of Gamma which is shown on the right of Figure 2.3. We impose vertex conditions shown on the left of Figure 2.4, where N stands for Neumann condition.

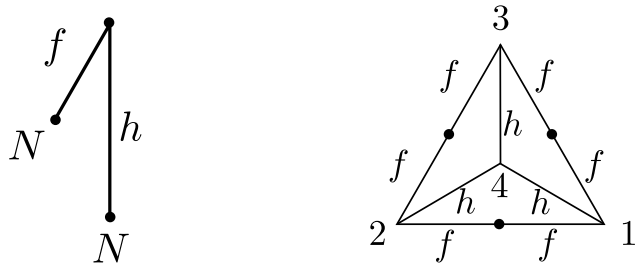

Figure 2.4: K_4 is covered by f and h.

If we have eigenfunctions f and h on the graph shown on the left of Figure 2.4, then K_4 can be covered by f and h as shown on the right of Figure 2.4 by transplanting them around. It is easy to see that the resulting function on the entire graph Gamma is an eigenfunction.

Let us calculate the eigenvalues of the graph on the left of Figure 2.4. Let f and h be defined by

$$f(x) = A_1 \cos(kx) + B_1 \sin(kx),$$
$$h(x) = A_2 \cos(kx) + B_2 \sin(kx)$$

Neumann vertex conditions on the left of Figure 2.4 implies that

$$\begin{cases} h'(a) = 0 \\ f'(b/2) = 0 \end{cases}.$$

Neumann vertex condition and continuity condition on vertex 3 implies that

$$\begin{cases} 2f'(0) + h'(0) = 0 \\ f(0) = h(0) \end{cases}.$$

Combine all these conditions, we get

$$\begin{cases} -A_2 \sin(ka) + B_2 \cos(ka) = 0 \\ -A_1 \sin(bk/2) + B_1 \cos(bk/2) = 0 \\ 2B_1 + B_2 = 0 \\ A_1 = A_2 \end{cases}.$$

This means that $\lambda = k^2$ must satisfies

$$2\cos(ak)\sin(bk/2) + \cos(bk/2)\sin(ak) = 0.$$

Using the identities

$$\sin(x) = \frac{e^{ix} - e^{-ix}}{2i}$$

and

$$\cos(x) = \frac{e^{ix} + e^{-ix}}{2},$$

we can rewrite the expression as

$$e^{i2ak} - e^{ibk} - 3e^{i(2a+b)k} + 3 = 0,$$

which is a factor of $S(k)$.

If we have an eigenfunction f and $h = 0$ on the graph as shown on the left of

Figure 2.5, where D stands for Dirichlet condition, then K_4 can be covered by f and g as shown on the right of Figure 2.5 by transplanting them around. Again we get a valid eigenfunction of the entire graph.

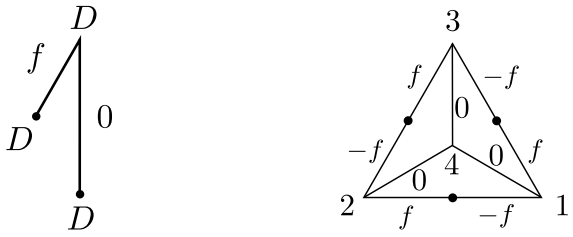

Figure 2.5: K_4 is covered by f and 0.

From the vertex conditions, we get

$$\begin{cases} f(0) = 0 \\ f(b/2) = 0 \end{cases}.$$

This implies that

$$\sin(bk/2) = 0$$

or

$$e^{ibk} - 1 = 0,$$

which is another factor of $S(k)$.

If we have eigenfunctions f_1, f_2 and h on the graph as shown on the left of Figure 2.6, then K_4 can be covered by f_1, f_2 and g as shown on the right two subgraphs of Figure 2.6 by transplanting them around. This time we get two linearly independent eigenfunctions of the whole graph.

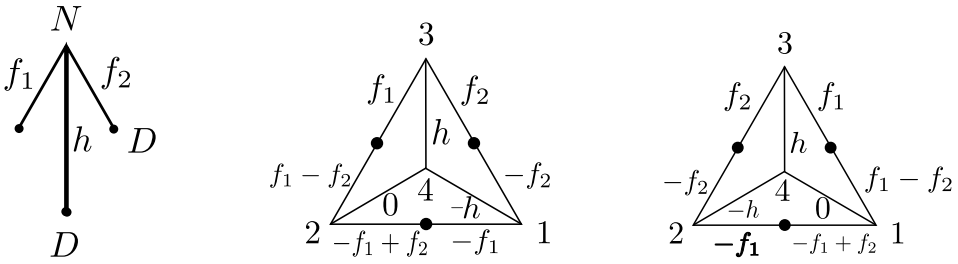

Figure 2.6: K_4 is covered by f_1, f_2 and h.

Define

$$f_i(x) = A_i \cos(kx) + B_i \sin(kx) \quad \text{for } i = 1, 2$$

and

$$h(x) = A_3 \cos(kx) + B_3 \sin(kx).$$

Continuity conditions at vertices $3, 4$ imply that

$$\begin{cases} f_1(0) = f_2(0) \\ f_2(0) = h(0) \\ h(a) = 0 \end{cases}.$$

Continuity conditions in the middle of edges $(1, 3)$ and $(2, 3)$ imply that

$$\begin{cases} f_2(b/2) = 0 \\ f_2'(b/2) - f_1'(b/2) = f_1'(b/2) \end{cases}.$$

Neumann condition at vertex 3 implies that

$$f_1'(0) + f_2'(0) + h'(0) = 0.$$

Combine all these conditions together, we get

$$\begin{cases} A_1 = A_2 \\ A_2 = A_3 \\ A_3\cos(ak) + B_3\sin(ak) = 0 \\ A_2\cos\left(bk/2\right) + B_2\sin\left(bk/2\right) = 0 \\ -A_2\sin\left(bk/2\right) + B_2\cos\left(bk/2\right) = 2\left(-A_1\sin\left(bk/2\right) + B_1\cos\left(bk/2\right)\right) \\ B_1 + B_2 + B_3 = 0 \end{cases}.$$

Then $\lambda = k^2$ must satisfies

$$\sin(ak) + \cos(ak)\sin(bk) + 2\cos(bk)\sin(ak) = 0$$

or

$$e^{i2ak} - e^{i2bk} - 2e^{ibk} + 2e^{i(2a+b)k} + 3e^{i2(a+b)k} - 3 = 0.$$

Since we have two linear independent eigenfunctions, the corresponding eigenvalues are twice degenerate, giving rise to the factor

$$\left(e^{i2ak} - e^{i2bk} - 2e^{ibk} + 2e^{i(2a+b)k} + 3e^{i2(a+b)k} - 3\right)^2$$

in $S(k)$.

These graphs corresponds to irreducible representations of the group of symmetries of the original graph through a construction called "quotient graph" by Band *et al.* [12]. In Section 4, we study these ideas on the level of scattering matrices $S(k)$.

3. SIMPLICITY OF EIGENVALUES AND NON-VANISHING OF EIGENFUNCTIONS OF A QUANTUM GRAPH*

The question we address here is when is it typical (with respect to variation of edge lengths) for a graph to have simple spectrum and to have eigenfunctions that do not vanish on vertices of the graph. To motivate our results, we first consider examples which turn out to be the only cases one needs to take special care about.

3.1 Main results

Definition 3.1.1. A *loop* is a chain of vertices $v,\ v_1,\ \ldots, v_n,\ v$ connected by edges, with each of the intermediate vertices $v_1, \ldots, v_n$ having degree 2. We include the possibility of having $n = 0$, in which case v is connected to itself by a looping edge.

By Remark 2.1.10, a looping edge is equivalent to a loop with intermediate vertices with $\alpha_{v_j} = 0$, see Figure 3.1.

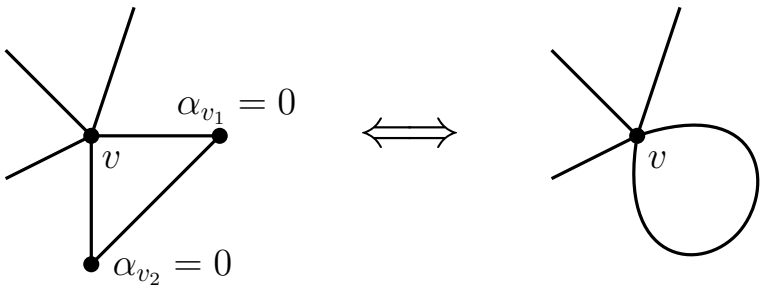

Figure 3.1: If the vertex conditions $\alpha_{v_1} = \alpha_{v_2} = 0$ with $\deg(v_1) = \deg(v_2) = 2$, the loop is equivalent to a looping edge.

Example 3.1.2. Let L be a graph consisting of one looping edge with no vertices. We will call such a graph a *circle*. By Remark 2.1.10 it can be equivalently represented as a cycle graph (a number of vertices connected into a closed chain) with all vertices having $\alpha_v = 0$. It is easy to see that the spectrum of the graph is

$$0,\ \left(\frac{2\pi}{\ell}\right)^2,\ \left(\frac{2\pi}{\ell}\right)^2,\ \left(\frac{4\pi}{\ell}\right)^2,\ \left(\frac{4\pi}{\ell}\right)^2, \dots$$

where ℓ is the length of the looping edge. We note that the double degeneracies in the spectrum *cannot* be resolved by changing the edge length.

The eigenfunctions can be represented as

$$C_1 \cos\left(\sqrt{\lambda}x\right) + C_2 \sin\left(\sqrt{\lambda}x\right) = A \sin\left(\sqrt{\lambda}x + \theta\right), \tag{3.1.1}$$

with constants C_1 and C_2 (or A and θ) arbitrary. Here λ is the eigenvalue and the origin $x = 0$ can be put in an arbitrary location on the graph. It is important to note that for any eigenvalue $\lambda \neq 0$ and any point on the graph, there is an eigenfunction which vanishes at that point.

Example 3.1.3. Consider a graph Γ with a looping edge L, see Figure 3.1. We assume that there are no other (non-trivial) vertices on the loop. The condition at the attachment point v is of δ-type with arbitrary α_v.

If ℓ is the length of the loop, then $(2\pi n/\ell)^2$ is an eigenvalue of Γ for any integer $n > 0$. We demonstrate this by constructing an eigenfunction of Γ. On the loop we take the function f to be equal to the eigenfunction of the corresponding circle, equation (3.1.1), chosen to vanish at the attachment point v. The function f is extended to the rest of the graph Γ by setting it to 0 identically. This obviously

makes f continuous and, since f is an eigenfunction with respect to the loop,

$$\sum_{e\in E_v(\Gamma)} \frac{df}{dx_e}(v) = \sum_{e\in E_v(L)} \frac{df}{dx_e}(v) = 0 = \alpha f(v) \tag{3.1.2}$$

for any α. We thus have an eigenfunction of Γ which is supported exclusively on the loop L; in particular it is zero on all vertices of Γ. Moreover, such an eigenfunction *cannot* be destroyed by changing the edge lengths of graph Γ.

We also note, that the eigenfunction that is supported exclusively on one loop is unique (for a given value of λ). This can be easily seen as the eigenfunction satisfies the Dirichlet problem on the looping edge, which has simple spectrum (see Example 2.2.3).

It turns out that having no other vertices on the loop is an essential feature of Example 3.1.3.

Lemma 3.1.4. *Let* Γ *be a graph with* δ*-type conditions at vertices. Suppose* L *is loop in* Γ *which has at least one vertex with* $\alpha_v \neq 0$ *on it, other than the attachment vertex. Then there is a small modification of edge lengths of* Γ*, after which* Γ *has no eigenfunctions* f *supported exclusively on the loop* L*.*

This lemma, proved in Section 3.3, motivates the following definition.

Definition 3.1.5. A *pure loop* is a loop with no vertices v_j having $\alpha_{v_j} \neq 0$, other than, possibly, the attachment point v. In fact, in what follows, by a "loop" we will always mean a pure loop, unless explicitly stated otherwise. As mentioned already, a graph consisting of one pure loop is called a *circle*; a graph consisting of an impure loop will be called an *impure loop graph*.

Now we are able to formulate our main result.

Theorem 3.1.6. *Let Γ be a connected graph with δ-type conditions at vertices. If Γ is not equivalent to a circle, then, after a small modification of edge lengths, the new graph $\tilde{\Gamma}$ will satisfy the following genericity conditions*

(i) $\sigma(\tilde{\Gamma})$ is simple, and

(ii) for each eigenfunction f of $\tilde{\Gamma}$,

(a) either $f(v) \neq 0$ for each vertex v, or

(b) $\operatorname{supp} f = L$ for only one loop L of $\tilde{\Gamma}$.

More precisely, in the space of all possible edge lengths, the set on which the above conditions are satisfied is residual (also called comeagre).

Remark 3.1.7. In [39], Friedlander proved that the spectrum of a connected metric graph with Neumann vertex conditions that is different from a circle can be made simple after a small pertubation. We extend his result to graphs with arbitrary δ-type vertex conditions and we show that the eigenfunctions are generic. Our proofs are more elementary than those of [39].

Remark 3.1.8. A *residual* or *comeagre* set is a set whose complement is *meagre*. In other words, a residual set is a countable intersection of open dense sets. Informally, a residual set is "large". In particular, since all spaces we will be dealing with (namely, the space of all possible lengths or the space of all points on a graph) are complete metric spaces, by Baire Category Theorem a residual set is dense.

We will show that in the vicinity of any choice of edge length, there is a residual set of lengths on which the theorem holds. As a direct consequence, it holds on a residual set with respect to the whole space of all possible edge lengths, which can be identified with $\mathbb{R}_+^E$.

3.2 Tools and ideas of the proof

In this section we collect the main tools and explain the basic ideas behind the proofs.

Lemma 3.2.1. *Let x be a point on the edge e. Then, in any neighborhood of x there is a residual set of y such that for all eigenfunctions f_n* either *$f_n(y) \neq 0$* or *$f_n \equiv 0$ on the edge e.*

Similarly, given a sequence of values $\{\phi_n\}$, all of them non-zero, there is a residual set of y such that for all normalized eigenfunctions f_n with $\lambda_n > 0$ we have $f_n(y) \neq \phi_n$.

Proof. Fix a neighborhood of x. Any eigenfunction f that is not identically zero on e has only finitely many zeros in the neighborhood: otherwise there is an accumulation point for zeros at which $f = f' = 0$ and, therefore, $f \equiv 0$. The union of the zero points over all possible n is a countable set. On the other hand, the neighborhood has uncountably many points to choose from.

The second part of the lemma is proved analogously, only one need not worry about f_n vanishing identically on the edge. □

The proof of Theorem 3.1.6 is built around modifications made to the structure of a graph. The following theorem describes the type of modification we find useful and its effect on the spectrum. We denote by Γ_α a compact quantum graph with a distinguished vertex v. Arbitrary self-adjoint conditions are fixed at all vertices other than v, while v is endowed with the δ-type condition with coefficient α.

Theorem 3.2.2 (Berkolaiko–Kuchment [21] and [22, Theorem 3.1.8])**.** *Let $\Gamma_{\alpha'}$ be the graph obtained from the graph Γ_α by changing the coefficient of the condition at vertex v from α to α'. If $-\infty < \alpha < \alpha' \leq \infty$ (where $\alpha' = \infty$ corresponds to the*

Dirichlet condition), then

$$\lambda_{n-1}(\Gamma_{\alpha'}) \leq \lambda_n(\Gamma_\alpha) \leq \lambda_n(\Gamma_{\alpha'}). \tag{3.2.1}$$

If the eigenvalue $\lambda_n(\Gamma_\alpha)$ is simple and its eigenfunction f is such that either $f(v)$ or $\sum f'(v)$ is non-zero, then the inequalities can be made strict,

$$\lambda_{n-1}(\Gamma_{\alpha'}) < \lambda_n(\Gamma_\alpha) < \lambda_n(\Gamma_{\alpha'}). \tag{3.2.2}$$

If $\alpha' < \alpha$, the inequalities are adjusted accordingly,

$$\lambda_n(\Gamma_{\alpha'}) < \lambda_n(\Gamma_\alpha) < \lambda_{n+1}(\Gamma_{\alpha'}). \tag{3.2.3}$$

3.3 Proofs of the main results

We begin by establishing the following auxiliary result.

Lemma 3.3.1. *Let Γ be an impure loop graph, i.e. a graph consisting of one loop with at least one vertex with coefficient $\alpha_v \neq 0$. After a small adjustment of edge lengths, its eigenvalues can be made simple.*

Proof. We prove the lemma by induction on the number of vertices with $\alpha_v \neq 0$.

Let Γ_1 be a loop with one vertex v and ℓ be the length of the loop. Parametrize the loop with a coordinate x such that $x = 0$ corresponds to v, $x > 0$ in the clockwise direction and $x < 0$ in the anticlockwise direction. Since Γ_1 has reflection symmetry, every eigenfunction is either odd or even, see Figure 3.2.

If f is odd, it satisfies $f(-x) = -f(x)$ for each point x. In particular, $f(0) = 0$ and, by continuity, $f(\ell/2) = f(-\ell/2) = -f(\ell/2) = 0$. Solving the equation $Hf =$

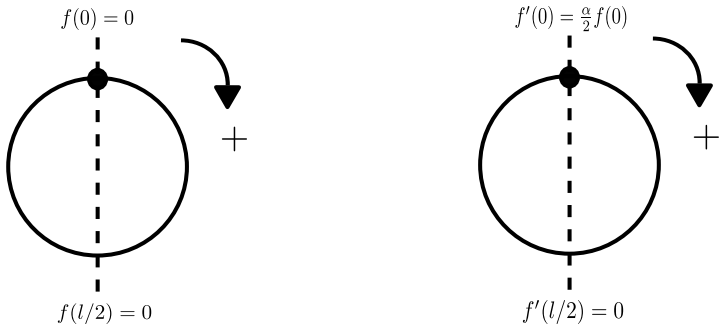

Figure 3.2: A loop with one vertex and the structure of the odd (left) and even (right) eigenfunctions.

λf, we have $f(x) = \sin(\sqrt{\lambda}x)$ and

$$\sqrt{\lambda} = 2k\pi/\ell, \qquad k \in \mathbb{N}. \tag{3.3.1}$$

If f is even, i.e. $f(-x) = f(x)$ for every point x. Since $f'(\ell/2) = -f'(-\ell/2)$ by symmetry and $f'(\ell/2) - f'(-\ell/2) = 0$ by Neumann vertex condition at $\ell/2$, we have $f'(\ell/2) = 0$. At $x = 0$,

$$\sum_{e \in E_0} \frac{df}{dx_e}(0) = \alpha_0 f(0),$$

i.e. $2f'_+(0) = \alpha_0 f(0)$, where f'_+ denotes the one-sided derivative taken at 0 in the positive direction. Solving the equation $Hf = \lambda f$, we have

$$2\sqrt{\lambda} \sin\left(\sqrt{\lambda}\ell/2\right) = \alpha_0 \cos\left(\sqrt{\lambda}\ell/2\right). \tag{3.3.2}$$

The roots of equation (3.3.2) cannot coincide with (3.3.1): the substitution of $\sqrt{\lambda} = 2k\pi/l$ into (3.3.2) results in $0 = \pm\alpha_0$, which contradicts our assumptions. Hence we proved the base case for the induction.

Suppose the statement is true for any impure loop graph with n nonzero vertex

conditions. Consider Γ, an impure loop graph with $n+1$ nonzero vertex conditions. Pick any vertex v and change its vertex condition to Neumann; using inductive hypothesis, adjust the edge lengths to obtain a graph Γ' with simple spectrum. By Lemma 3.2.1 it is now possible to pick a point near the former position of the vertex v, where none of the eigenfunctions are zero. Note that the eigenfunctions cannot vanish on an open subset of the graph, since the unique continuation holds for the impure loop graph. Now we change the vertex condition at the new v back to α_v and use the strict inequalities in Theorem 3.2.2 to conclude that the spectrum is still simple. □

We are now ready to prove Lemma 3.1.4.

Proof of Lemma 3.1.4. Split the loop L at the attachment point v from Γ, see Figure 3.3. Assign Neumann vertex condition to the former attachment point on the loop and keep other vertex conditions unchanged.

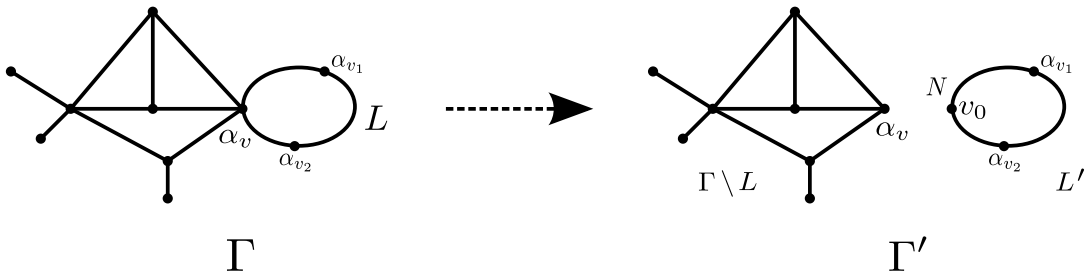

Figure 3.3: Modifications to graph Γ.

Apply Lemma 3.3.1 to L so that $\sigma(L')$ is simple for the changed length loop L'. Furthermore, by Lemma 3.2.1, we can pick a point v_0 near the former attachment point so that each eigenfunction f of L' is nonzero at v_0. Attach L' back to $\Gamma \setminus L$ at v_0. Then the new graph Γ' satisfies the same vertex conditions everywhere as Γ.

If there exists an eigenfunction g of Γ' with $\operatorname{supp} g = L'$, then necessarily $g(v_0) = 0$ and g is an eigenfunction of the loop L' (see equation (3.1.2)), which is a contradiction. □

Before we start the proof of the main theorem, we make some observations.

Remark 3.3.2. If $\lambda = 0$, then the corresponding eigenfunction f of Γ is a constant on every edge, which therefore must be the same (non-zero!) constant throughout the graph by continuity. We conclude that the eigenvalue $\lambda = 0$ is simple and f is non-zero on every vertex. Hence, Theorem 3.1.6 holds for $\lambda = 0$.

Now, we are ready to prove the main theorem.

Proof of Theorem 3.1.6. We may assume $\lambda \neq 0$ by Remark 3.3.2.

We will prove the result by an induction on the number of edges of the graph. If Γ consists of one edge which is not a loop, the statement holds by classical Sturm-Liouville theory. The case of a loop with no non-trivial δ-type vertices is specifically excluded by the assumptions of the theorem. The case of a loop with one vertex v with a non-zero δ-type condition we view as a pure loop with an attachment point (just not attached to anything!). The spectrum is simple by Lemma 3.3.1, while part (ii)(b) of the theorem is true automatically. A loop with more than one non-zero condition is already a graph with at least two edges.

The plan for the inductive step is as follows. First we establish part (i) for a graph Γ if *both parts* of the theorem hold for every graph with a smaller number of edges. Then we will establish part (ii) assuming, in addition to the above, that the spectrum of Γ is simple.

Consider Γ, a connected graph with n edges, satisfying δ-type conditions with coefficients α_v for each vertex v. For the proof of part (i) we consider three cases.

Part (i), case 1. Γ has no loops or cycles, i.e. it is a tree.

Choose an edge e leading to a leaf (a vertex of degree 1) of the tree and split it from the tree. The new one-edge graph we denote by Γ_1 while the rest of the tree is denoted by Γ_2. The attachment point v of that edge is split into two vertices, $v_1 \in \Gamma_1$ and $v_2 \in \Gamma_2$, see Figure 3.4. We assign Neumann condition to vertex v_1. The vertex v_2 inherits the δ-type condition with the constant α_v (which may also be 0), while all other vertices keep their previous conditions.

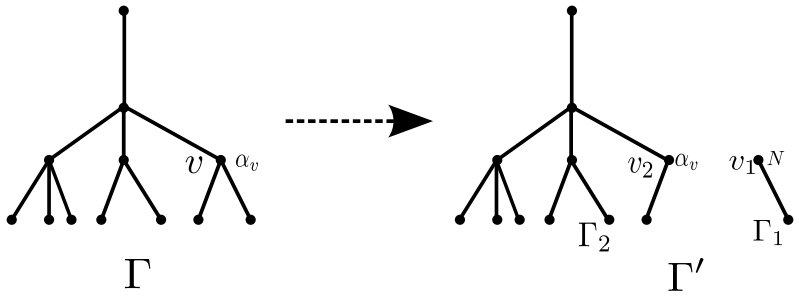

Figure 3.4: Part (i), case 1: splitting away an edge from a tree.

Adjust the edge lengths of Γ_1 and Γ_2 so that

1. both graphs Γ_1 and Γ_2 satisfy (i) and (ii), and

2. $\sigma(\Gamma_1) \cap \sigma(\Gamma_2) = \{0\}$.

Note that $\sigma(\Gamma_1)$ is a set of strictly decreasing functions of the edge length and will have a nonempty intersection with the discrete set $\sigma(\Gamma_2)$ on a meagre set of lengths of e. Altogether, conditions (1) and (2) above are satisfied on a residual set of edge lengths.

Glue v_1 and v_2 back together and call the resulting vertex $\tilde{v}$. The new graph $\tilde{\Gamma}$ has the same vertex conditions as Γ. We claim that the spectrum of Γ is simple. Assume

the contrary, $\lambda \in \sigma(\tilde{\Gamma})$ is multiple with corresponding eigenfunctions f_i. Then we can find a non-zero linear combination $f = \sum a_i f_i$, which is still an eigenfunction of $\tilde{\Gamma}$, such that it is also an eigenfunction *with respect to the graph* Γ_1, i.e. $f'(\tilde{v}) = 0$ along the edge e. Since

$$\alpha_v f(\tilde{v}) = \sum_{e' \in E_{\tilde{v}}} \frac{df}{dx_{e'}}(\tilde{v}) = \sum_{e' \in E_{\tilde{v}} \setminus \{e\}} \frac{df}{dx_{e'}}(\tilde{v}),$$

the function f is also an eigenfunction with respect to the graph Γ_2.

If f is non-zero on both Γ_1 and Γ_2, condition (2) is violated. If f is zero on one of them, it is zero on $\tilde{v}$ which violates condition (1). Therefore, the spectrum of $\tilde{\Gamma}$ is simple.

Part (i), case 2. Γ contains at least one loop.

For each loop L of Γ, we repeat the steps of the previous case, namely,

1. split L away from the rest of Γ at the attachment point v, see Figure 3.5. For $\Gamma \setminus L$, keep α_v vertex condition for the attachment point v_1 and keep all other vertex conditions unchanged. Adjust the lengths of $\Gamma \setminus L$ so that

   $$\Gamma \setminus L \text{ satisfies (i) and (ii)},$$

2. assign Neumann vertex condition to the attachment point v_2 on L; adjust L so that

   $$\sigma(L) \cap \sigma(\Gamma \setminus L) = \{0\},$$

   and glue L back to Γ.

The above conditions can be satisfied for each loop on a residual set of lengths of the graph Γ. Therefore, it can be satisfied for all loops L *simultaneously* on the

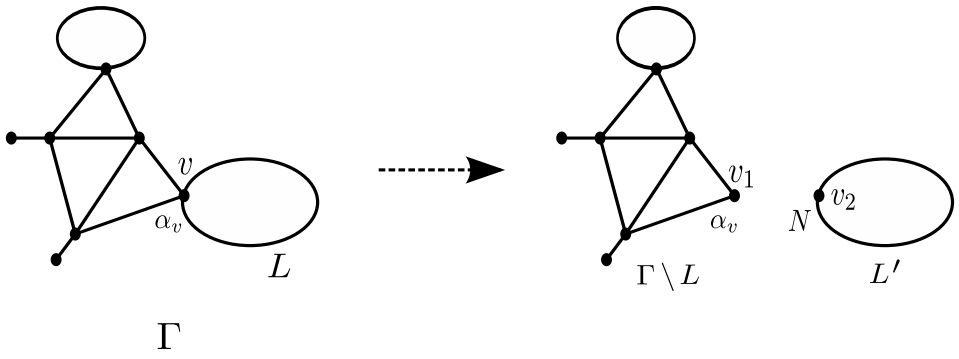

Figure 3.5: Part (i), case 2: splitting away a loop.

intersection of residual sets which is also residual.

Let us first consider λ that is an eigenvalue of some loop L. By Example 3.1.3, $\lambda = (2\pi n/L)^2 \in \sigma(\Gamma)$. Here we abuse the notation slightly by using L to denote both the subgraph containing the looping edge and the length of that edge.

We want to show that the above λ is simple in the spectrum $\sigma(\Gamma)$. Assume the contrary, there is at least one eigenfunction f which is not identically zero on $\Gamma \setminus L$. Transform f by flipping the loop; this is still an eigenfunction which we will denote by $\tilde{f}$. The function $g = (f + \tilde{f})/2$ has the following properties: it is an eigenfunction of Γ, not identically zero on $\Gamma \setminus L$, and its derivatives into the edge L from both sides agree, i.e.

$$g'_L(0) = -g'_L(L).$$

Moreover, we know that g on the edge L takes the form $g = \sin(2\pi nx/L + \theta)$ which by direct computation implies that

$$g'_L(0) = -g'_L(L) = 0.$$

Therefore, the function g satisfies the δ-type conditions at the attachment point v

also with respect to the graph $\Gamma \setminus L$. Thus we get $\lambda \in \sigma(\Gamma \setminus L)$ in contradiction to condition (2) above.

Now, if λ is not an eigenvalue of any loop of Γ, and is multiple, we can find $f = \sum_{i=1}^{2} a_i f_i$ such that f satisfies Neumann vertex condition with respect to some loop L. It must be identically zero on L (otherwise λ is an eigenvalue of L), therefore at the attachment point $f(v) = 0$. Since f is an eigenfunction on the graph $\Gamma \setminus L$, which satisfies (ii), it must be supported on some other loop L', resulting in a contradiction.

Part (i), case 3. Γ contains at least one cycle and no loops.

Pick a vertex v on the cycle such that $\deg(v) \geq 3$. Split Γ at v so that $\deg(v_1) = 2$, $\deg(v_2) \geq 1$, and the graph is still connected (this is possible precisely because v is on a cycle). For the new graph Γ', assign Neumann vertex condition to v_1 and α_v vertex condition to v_2, and keep other vertex conditions unchanged, see Figure 3.6. The vertex v_1 is now trivial, hence Γ' has effectively one edge less than Γ. We can thus use induction and adjust Γ' to satisfy conditions (i) and (ii).

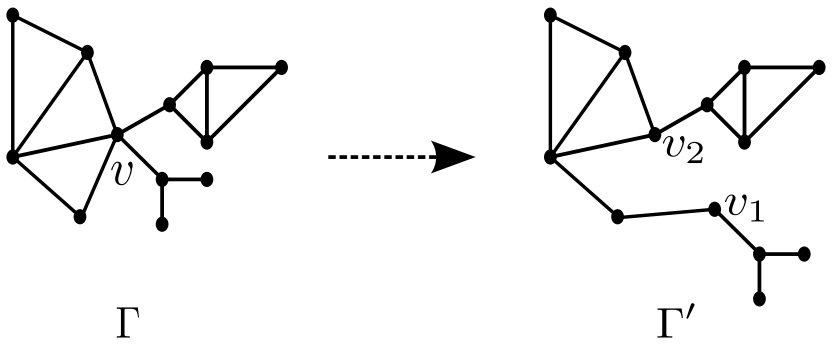

Figure 3.6: Part (i), case 3: splitting a graph with a cycle; each of the new vertices is not on a loop.

First, we show that we can always find a new vertex v_1' near v_1 so that $f(v_1') \neq f(v_2)$ for each eigenfunction f of Γ'. Because our modification of Γ may have created

loops, we need to consider three possibilities:

1. neither v_1 nor v_2 is on a loop. Then Γ' has no loops. Since Γ' satisfies (i) and (ii), $f(v_2) \neq 0$. By Lemma 3.2.1, there exists v_1' so that $f(v_1') \neq f(v_2)$.

2. only one of v_1 and v_2 is on a loop. After relabeling, we may assume that v_1 is on a loop we denote L and v_2 is not on a loop. Since Γ' satisfies (i) and (ii), for each eigenfunction, is not identically 0 in the neighborhood of v_1 and we can again apply Lemma 3.2.1, whether $f(v_2)$ is zero or not.

3. both of v_1 and v_2 are on (pure!) loops, see Figure 3.7. Then $\alpha_v = 0$ and both v_1 and v_2 may be adjusted. Since the eigenfunction cannot vanish identically around both v_1 and v_2 at the same time, we can again use Lemma 3.2.1 to make adjustments until $f(v_1') \neq f(v_2')$.

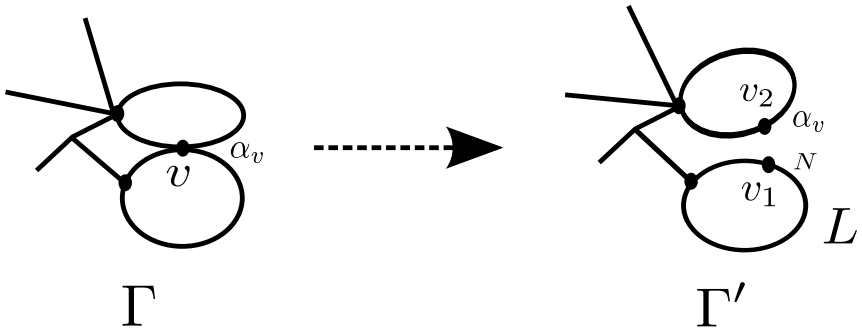

Figure 3.7: Part (i), case 3: splitting a graph with a cycle; both new vertices are on loops.

Now glue v_1' and v_2 (or v_2', if appropriate) together and call the vertex $\tilde{v}$. Note that the new graph $\tilde{\Gamma}$ has the same vertex conditions as Γ. Assume that $\lambda \in \sigma(\tilde{\Gamma})$ is multiple with eigenfunctions f_i. Similarly to above, we can find $f = \sum a_i f_i$, still an

eigenfunction of $\tilde{\Gamma}$, such that it satisfies Neumann condition with respect to edges that were connected to v_1',

$$\sum_{e \in E_{v_1'}} \frac{df}{dx_e}(v_1') = 0.$$

Then f also satisfies α_v vertex condition at v_2. Therefore, f is an eigenfunction of Γ', which means $f(v_1') \neq f(v_2)$, contradicting the fact that f is continuous at $\tilde{v}$ for $\tilde{\Gamma}$. Hence λ is simple.

Proof of part (ii). We will show the statement on a single vertex basis, that is we fix a vertex v and show that each eigenfunction is either non-zero at v or is supported on a loop. This is achieved by small modifications of the graph and holds on a residual set of lengths. As a result will hold at every v on an intersection of residual sets, which is also residual.

First, we assume that the vertex v has Neumann conditions. We may assume that the spectrum of Γ is simple. Also, after a series of modifications we may assume that for each edge e of the graph, $\Gamma \setminus e$ satisfies (i) and (ii). If removing e disconnects the graph, we assume that each of the two components satisfies the assumptions. In the special case when removing an edge creates a new loop, we also ask that the loop states do not vanish at the point where the edge was attached (again achievable by a small movement of the attachment point).

Now let (λ, f) be the n-th eigenpair of Γ such that f vanishes at the chosen vertex v, $f(v) = 0$.

Case 1: $f|_e \equiv 0$ for some edge e incident to v.

Now $f(u) = f(v) = 0$ for the end points u, v of the edge e and f is also an eigenfunction of $\Gamma \setminus e$. Since $\Gamma \setminus e$ satisfies (i) and (ii), $\operatorname{supp} f = L$ for a loop L in $\Gamma \setminus e$. If this loop is present in Γ, we have nothing further to prove. If the loop is not present in Γ, then either u or v lies on the loop and we get a contradiction with

the conditions imposed on $\Gamma \setminus e$ above.

Case 2: $f|_e \not\equiv 0$ for each edge e incident to v.

Parametrizing the edges incident to v so that $x = 0$ at v, we have

$$\begin{cases} -\dfrac{d^2}{dx^2} f = \lambda f =: k^2 f \\ \sum_{e \in E_v} \dfrac{df}{dx_e}(0) = 0 \\ f(0) = 0 \end{cases}, \tag{3.3.3}$$

and therefore

$$f_e(x) = A_e \sin(kx) \qquad \text{and} \qquad \sum_{e \in E_v} A_e = 0.$$

Note that each coefficient $A_e \neq 0$ since $f|_e \not\equiv 0$. At v, we will shorten the edges with $f_e' = A_e > 0$ and lengthen edges with $f_e' < 0$ in a way which will be controlled by a (small) parameter ϵ. Namely, we ask that $f_e(\tilde{v}) = \epsilon$, where $\tilde{v}$ denotes the new position of the vertex v and the function f_e is kept as before, see Figure 3.8.

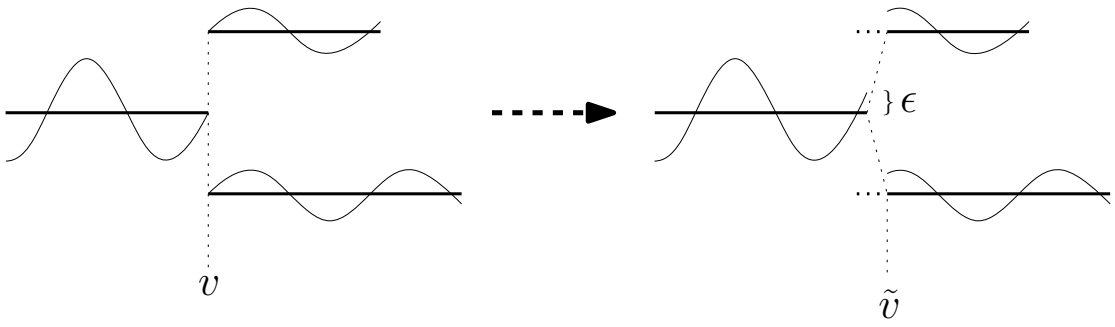

Figure 3.8: Part (ii), case 2: modifying the edge lengths so that $f_e(v)$ becomes equal to ϵ.

In this way, f is still continuous at $\tilde{v}$ and satisfies δ-type vertex condition for some parameter α', which we compute as follows. The new position of the vertex $\tilde{v}$

on edge e is determined by the equation $f_e(x_e) = \epsilon$, or

$$x_i = 1/k \arcsin(\epsilon/A_i).$$

We now find the coefficient α'_v from the condition

$$\sum_{e \in E_v} \frac{df}{dx_e}(\tilde{v}) = \alpha'_v f(\tilde{v}) = \alpha'_v \epsilon,$$

leading to

$$\alpha'_v = \frac{1}{\epsilon} \sum_{e \in E_v} f'_e(\tilde{v}) = \frac{1}{\epsilon} \sum_{e \in E_v} kA_e \cos(kx_e) = -\frac{k\epsilon}{2} \sum_{e \in E_v} \frac{1}{A_e} + O(\epsilon^2) = O(\epsilon).$$

We now consider two families of graphs, continuously depending on the parameter ϵ: Γ' which has the modified edge lengths and the Neumann condition at the vertex v and Γ'' which in addition to changed lengths has $\alpha'_v = \alpha'_v(\epsilon)$ condition computed above.

If the parameter ϵ is small enough, the eigenvalues of three graphs Γ, $\Gamma'(\epsilon)$ and $\Gamma''(\epsilon)$ are still in correspondence. More precisely, for any k and small enough ϵ, the eigenvalue $\lambda_k(\Gamma_1)$ is closer to $\lambda_k(\Gamma_2)$ than to any other eigenvalue of Γ_2 for any two graphs Γ_1 and Γ_2.

We now claim that the n-th eigenfunction of Γ' doesn't vanish on v. Indeed, if $f(v) = 0$, then it is also an eigenfunction of Γ'' (condition (2.1.2) will be satisfied for any α_v) and must have index n due to the correspondence of eigenvalues, but we explicitly constructed the n-th eigenfunction of Γ'' above to have value ϵ on the vertex v. This completes the proof of case 2.

Finally, we have to consider the vertex v with non-Neumann condition: $\alpha_v \neq 0$.

In this case we make edge length adjustments to the graph Γ_0 obtained from Γ by setting $\alpha_v = 0$. Once condition (ii) is satisfied for Γ_0 at v, it is also satisfied for Γ at v. Indeed, if an eigenfunction of Γ vanishes at v, it automatically becomes the eigenfunction of Γ_0, still vanishing at v, which is a contradiction. □

3.4 An application: connectedness of the secular manifolds

In this section we will deal only with graphs with Neumann or Dirichlet vertex conditions. For such a graph Γ it is possible to find the eigenvalues $\lambda = k^2$ as the solutions of the equation

$$F_\Gamma(k) := C \det\left(e^{-ikL/2}\mathbb{I} - e^{ikL/2}S\right) = 0, \tag{3.4.1}$$

where all matrices have dimension $2E$ with E being the number of edges of the graph; they should be thought as operating on vectors indexed by the directed edges of the graph (each edge corresponds to two directed edges, refer to previous definition of bonds in Section 2). The matrix $\mathbb{I}$ is the identity matrix, L is the diagonal matrix populated with the edge lengths and S is a unitary matrix with real entries of known form [61] (the precise form is irrelevant to our discussion). The constant C can be chosen so that F_Γ is real for real k.

Each length appears in the matrix L twice: once for each direction of the edge. As a consequence, the diagonal matrix e^{ikL} has two entries $e^{ik\ell_e}$ for each edge e. Substituting $k\ell_e$ with the torus variables $\varkappa_e \in [0, 2\pi)$, we get the function $\Phi_\Gamma(\varkappa_1, \ldots, \varkappa_E)$ such that

$$\Phi_\Gamma(k\ell_1, \ldots, k\ell_E) = F_\Gamma(k).$$

The solutions $\vec{\varkappa}$ of $\Phi_\Gamma(\vec{\varkappa}) = 0$ form an algebraic subvariety Σ_Γ of the torus $\mathbb{T}^E$. We call Σ_Γ the *secular manifold* of the graph Γ. The study of Σ_Γ as a tool of

understanding eigenvalues of a quantum graphs was pioneered by Barra and Gaspard [13]. An important question is weather the secular manifold is reducible, i.e. if Φ can be decomposed as a product of two analytic functions.

It has been conjectured by Colin de Verdière [32] that the secular manifold is reducible if and only if the graph has a symmetry which is preserved under any change of edge lengths. It can be shown (see [32] for a partial proof) that such a symmetry only exists if the graph is an interval, a circle, a mandarin [10] or has some loops. It is also conjectured that the set of the non-smooth points has co-dimension 2 with respect to the manifold Σ_Γ.

In this section we prove a related result for a family of quantum graphs. We start with some terminology from [32] (whose term for Σ_Γ is "determinant manifold"). A point of Σ_Γ is *smooth* if the differential of Φ_Γ at this point is non-zero. A point $\vec{\varkappa} \neq 0$ is smooth if and only if 1 is a non-degenerate eigenvalue of the graph Γ with edge lengths set to $\ell_e = \varkappa_e$ or, more generally, if $\lambda = k^2$ is an eigenvalue of Γ with lengths ℓ_e such that $\vec{\varkappa} = k\ell_e \mod 2\pi$. In what follows we will omit the "modulo 2π" from the description of points on the torus, to keep the notation compact.

Theorem 3.4.1. *Let the graph Γ have no loops and have a vertex of degree one. Then the set of smooth points of Σ_Γ has two connected components.*

Example 3.4.2. Consider a star graph with three edges (v_0, v_1), (v_0, v_2) and (v_0, v_3) (see Figure 3.9) with Neumann condition at the central vertex v_0 and Dirichlet conditions at the leaves v_1, v_2, v_3.

There are three edges and therefore three torus variables. As we shown in Section 2, the secular function of such a graph has the form

$$\Phi_{\mathrm{star,D}}(\vec{\varkappa}) = \sum_{j=1}^{3} \sin(\varkappa_j)\sin(\varkappa_{j+1})\cos(\varkappa_{j+2}), \tag{3.4.2}$$

Figure 3.9: A star graph with three edges and a mandarin graph with three edges.

where indices of $\varkappa$ are taken modulo 3. The secular manifold for the graph is shown in Figure 3.10. There are four sheets visible but they match pairwise under the torus periodicity. The two sheets touch each other through the conical points of non-smoothness. Similar pictures result if we consider the star graph with Neumann conditions at the leaves, which results in the secular determinant

$$\Phi_{\mathrm{star,N}}(\vec{\varkappa}) = \sum_{j=1}^{3} \cos(\varkappa_j)\cos(\varkappa_{j+1})\sin(\varkappa_{j+2}) = \Phi_{\mathrm{star,D}}(\vec{\varkappa} - \pi/2). \tag{3.4.3}$$

Proof of Theorem 3.4.1. Choose the edge lengths in such a way that

1. the eigenvalue spectrum of Γ is simple and eigenfunctions do not vanish at vertices,

2. the edge lengths are rationally independent.

Denote the vector of the edge lengths by $\vec{\ell}_0$.

Condition (2) implies that the flow $k \mapsto k\vec{\ell}_0$ is ergodic on the torus, and its intersections with the secular manifold are dense in it. The closure of the odd-numbered intersections (within the set of smooth points of Σ_Γ) forms one component and the even-numbered intersections, the other. We will prove that they are mutually disjoint and connected.

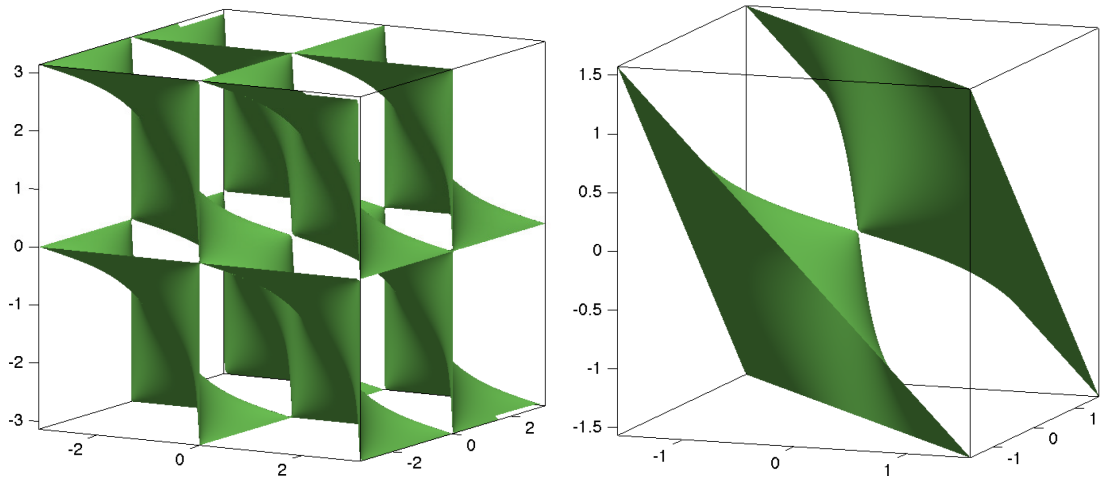

Figure 3.10: Secular manifold of the star graph is shown on the left. It is over $[-\pi, \pi]^3$. Of the four sheets visible, the first and third are parts of the same sheet by the torus periodicity; same for the sheets two and four. A detail of the plot over $[-\pi/2, \pi/2]^3$ is shown on the right.

It is known (see, for example, [4] or [32]) that the gradient of Φ_Γ has either all non-negative components or all non-positive components. Since $k_n = \sqrt{\lambda_n}$ are simple roots of the real-valued function $F_\Gamma(k) = \Phi_\Gamma(k\vec{\ell}_0)$, the derivatives $F'_\Gamma(k_n)$ alternate in sign and therefore the gradient is non-negative on one of the components we defined and non-positive on the other. At a point of intersection of the two components, the gradient must vanish which contradicts the definition of the components.

Let now $\vec{\varkappa}_1$ and $\vec{\varkappa}_2$ be the two points on the same component (without loss of generality, take the component of even-numbered eigenvalues). Surround them by small open neighbourhoods U_1 and U_2, such that $U_j \cap \Sigma_\Gamma$ are connected and contain only smooth points of the same component. From definition of the components we can find two eigenvalues $\lambda_{2n_1} = k_1^2$ and $\lambda_{2n_2} = k_2^2$, $n_1 < n_2$, such that $k_j\vec{\ell}_0 \in U_j \cap \Sigma_\Gamma$, $j = 1, 2$. We now need to show that the points $k_1\vec{\ell}_0$ and $k_2\vec{\ell}_0$ can be connected by a path on Σ_Γ which does not pass through any singular points.

Denote by v the vertex of degree 1 and by e_1 the edge leading to it. The vertex condition at v can be written as

$$\cos(\theta/2)\frac{df}{dx_{e_1}}(v) = \sin(\theta/2)f(v), \tag{3.4.4}$$

with $\theta = \theta_v$ equal to 0 for Neumann and π for Dirichlet. Now we start with the eigenvalue $\lambda = k_2^2$ and continue it analytically by changing θ. According to [21, Thm 6.1] (see also [22, Thm 3.1.13]), the eigenvalue $\lambda(\theta)$ is an analytic function unless there exists an eigenfunction of the graph Γ which satisfies both Dirichlet and Neumann conditions (and thus any other δ-type conditions) at the vertex v. Such an eigenfunction would have to be identically zero on the edge e_1, which we ruled out in condition (1) above. Therefore, $\lambda(\theta)$ is analytic and passes through every eigenvalue of Γ at the points $\theta = 2\pi n + \theta_v$, $n \in \mathbb{Z}$, $n \geq n_0$. In particular, for $n = \tilde{n} := 2(n_1 - n_2) < 0$ we will have $\lambda(\theta) = k_1^2$.

We will now map this λ-path, parametrized by θ decreasing from θ_v to $2\pi\tilde{n} + \theta_v$, to a path on the secular manifold Σ_Γ. Starting with an eigenfunction f on Γ with the vertex condition at v specified by θ, we prolong the edge e_1 to have the length

$$\ell_{e_1}(\theta) := \ell_{0,e_1} + \frac{\theta_v - \theta}{2\sqrt{\lambda(\theta)}}. \tag{3.4.5}$$

A direct calculation shows that the eigenfunction f continued as a sine wave with the same amplitude past the old location of the vertex v will satisfy condition (3.4.4) with $\theta = \theta_v$ at the new location of v.

Define the vector-function $\vec{\ell}(\theta)$ by using (3.4.5) for the component corresponding to e_1 and keeping all other components equal to the corresponding components of $\vec{\ell}_0$. The above discussion shows that the point $\vec{\varkappa}(\theta) = \sqrt{\lambda(\theta)}\vec{\ell}(\theta)$ will remain on the

secular manifold for all θ between θ_v and $2\pi\tilde{n}+\theta_v$ and will pass only through points of multiplicity 1, which are exactly the points of smoothness. This path connects the points $k_1\vec{\ell}_0$ and $k_2\vec{\ell}_0$ as required. The seeming mismatch of lengths at $\theta = 2\pi\tilde{n}+\theta_v$ is due to the modular arithmetic on the torus; here we use the fact that $\tilde{n}$ is even. $\square$

Remark 3.4.3. An identical theorem can be proved for a graph with a bridge, i.e. an edge whose removal disconnects the graph. The method of proof is the same with a point an the bridge being the location where the variable δ-type condition is introduced and the resulting eigenfunction is related to the eigenfunction of the original graph with a longer edge. Whether the same result holds for graphs without such edges (such as the tetrahedron graph — the complete graph on 4 vertices) is still unknown.

Example 3.4.4. The following example shows that there is no direct link between reducibility of the secular manifold and its connectedness. For the mandarin graph with three edges (see Figure 3.9), the secular determinant is reducible: it decomposes into a product of the secular determinants of Dirichlet and Neumann stars due to the reflection symmetry,

$$\Phi_{\text{mandarin}}(\vec{\varkappa}) = \Phi_{\text{star,D}}(\vec{\varkappa}/2)\cdot\Phi_{\text{star,N}}(\vec{\varkappa}/2),$$

see equations (3.4.2) and (3.4.3). Note that while the conditions of Theorem 3.4.1 (or Remark 3.4.3) are not satisfied, the secular manifold still has two connected components, see Figure 3.11.

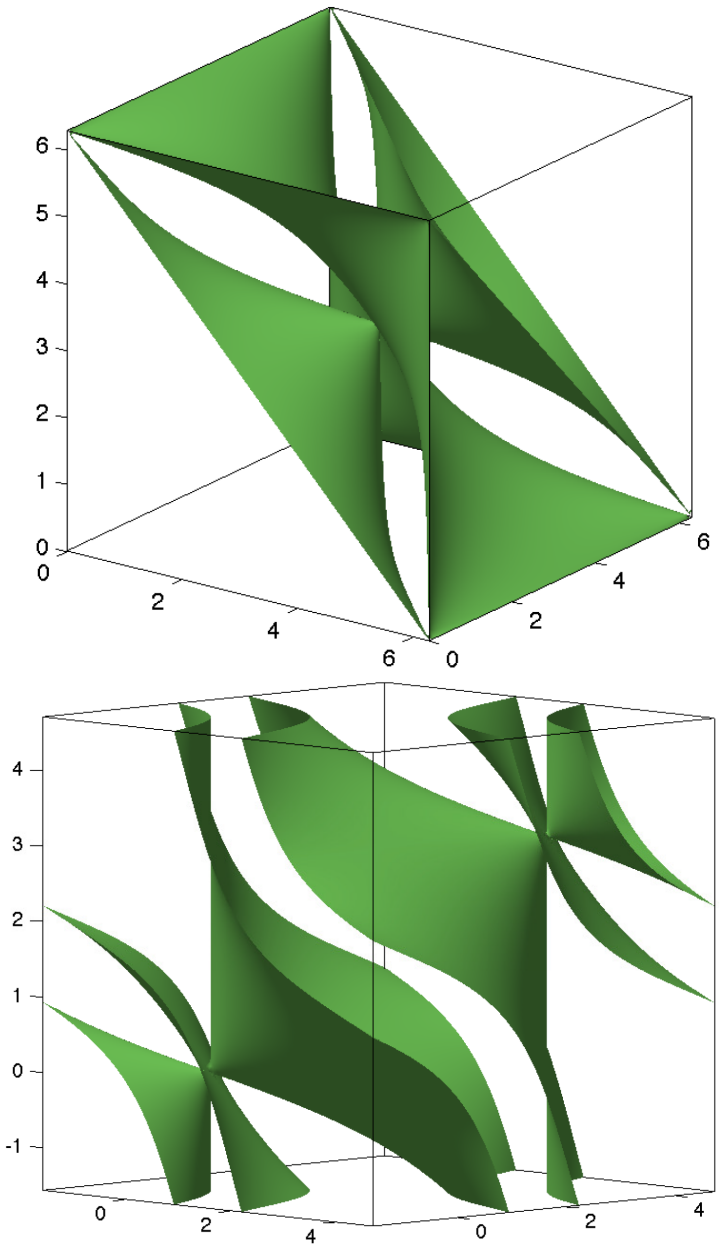

Figure 3.11: Secular manifold of the mandarin graph is shown. The top is shown over $[0, 2\pi]^3$ and, to provide another perspective, the bottome is over $[-\pi/2, 3\pi/2]^3$.

4. SYMMETRY OF QUANTUM GRAPHS AND FACTORIZATION OF THE SPECTRAL DETERMINANT

We study the spectral determinant of symmetric compact quantum graphs with Neumann vertex conditions. We find that it factorizes into a product of factors corresponding to irreducible representation of the group of symmetry. The factorization is traced back to a block-diagonal form of the scattering matrix. We present and prove a computational algorithm for finding the change of basis which brings the scattering matrix to this block-diagonal form.

4.1 Examples

To motivate our results, we first consider some examples. We remind the reader that the spectrum of a graph with Neumann vertex condition can be found via secular determinant by the following theorem.

Theorem 4.1.1 ([22])**.** *Consider the eigenvalue problem (2.2.1) on a graph with Neumann vertex conditions (2.1.2), i.e.* $\alpha_v = 0$ *for each* v *on the graph. Then* $\lambda = k^2$ *is an eigenvalue iff* k *satisfies the secular equation*

$$\det((\mathbb{I} - S(k))) = 0.$$

Example 4.1.2. Consider the lollipop graph with Neumann conditions everywhere as we shown in Section 2. We see that the secular determinant factorizes as show in equation (2.2.5). The lollipop graph is symmetric with respect to flipping the loop. The group of symmetries is thus isomorphic to $\mathbb{Z}_2$.

Example 4.1.3. Consider the star graph with three edges and Neumann vertex conditions, see Figure 4.1.

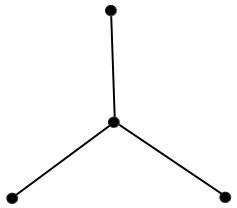

Figure 4.1: A star graph with edges of equal length.

Let the all edge lengths be equal to a. The secular determinant can be computed as

$$\det(\mathbb{I} - S(k)) = -(e^{ika} + 1)(e^{ika} - 1)(e^{i2ka} + 1)^2.$$

Because of the square term, the spectrum cannot be simple by Theorem 4.1.1. The group of symmetries, in this case, is

$$S_3 = \{(1), (12), (13), (23), (123), (132)\}.$$

Example 4.1.4. Consider the complete graph $\Gamma = K_4$ with Neumann conditions on vertices $1, 2, 3, 4$, where vertex 4 is located at the center. Let a, b be the lengths of inside edges and outside edges. As we compute in Section 2, the secular determinant is

$$\begin{aligned}\det(\mathbb{I} - S(k)) =& \frac{1}{27} \cdot \left(3e^{ik(2a+b)} - e^{i2ak} + e^{ibk} - 3\right) \cdot \left(e^{ibk} - 1\right) \\ & \cdot \left(3e^{i2(a+b)k} + 2e^{ik(2a+b)} + e^{i2ak} - e^{i2bk} - 2e^{ibk} - 3\right)^2.\end{aligned}$$

Because of the square term, the spectrum cannot be simple by Theorem 4.1.1, irrespectively of the choice of lengths a and b. This graph is symmetric under any permutation of vertices 1,2, and 3. Hence the group of symmetries is S_3. We will consider this example in more details below.

Now, the question is whether we can interpret the factorizations of the secular determinant. We introduce some definitions from representation theory, see [85].

Definition 4.1.5. A *representation* of a group G is a homomorphism $\rho : G \to GL(V)$ for some (finite-dimensional) complex vector space V. The dimension of V is called the *degree* of ρ.

A representation $\rho : G \to GL(V)$ of a group G is said to be *irreducible* if the only G-invariant subspaces of V are $\{0\}$ and V.

The *character* $\chi_\rho : G \to \mathbb{C}$ of ρ is defined by setting $\chi_\rho = Tr(\rho)$.

Theorem 4.1.6 ([85])**.** *Let $\rho_1, \ldots, \rho_n$ be a complete set of representatives of the equivalence classes of irreducible representations (irreps) of G. Then*

$$\rho \sim m_{\rho_1}\rho_1 \oplus m_{\rho_2}\rho_2 \oplus \cdots \oplus m_{\rho_s}\rho_n,$$

where

$$m_{\rho_j} = \langle \chi_\rho, \chi_{\rho_j} \rangle \coloneqq \frac{1}{|G|} \sum_{g \in G} \chi_\rho(g)\overline{\chi_{\rho_j}(g)}$$

for each $j = 1, \ldots, n$. Consequently, the decomposition of ρ into irreducible constituents is unique and ρ is determined up to equivalence by its character.

Example 4.1.7. Consider the graph $\Gamma = K_4$ in Example 4.1.4 again. We will construct a representation and explore the connections between the factorizations of secular determinant (2.2.8) and the multiplicities m_j's in the decomposition of the representation (4.1.6).

As mentioned above, for $a \neq b$ the symmetric group of the graph Γ is $G = S_3$, where we describe a symmetry transformation as a permutation of vertices. For example, if we apply $g = (12) \in S_3$ to Γ, we switch the vertex 1 with vertex 2, i.e. flipping Γ along edge e_{34}, see Figure 4.2.

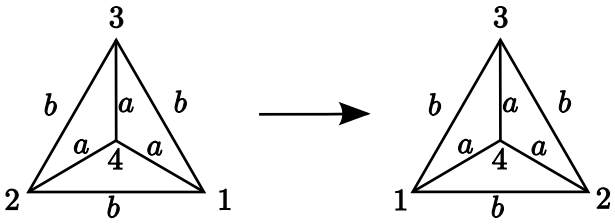

Figure 4.2: Apply $g = (12) \in S_3$ to Γ.

Consider the vector space $V = \mathbb{C}^{12}$. We relabel the standard basis for $\mathbb{C}^{12}$ using the notation e_{ij} for the basis vector corresponding to the bond (i, j) of the graph. We order bonds as follows. Denote by N the number of vertices of Γ. First list all e_{ij}'s such that for each $i = 1, \cdots, N$, j runs through $i + 1$ to N. Second, reverse all the bonds by listing all e_{ij}'s such that for each $j = 1, \cdots, N$, i runs through $j + 1$ to N. The identity matrix is then

$$\mathbb{I}_{12\times 12} = (e_{12}, e_{13}, e_{14}, e_{23}, e_{24}, e_{34}, e_{21}, e_{31}, e_{41}, e_{32}, e_{42}, e_{43}).$$

We define a representation $M = \{M_g : g \in S_3\}$ as a permutation of the basis vectors which reflects the permutation of bonds by the action of g. For example, $M_{(12)}$ represents the graph Γ after applying group action $g = (12) \in S_3$ so that

$$M_{(12)} = (e_{21}, e_{23}, e_{24}, e_{13}, e_{14}, e_{34}, e_{12}, e_{32}, e_{42}, e_{31}, e_{41}, e_{43}).$$

Note that the character of M is just the number of basis vectors fixed by M.

There are three irreps of $G = S_3$, namely, the identity representation R_i

$$R_i = \{\rho_i(g) = (1) : g \in S_3\},$$

the sign representation R_s

$$R_s = \{\rho_s(g) = (\text{sign}(g)) : g \in S_3\},$$

where

$$\text{sign}(g) = \begin{cases} 1 & \text{if } g \text{ is even} \\ -1 & \text{if } g \text{ is odd} \end{cases},$$

and a 2-D representation R_{2d}

$$R_{2d} = \left\{ \begin{array}{lll} (1) \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, & (12) \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & (13) \mapsto \begin{pmatrix} 0 & \omega \\ \omega^2 & 0 \end{pmatrix}, \\ (23) \mapsto \begin{pmatrix} 0 & \omega^2 \\ \omega & 0 \end{pmatrix}, & (123) \mapsto \begin{pmatrix} \omega & 0 \\ 0 & \omega^2 \end{pmatrix}, & (132) \mapsto \begin{pmatrix} \omega^2 & 0 \\ 0 & \omega \end{pmatrix} \end{array} \right\},$$

where ω is the primitive cubic root of 1.

Using the character table of S_3, see Table 4.1, we may compute each m_ρ as stated in Theorem 4.1.6.

$$\begin{aligned} m_i &= \langle \chi_M, \chi_i \rangle = 1/6 \left(\chi_{M_{(1)}} \chi_{i_{(1)}} \cdot 1 + \chi_{M_{(12)}} \chi_{i_{(12)}} \cdot 3 + \chi_{M_{(123)}} \chi_{i_{(123)}} \cdot 2 \right) = 3, \\ m_s &= \langle \chi_M, \chi_s \rangle = 1/6 \left(\chi_{M_{(1)}} \chi_{s_{(1)}} \cdot 1 + \chi_{M_{(12)}} \chi_{s_{(12)}} \cdot 3 + \chi_{M_{(123)}} \chi_{s_{(123)}} \cdot 2 \right) = 1, \\ m_{2d} &= \langle \chi_M, \chi_{2d} \rangle = 1/6 \left(\chi_{M_{(1)}} \chi_{2d_{(1)}} \cdot 1 + \chi_{M_{(12)}} \chi_{2d_{(12)}} \cdot 3 + \chi_{M_{(123)}} \chi_{2d_{(123)}} \cdot 2 \right) = 4. \end{aligned}$$

Therefore, we have

$$M \sim 3R_i \oplus R_s \oplus 4R_{2d}. \tag{4.1.1}$$

We may also compute each m_ρ using the following method. According to the

S_3	(1)	(12)	(123)
size of conjugacy class	1	3	2
χ_i	1	1	1
χ_s	1	-1	1
χ_{2d}	2	0	-1
χ_M	12	2	0

Table 4.1: Character table of S_3.

character table, see Table 4.1, we know that

$$\begin{cases} m_i + m_s + 2m_{2d} = 12 \\ m_i - m_s = 2 \\ m_i + m_s - m_{2d} = 0 \end{cases},$$

which implies that

$$\begin{cases} m_i = 3 \\ m_s = 1 \\ m_{2d} = 4 \end{cases}.$$

Compare the factorizations (2.2.8) of the secular determinant of Γ with the decomposition (4.1.1) of the representation M. We will show that

$$R_i \text{ corresponds to } 3e^{ik(2a+b)} - e^{i2ak} + e^{ibk} - 3,$$
$$R_s \text{ corresponds to } e^{ibk} - 1,$$

and

$$R_{2d} \text{ corresponds to } \left(3e^{i2(a+b)k} + 2e^{ik(2a+b)} + e^{i2ak} - e^{i2bk} - 2e^{ibk} - 3\right)^2.$$

We will also show that

(a) the dimensions of the irreps are the same as the powers of the corresponding factors.

(b) the multiplicities of the irreps m_j's are the degrees of the polynomials inside the parentheses, where the polynomials are expressed in terms of variables

$$z_a = e^{ika} \quad \text{and} \quad z_b = e^{ikb}.$$

4.2 Main results

To extract the part of the operator $S(k)$ acting on a space $\mathbb{C}^{12}$ corresponding to a representation ρ, we need to find the subspace of $\mathbb{C}^{12}$ which transforms according to ρ. More precisely, we are looking for "equivariant vectors" $\phi^1, \ldots, \phi^d$ such that the matrix $\phi = \begin{bmatrix} \phi^1 & \ldots & \phi^d \end{bmatrix}$ satisfies $M_g\phi = \phi\rho(g)$, where $m = \dim X$ and $d = \dim \rho$.

For a $m \times d$ matrix $\phi = \begin{bmatrix} \phi^1 & \cdots & \phi^d \end{bmatrix}$, we define the reshuffling operator

$$\tau_d(\phi) \coloneqq \begin{pmatrix} \phi^1 \\ \vdots \\ \phi^d \end{pmatrix} = \sum_{j=1}^{d} e_j \otimes \phi_j,$$

where $e_j = (0 \ \cdots \ 0 \ 1 \ 0 \ \cdots \ 0)^T$ with 1 on the jth spot is a d-dimensional vector.

Lemma 4.2.1. *Let S be a subset of the group of symmetry G. Then ϕ satisfies intertwining relation $M_g\phi = \phi\rho(g)$ for each $g \in S$ if and only if*

$$\tau_d(\phi) \in \bigcap_{g \in S} \ker \left(\mathbb{I}_d \otimes M_g - \rho(g)^T \otimes \mathbb{I}_m \right).$$

Proof. Note that

$$
\begin{aligned}
&M_g\phi = \phi\rho(g) \text{ for each } g \in S \\
&\Leftrightarrow M_g \left[\phi^1 \ \cdots \ \phi^d\right] = \left[\phi^1 \ \cdots \ \phi^d\right] \rho(g) \\
&\Leftrightarrow \text{for each } r = 1, \ldots, d, \ M_g\phi^r = \left((\rho(g))_{1,r} \, \phi^1 + \cdots + (\rho(g))_{d,r} \, \phi^d \right) \\
&\Leftrightarrow \begin{pmatrix} M_g\phi^1 \\ \vdots \\ M_g\phi^d \end{pmatrix} = \begin{pmatrix} \left(\rho(g)^T\right)_{1,1} \phi^1 + \cdots + \left(\rho(g)^T\right)_{1,d} \phi^d \\ \vdots \\ \left(\rho(g)^T\right)_{d,1} \phi^1 + \cdots + \left(\rho(g)^T\right)_{d,d} \phi^d \end{pmatrix} \\
&\Leftrightarrow \mathbb{I}_d \otimes M_g \begin{pmatrix} \phi^1 \\ \vdots \\ \phi^d \end{pmatrix} = \rho(g)^T \otimes \mathbb{I}_m \begin{pmatrix} \phi^1 \\ \vdots \\ \phi^d \end{pmatrix} \\
&\Leftrightarrow \tau_d(\phi) \in \bigcap_{g \in S} \ker \left(\mathbb{I}_d \otimes M_g - \rho(g)^T \otimes \mathbb{I}_m \right).
\end{aligned}
$$

□

The following theorems, see [83], will be used frequently in our proofs.

Theorem 4.2.2 (Schur's Lemma, First Form)**.** *Let U be an irreducible representation of G on X. Let $T \in Hom(X)$ obey*

$$TU(x) = U(x)T \quad \textit{all } \ x \in G.$$

Then $T = c\mathbb{I}$ for some constant c.

Theorem 4.2.3 (Schur's Lemma, Second Form)**.** *Let U, V be two inequivalent irreps of a finite group G on spaces X, Y. If $T : X \to Y$ is such that*

$$TU(x) = V(x)T \quad \textit{all } \ x \in G,$$

then $T = 0$.

Lemma 4.2.4. *Let* M *be a representation of the symmetric group* G*. For each irrep* ρ *of* G*, we define*

$$\Phi_\rho \coloneqq \bigcap_{g \in G} \ker\left(\mathbb{I}_d \otimes M_g - \rho(g)^T \otimes \mathbb{I}_m\right), \tag{4.2.1}$$

where $d = \dim \rho$ *and* $m = \dim M$*. Let* $\{\phi_{\rho,j}\}_{j=1}^{n}$*, where* $n = \dim \Phi_\rho > 0$*, be an orthogonal basis of* Φ_ρ *normalized to* $||\phi_{\rho,j}||^2 = d$*. Reshuffle each* $\phi_{\rho,j}$*, which is a* $md \times 1$ *vector, into a matrix* $\Psi_{\rho,j} = \tau_d\left(\Phi_{\rho,j}\right)$ *with columns denoted by* $\phi^i_{\rho,j}$*, i.e.*

$$\tau_d\left(\Phi_{\rho,j}\right) = \psi_{\rho,j} = \left[\phi^1_{\rho,j} \;\; \phi^2_{\rho,j} \;\; \cdots \;\; \phi^d_{\rho,j}\right].$$

Then for each ρ*, we have*

$$\psi^*_{\rho,j_1}\psi_{\rho,j_2} = \delta_{j_1,j_2}\mathbb{I}_d, \tag{4.2.2}$$

and for all irreps $\rho_1 \neq \rho_2$ *and* $j_1, j_2 \in \{1, \ldots, n\}$*,*

$$\psi^*_{\rho_1,j_1}\psi_{\rho_2,j_2} = \mathbb{O}_{d_1 \times d_2}, \tag{4.2.3}$$

where $\mathbb{O}_{d_1 \times d_2}$ *is the zero matrix of size* $d_1 \times d_2$*.*

Proof. Inspired by Schur's Lemma (see Theorem 4.2.2), for each fixed irrep ρ, we start with

$$M_g\psi_{\rho,j} = \psi_{\rho,j}\rho(g). \tag{4.2.4}$$

Since both representations, M_g and $\rho(g)$, are unitary, we have $M_g^* = M_{g^{-1}}$ and $\rho(g)^* = \rho(g^{-1})$. Replacing g by g^{-1} in equation (4.2.4), we get

$$M_g^*\psi_{\rho,j} = \psi_{\rho,j}\rho(g)^*.$$

Taking adjoints, we obtain

$$\psi^*_{\rho,j} M_g = \rho(g)\psi^*_{\rho,j}. \tag{4.2.5}$$

Now,

$$\begin{aligned}
\psi^*_{\rho_1,j_1}\psi_{\rho_2,j_2}\rho_2(g) &= \psi^*_{\rho_1,j_1} M_g \psi_{\rho_2,j_2} && \text{by equation (4.2.4)} \\
&= \rho_1(g)\psi^*_{\rho_1,j_1}\psi_{\rho_2,j_2}. && \text{by equation (4.2.5)}
\end{aligned}$$

If $\rho_1 \neq \rho_2$, Theorem 4.2.3 implies that

$$\psi^*_{\rho_1,j_1}\psi_{\rho_2,j_2} = \mathbb{O}_{d_1\times d_2}.$$

If $\rho_1 = \rho_2 = \rho$, Theorem 4.2.2 implies that

$$\psi^*_{\rho,j_1}\psi_{\rho,j_2} = a\mathbb{I}_d$$

for some constant a. The trace on the left side is

$$\begin{aligned}
Tr\left(\psi^*_{\rho,j_1}\psi_{\rho,j_2}\right) &= \langle \phi^1_{\rho,j_1}, \phi^1_{\rho,j_2}\rangle + \langle \phi^2_{\rho,j_1}, \phi^2_{\rho,j_2}\rangle + \cdots + \langle \phi^d_{\rho,j_1}, \phi^d_{\rho,j_2}\rangle \\
&= \langle \phi_{\rho,j_1}, \phi_{\rho,j_2}\rangle \\
&= \delta_{j_1,j_2} d
\end{aligned}$$

using the fact that $\{\phi_{\rho,j}\}_{j=1}^n$ is an orthogonal basis of Φ_ρ while the trace on the right is

$$Tr(a\mathbb{I}_d) = ad.$$

Therefore, $a = \delta_{j_1,j_2}$. □

Remark 4.2.5. Let S be the set of generators of G, then

$$\bigcap_{g\in G} \ker\left(\mathbb{I}_d \otimes M_g - \rho(g)^T \otimes \mathbb{I}_m\right) = \bigcap_{s\in S} \ker\left(\mathbb{I}_d \otimes M_s - \rho(s)^T \otimes \mathbb{I}_m\right).$$

One direction $\bigcap_{g\in S} \ker\left(\mathbb{I}_d \otimes M_g - \rho(g)^T \otimes \mathbb{I}_m\right) \supseteq \bigcap_{g\in G} \ker\left(\mathbb{I}_d \otimes M_g - \rho(g)^T \otimes \mathbb{I}_m\right)$ is clearly true. To prove the other direction, note that for each $j = 1, 2$ and $g_j \in G$, $M_\rho(g_j)\phi = \phi M_\alpha(g_j)$ implies that $M_\rho(g_1g_2)\phi = \phi M_\alpha(g_1g_2)$ since

$$\begin{aligned} M_\rho(g_1g_2)\phi &= M_\rho(g_1)M_\rho(g_2)\phi \\ &= M_\rho(g_1)\phi M_\alpha(g_2) \\ &= \phi M_\alpha(g_1)M_\alpha(g_2) \\ &= \phi M_\alpha(g_1g_2). \end{aligned}$$

For each $\phi \in \bigcap_{s\in S} \ker\left(\mathbb{I}_d \otimes M_s - \rho(s)^T \otimes \mathbb{I}_m\right)$, ϕ satisfies $M_\rho(s)\tau^{-1}(\phi) = \tau^{-1}(\phi)M_\alpha(s)$ for all $s \in S$ by Lemma 4.2.1. Then $M(g)\phi = \phi M(g)$ for all g that are products of generators, that is all $g \in G$. Therefore, $\phi \in \bigcap_{g\in G} \ker\left(\mathbb{I}_d \otimes M_g - \rho(g)^T \otimes \mathbb{I}_m\right)$.

Corollary 4.2.6. *Vectors $\{\phi^r_{\rho,j}\}$ are orthonormal, i.e.*

$$\langle \phi^{r_1}_{\rho_1,j_1}, \phi^{r_2}_{\rho_2,j_2} \rangle = \begin{cases} 1 & \text{if } \rho_1 = \rho_2, j_1 = j_2, r_1 = r_2 \\ 0 & \text{otherwise} \end{cases}.$$

Proof. By writing out equations (4.2.2) and (4.2.3), we see the statement is true. □

Theorem 4.2.7. *For each irrep ρ, let Φ_ρ and $\phi^1_{\rho,j}, \ldots, \phi^d_{\rho,j}$ be defined as in Lemma 4.2.4 for a representation M. For each fixed ρ, define*

$$\tilde{\Psi}_\rho \coloneqq \begin{pmatrix} \phi^1_{\rho,1} & \cdots & \phi^d_{\rho,1} & \phi^1_{\rho,2} & \cdots & \phi^d_{\rho,2} & \cdots\cdots & \phi^1_{\rho,n} & \cdots & \phi^d_{\rho,n} \end{pmatrix}.$$

Now assume that the irrep ρ runs from $\rho_1, \ldots, \rho_L$ for some L, where L is the number of irreps of the group G. If we define

$$\Psi \coloneqq \begin{pmatrix} \tilde{\Psi}_{\rho_1} & \cdots \tilde{\Psi}_{\rho_L} \end{pmatrix},$$

then Ψ is unitary and it will block diagonalize M. Furthermore, for each irrep ρ,

$$m_\rho = n = \dim \Psi_\rho,$$

where m_ρ is the multiplicity in Theorem 4.1.6.

Proof. Note that equations (4.2.2) and (4.2.3) show that Ψ is unitary.

For a fixed irrep ρ, we know that

$$\mathbb{I}_d \otimes M_g \begin{pmatrix} \phi^1_{\rho,j} \\ \vdots \\ \phi^d_{\rho,j} \end{pmatrix} = \rho(g) \otimes \mathbb{I}_m \begin{pmatrix} \phi^1_{\rho,j} \\ \vdots \\ \phi^d_{\rho,j} \end{pmatrix}$$

by the definition of Φ_ρ. More precisely, writing the equality out, we have

$$\begin{pmatrix} M_g \phi^1_{\rho,j} \\ \vdots \\ M_g \phi^d_{\rho,j} \end{pmatrix} = \begin{pmatrix} \rho(g)_{1,1}\phi^1_{\rho,j} + \cdots + \rho(g)_{d,1}\phi^d_{\rho,j} \\ \vdots \\ \rho(g)_{1,d}\phi^1_{\rho,j} + \cdots + \rho(g)_{d,d}\phi^d_{\rho,j} \end{pmatrix},$$

which implies that

$$M_g \phi^r_{\rho,j} = \sum_{s=1}^{d} \rho(g)_{s,r} \phi^s_{\rho,j}$$

for each $r = 1, \ldots, d$.

Now, for two irreps ρ_1, ρ_2 (including the case $\rho_1 = \rho_2$),

$$\left(\phi^{r_2}_{\rho_2,j_2}\right)^* M_g \phi^{r_1}_{\rho_1,j_1} = \sum_{s=1}^{d} \rho_1(g)_{s,r_1} \left(\phi^{r_2}_{\rho_2,j_2}\right)^* \phi^{s}_{\rho_1,j_1} = \delta_{\rho_1,\rho_2}\delta_{j_1,j_2}\rho_1(g)_{r_2,r_1}.$$

Note that each $\phi_{\rho,j}, j = 1, \ldots, n$ is of size $m \times 1$. If we list all $\phi_{\rho,j}$'s as defined in Ψ, we see from the above equation that each nonzero block is of size $d \times d$, where $d = \dim \rho$. There are $n = \dim \Psi_\rho$ blocks, indexed by j, corresponding to ρ. These blocks are identical. Since the decomposition into irreps is unique by Theorem 4.1.6, we know that $m_\rho = n = \dim \Psi_\rho$. □

In fact, as we can see from the following theorem, not only M can be block diagonalized, but also $S(k)$. Note that the vectors $\{\phi^r_{\rho,j}\}$ should be ordered differently.

Theorem 4.2.8. *For each irrep ρ, let Φ_ρ and $\phi^1_{\rho,j}, \ldots, \phi^d_{\rho,j}$ be defined as in Lemma 4.2.4 for a graph Γ. For each fixed ρ, define*

$$\tilde{\Phi}_\rho \coloneqq \begin{pmatrix} \phi^1_{\rho,1} & \cdots & \phi^1_{\rho,n} & \phi^2_{\rho,1} & \cdots & \phi^2_{\rho,n} & \cdots\cdots & \phi^d_{\rho,1} & \cdots & \phi^d_{\rho,n} \end{pmatrix}.$$

Now assume that the irrep ρ runs from $\rho_1, \ldots, \rho_L$, where L is the number of irreps of the group G. If we define

$$\Phi \coloneqq \begin{pmatrix} \tilde{\Phi}_{\rho_1} & \cdots \tilde{\Phi}_{\rho_L} \end{pmatrix},$$

then Φ is unitary and it will block diagonalize the scattering matrix $S(k)$ of Γ. Furthermore, blocks of the same irreps are identical.

Proof. Note that equations (4.2.2) and (4.2.3) show that Φ is unitary.

Since the graph Γ is symmetric with respect to $g \in G$, we know that

$$M_g S(k) = S(k) M_g$$

for each $g \in G$. Now,

$$\begin{aligned}
\psi^*_{\rho_1,j_1} S(k) \psi_{\rho_2,j_2} \rho_2(g)^* &= \psi^*_{\rho_1,j_1} S(k) M_g \psi_{\rho_2,j_2} && \text{by equation (4.2.4)} \\
&= \psi^*_{\rho_1,j_1} M_g S(k) \psi_{\rho_2,j_2} \\
&= \rho_1(g)^* \psi^*_{\rho_1,j_1} S(k) \psi_{\rho_2,j_2}. && \text{by equation (4.2.5)}
\end{aligned}$$

By Theorem 4.2.2 and Theorem 4.2.3, we know that

$$\psi^*_{\rho_1,j_1} S(k) \psi_{\rho_2,j_2} = \delta_{\rho_1,\rho_2} C(S(k), j_1, j_2) \mathbb{I} \tag{4.2.6}$$

for some constant C depending on $S(k), j_1$, and j_2. That is,

$$\langle \phi^{r_1}_{\rho_1,j_1}, S(k) \phi^{r_2}_{\rho_2,j_2} \rangle = \delta_{\rho_1,\rho_2} \delta_{r_1,r_2} C(S(k), j_1, j_2).$$

We can see from equation (4.2.6) that we get d blocks, indexed by r, and that blocks from the same irreps are identical. □

Example 4.2.9. Consider again the star graph from Example 4.1.3. Let all edge lengths be equal to a. The group of symmetry is S_3. We will find the null spaces as indicated in Lemma 4.2.4 and apply Theorem 4.2.7 and 4.2.8.

Note that the number of elements in the representation set $M = \{M_g : g \in S_3\}$ is 6, which is the size of S_3. We only list the generators of the set M here. Other representations $M_g \in M$ can be otained similarly by switching corresponding column

vectors.

$$
\begin{aligned}
M_{(1)} &= \mathbb{I}_6 \\
&= (e_{(14)} \;\; e_{(24)} \;\; e_{(34)} \;\; e_{(41)} \;\; e_{(42)} \;\; e_{(43)}), \\
M_{(12)} &= (e_{(24)} \;\; e_{(14)} \;\; e_{(34)} \;\; e_{(42)} \;\; e_{(41)} \;\; e_{(43)}) \\
&= \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}, \\
M_{(13)} &= (e_{(34)} \;\; e_{(24)} \;\; e_{(14)} \;\; e_{(43)} \;\; e_{(42)} \;\; e_{(41)}) \\
&= \begin{pmatrix}
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 0
\end{pmatrix}.
\end{aligned}
$$

The character of M is shown as in Table 4.2.

By Theorem 4.1.6, we know that

$$M \sim 2R_i \oplus 2R_{2d}.$$

We may compute S and $D(k)$ as follows.

S_3	(1)	(12)	(123)
size of conjugacy class	1	3	2
χ_i	1	1	1
χ_s	1	-1	1
χ_{2d}	2	0	-1
χ_M	6	2	0

Table 4.2: Character table of M.

$$S = \begin{pmatrix} 0 & 0 & 0 & -1/3 & 2/3 & 2/3 \\ 0 & 0 & 0 & 2/3 & -1/3 & 2/3 \\ 0 & 0 & 0 & 2/3 & 2/3 & -1/3 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

and

$$D(k) = e^{ika}\mathbb{I}_6.$$

For the identity representation R_i, equation (4.2.1) (for Φ_i) becomes

$$\Phi_i = \ker \begin{pmatrix} M_{(12)} - \mathbb{I}_{12} \\ M_{(13)} - \mathbb{I}_{12} \end{pmatrix} =: \operatorname{span}\left\{ (\phi^1_{i,1} \;\; \phi^1_{i,2}) \right\},$$

where

$$\phi^1_{i,1} = 1/\sqrt{3}(0,0,0,1,1,1)^T,$$
$$\phi^1_{i,2} = 1/\sqrt{3}(1,1,1,0,0,0)^T.$$

Here we may take the kernel over the generators (12) and (13) of S_3 by Remark 4.2.5.

For the sign representation R_s, equation (4.2.1) (for Φ_s) becomes

$$\Phi_s = \ker \begin{pmatrix} M_{(12)} + \mathbb{I}_{12} \\ M_{(13)} + \mathbb{I}_{12} \end{pmatrix} = \{0\}.$$

For the $2d$ representation R_{2d}, equation (4.2.1) (for Φ_{2d}) becomes

$$\begin{aligned} \Phi_{2d} &= \ker \begin{pmatrix} \mathbb{I}_2 \otimes M_{(12)} - \rho_{2d}^T(12) \otimes \mathbb{I}_{12} \\ \mathbb{I}_2 \otimes M_{(13)} - \rho_{2d}^T(13) \otimes \mathbb{I}_{12} \end{pmatrix} \\ &= \ker \begin{pmatrix} M_{(12)} & -\mathbb{I}_{12} \\ -\mathbb{I}_{12} & M_{(12)} \\ M_{(13)} & -\omega^2 \mathbb{I}_{12} \\ -\omega \mathbb{I}_{12} & M_{(13)} \end{pmatrix} \\ &=: \operatorname{span} \left\{ \begin{pmatrix} \phi_{2d,1}^1 & \phi_{2d,2}^1 \\ \phi_{2d,1}^2 & \phi_{2d,2}^2 \end{pmatrix} \right\}, \end{aligned}$$

where

$$\begin{aligned} \phi_{2d,1}^1 &= 1/\sqrt{3}(0,0,0,\omega,\omega^2,1)^T, \\ \phi_{2d,2}^1 &= 1/\sqrt{3}(\omega,\omega^2,1,0,0,0)^T, \\ \phi_{2d,1}^2 &= 1/\sqrt{3}(0,0,0,\omega^2,\omega,1)^T, \\ \phi_{2d,2}^2 &= 1/\sqrt{3}(\omega^2,\omega,1,0,0,0)^T. \end{aligned}$$

By Theorem 4.2.7, the matrix

$$\Psi := \begin{pmatrix} \phi_{i,1}^1 & \phi_{i,2}^1 & \phi_{2d,1}^1 & \phi_{2d,1}^2 & \phi_{2d,2}^1 & \phi_{2d,2}^2 \end{pmatrix}$$

$$= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 & 0 & 0 & \omega & \omega^2 \\ 0 & 1 & 0 & 0 & \omega^2 & \omega \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & \omega & \omega^2 & 0 & 0 \\ 1 & 0 & \omega^2 & \omega & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

should block diagonalize M. Indeed, we have

$$\Psi^* M_{(12)} \Psi = \begin{pmatrix} \boxed{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & \boxed{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{0} & \boxed{1} & 0 & 0 \\ 0 & 0 & \boxed{1} & \boxed{0} & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{0} & \boxed{1} \\ 0 & 0 & 0 & 0 & \boxed{1} & \boxed{0} \end{pmatrix}$$

and

$$\Psi^* M_{(13)} \Psi = \begin{pmatrix} \boxed{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & \boxed{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{0} & \boxed{\omega^2} & 0 & 0 \\ 0 & 0 & \boxed{\omega} & \boxed{0} & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{0} & \boxed{\omega^2} \\ 0 & 0 & 0 & 0 & \boxed{\omega} & \boxed{0} \end{pmatrix}.$$

Note that the blocks of $\Psi^* M_g \Psi$ are the matrices $\rho(g)^T$ of the suitable ρ (two ρ_i and two ρ_{2d}).

According to Theorem 4.2.8, if we rearrange the vectors $\{\phi^r_{\rho,j}\}$, then the matrix

$$\Phi := (\phi^1_{i,1} \;\; \phi^1_{i,2} \;\; \phi^1_{2d,1} \;\; \phi^1_{2d,2} \;\; \phi^2_{2d,1} \;\; \phi^2_{2d,2})$$

$$= \frac{\sqrt{3}}{3} \begin{pmatrix} 0 & 1 & 0 & \omega & 0 & \omega^2 \\ 0 & 1 & 0 & \omega^2 & 0 & \omega \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & \omega & 0 & \omega^2 & 0 \\ 1 & 0 & \omega^2 & 0 & \omega & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}$$

should block diagonalize $S(k)$. Indeed, we have

$$\Phi^* S(k) \Phi = \begin{pmatrix} 0 & e^{ika} & 0 & 0 & 0 & 0 \\ e^{ika} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{ika} & 0 & 0 \\ 0 & 0 & -e^{ika} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{ika} \\ 0 & 0 & 0 & 0 & -e^{ika} & 0 \end{pmatrix}.$$

Example 4.2.10. Consider the group action $G = S_3$ acting on the complete graph K_4 again; see Example 4.1.4. We will find the null spaces as indicated in Lemma 4.2.4 and apply Theorem 4.2.7 and 4.2.8.

For the identity representation, equation (4.2.1) (for Φ_i) becomes

$$\Phi_i \in \ker \begin{pmatrix} M_{(12)} - \mathbb{I}_{12} \\ M_{(13)} - \mathbb{I}_{12} \end{pmatrix} =: \operatorname{span} \left\{ \begin{pmatrix} \phi^1_{i,1} & \phi^1_{i,2} & \phi^1_{i,3} \end{pmatrix} \right\},$$

where

$$\phi^1_{i,1} = 1/\sqrt{3}(1/\sqrt{2}, 1/\sqrt{2}, 0, 1/\sqrt{2}, 0, 0, 1/\sqrt{2}, 1/\sqrt{2}, 0, 1/\sqrt{2}, 0, 0)^T,$$

$$\phi^1_{i,2} = 1/\sqrt{3}(0,0,1,0,1,1,0,0,0,0,0,0)^T,$$
$$\phi^1_{i,3} = 1/\sqrt{3}(0,0,0,0,0,0,0,0,0,1,0,1,1)^T.$$

For the sign representation, equation (4.2.1) (for Φ_s) becomes

$$\Phi_s \in \ker \begin{pmatrix} M_{(12)} + \mathbb{I}_{12} \\ M_{(13)} + \mathbb{I}_{12} \end{pmatrix} =: \operatorname{span}\left\{\left(\phi^1_{s,1}\right)\right\},$$

where

$$\phi^1_{s,1} = 1/\sqrt{6}(-1,1,0,-1,0,0,1,-1,0,1,0,0)^T.$$

For the $2d$ representation, equation (4.2.1) (for Φ_{2d}) becomes

$$\begin{aligned}\Phi_{2d} &= \ker \begin{pmatrix} \mathbb{I}_2 \otimes M_{(12)} - \rho^T_{2d}(12) \otimes \mathbb{I}_{12} \\ \mathbb{I}_2 \otimes M_{(13)} - \rho^T_{2d}(13) \otimes \mathbb{I}_{12} \end{pmatrix} \\ &= \ker \begin{pmatrix} M_{(12)} & -\mathbb{I}_{12} \\ -\mathbb{I}_{12} & M_{(12)} \\ M_{(13)} & -\omega^2\mathbb{I}_{12} \\ -\omega\mathbb{I}_{12} & M_{(13)} \end{pmatrix} \\ &=: \operatorname{span}\left\{ \begin{pmatrix} \phi^1_{2d,1} & \phi^1_{2d,2} & \phi^1_{2d,3} & \phi^1_{2d,4} \\ \phi^2_{2d,1} & \phi^2_{2d,2} & \phi^2_{2d,3} & \phi^2_{2d,4} \end{pmatrix} \right\},\end{aligned}$$

where

$$\phi^1_{2d,1} = 1/\sqrt{3}(\omega^2,0,0,\omega,0,0,0,1,0,0,0,0)^T,$$
$$\phi^1_{2d,2} = 1/\sqrt{3}(0,\omega^2,0,0,0,0,\omega,0,0,1,0,0)^T,$$
$$\phi^1_{2d,3} = 1/\sqrt{3}(0,0,\omega^2,0,\omega,1,0,0,0,0,0,0)^T,$$

$$\phi^1_{2d,4} = 1/\sqrt{3}(0,0,0,0,0,0,0,0,\omega^2,0,\omega,1)^T,$$
$$\phi^2_{2d,1} = 1/\sqrt{3}(\omega,0,0,\omega^2,0,0,0,1,0,0,0,0)^T,$$
$$\phi^2_{2d,2} = 1/\sqrt{3}(0,\omega,0,0,0,0,\omega^2,0,0,1,0,0)^T,$$
$$\phi^2_{2d,3} = 1/\sqrt{3}(0,0,\omega,0,\omega^2,1,0,0,0,0,0,0)^T,$$
$$\phi^2_{2d,4} = 1/\sqrt{3}(0,0,0,0,0,0,0,0,\omega,0,\omega^2,1)^T.$$

By Theorem 4.2.7, the matrix

$$\Psi \coloneqq \left(\phi^1_{i,1}\ \phi^1_{i,2}\ \phi^1_{i,3}\ \phi^1_{s,1}\ \phi^1_{2d,1}\ \phi^2_{2d,1}\ \phi^1_{2d,2}\ \phi^2_{2d,2}\ \phi^1_{2d,3}\ \phi^2_{2d,3}\ \phi^1_{2d,4}\ \phi^2_{2d,4}\right)$$

should block diagonalize M. Indeed, for example, we have

$$\Psi^* M_{(12)} \Psi = \begin{pmatrix}
\boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \boxed{-1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \boxed{0} & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \boxed{1} & \boxed{0} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{1} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & \boxed{0} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{1} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & \boxed{0} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{1} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & \boxed{0}
\end{pmatrix}.$$

According to Theorem 4.2.8, if we rearrange the vectors $\{\phi^r_{\rho,j}\}$, then the matrix

$$\Phi \coloneqq (\phi^1_{i,1}\ \phi^1_{i,2}\ \phi^1_{i,3}\ \phi^1_{s,1}\ \phi^1_{2d,1}\ \phi^1_{2d,2}\ \phi^1_{2d,3}\ \phi^1_{2d,4}\ \phi^2_{2d,1}\ \phi^2_{2d,2}\ \phi^2_{2d,3}\ \phi^2_{2d,4})$$

should block diagonalize $S(k)$. Indeed, we have

$$\Phi^* S(k)\Phi = \begin{pmatrix} A^{S(k)}_{i,3\times 3} & 0 & 0 & 0 \\ 0 & B^{S(k)}_{s,1\times 1} & 0 & 0 \\ 0 & 0 & C^{S(k)}_{2d,4\times 4} & 0 \\ 0 & 0 & 0 & C^{S(k)}_{2d,4\times 4} \end{pmatrix},$$

where $A^{S(k)}_{i,3\times 3}, B^{S(k)}_{s,1\times 1}$, and $C^{S(k)}_{2d,4\times 4}$ are block matrices defined as below.

$$A^{S(k)}_{i,3\times 3} = \begin{pmatrix} 0 & 0 & e^{iak} \\ 2\sqrt{2}e^{ibk}/3 & e^{ibk}/3 & 0 \\ -e^{iak}/3 & 2\sqrt{2}e^{iak}/3 & 0 \end{pmatrix},$$

$$B^{S(k)}_{s,1\times 1} = \left(e^{ibk}\right),$$

and

$$C^{S(k)}_{2d,4\times 4} = \begin{pmatrix} -(1+\sqrt{3}i)e^{ibk}/9 & 0 & 2e^{ibk}/9 & -(1+\sqrt{3}i)e^{ibk}/18 \\ -(1+\sqrt{3}i)e^{iak}/9 & 0 & -e^{iak}/9 & (1+\sqrt{3}i)e^{iak}/9 \\ 0 & -e^{iak}/3 & 0 & 0 \\ (1+\sqrt{3}i)e^{ibk}/18 & 0 & 2e^{ibk}/9 & (1+\sqrt{3}i)e^{ibk}/9 \end{pmatrix}.$$

4.3 More symmetries for the tetrahedron

Note that the complete graph K_4 can support more symmetries than S_3. More precisely, if we let all edges be of equal length, the complete group of symmetries is S_4, which is generated by permutations $(12), (13)$, and (14). This is a permutation of all four vertices. In this section, we apply Lemma 4.2.4 to the tetrahedron.

There are five irreps of S_4, namely, the identity representation R_i

$$R_i = \{\rho_i(g) = (1) : g \in S_3\},$$

the sign representation R_s

$$R_s = \{\rho_s(g) = (\text{sign}(g)) : g \in S_3\},$$

where

$$\text{sign}(g) = \begin{cases} 1 & \text{if } g \text{ is even} \\ -1 & \text{if } g \text{ is odd} \end{cases},$$

a 2-D representation R_{2d}

$$R_{2d} = \left\{ (12) \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (13) \mapsto \begin{pmatrix} 0 & \overline{\omega} \\ \overline{\omega}^2 & 0 \end{pmatrix}, \quad (14) \mapsto \begin{pmatrix} 0 & \overline{\omega}^2 \\ \overline{\omega} & 0 \end{pmatrix} \right\},$$

where ω is the primitive cubic root of 1, and two 3-D representations $R_{3d,1}$ and $R_{3d,2}$ as follows

$$R_{3d-1} = \left\{ (12) \mapsto \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad (13) \mapsto \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad (14) \mapsto \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \right\},$$

and

$$R_{3d-2} = \left\{ (12) \mapsto \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (13) \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \quad (14) \mapsto \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \right\}.$$

The characters of the irreps are listed in Table 4.3, where we use the same repre-

sentation $M = \{M_g : g \in S_4\}$ as in Example 4.1.7.

S_4	(1)	(12)	(123)	(1234)	(12)(34)
size of conjugacy class	1	6	8	6	3
χ_i	1	1	1	1	1
χ_s	1	-1	1	-1	1
χ_{2d}	2	0	-1	0	2
χ_{3d-1}	3	-1	0	1	-1
χ_{3d-2}	3	1	0	-1	-1
χ_M	12	2	0	0	0

Table 4.3: Character table of S_4.

By Theorem 4.1.6, we know that

$$M \sim R_i \oplus R_{2d} \oplus R_{3d-1} \oplus 2R_{3d-2}.$$

Note that the sign representation R_s is absent from the expansion.

Similarly, we may find the vectors, up to a normalization factor, as stated in Lemma 4.2.4.

$$\begin{aligned}
\phi^1_{i,1} &= (1,1,1,1,1,1,1,1,1,1,1,1)^T, \\
\phi^1_{2d,1} &= (1,\omega^2,\omega,\omega,\omega^2,1,1,\omega^2,\omega,\omega,\omega^2,1)^T, \\
\phi^2_{2d,1} &= (1,\omega,\omega^2,\omega^2,\omega,1,1,\omega,\omega^2,\omega^2,\omega,1)^T, \\
\phi^1_{3d-1,1} &= (1,0,-1,1,0,1,-1,0,1,-1,0,-1)^T, \\
\phi^2_{3d-1,1} &= (-1,1,0,0,-1,1,1,-1,0,0,1,-1)^T, \\
\phi^3_{3d-1,1} &= (0,-1,1,1,-1,0,0,1,-1,-1,1,0)^T, \\
\phi^1_{3d-2,1} &= (0,-1,0,0,1,0,0,-1,0,0,1,0)^T,
\end{aligned}$$

$$\phi^1_{3d-2,2} = (-1,0,-1,1,0,-1,1,0,1,-1,0,1)^T,$$
$$\phi^2_{3d-2,1} = (0,0,-1,1,0,0,0,0,-1,1,0,0)^T,$$
$$\phi^2_{3d-2,2} = (-1,-1,0,0,1,1,1,1,0,0,-1,-1)^T,$$
$$\phi^3_{3d-2,1} = (-1,0,0,0,0,1,-1,0,0,0,0,1)^T,$$
$$\phi^3_{3d-2,2} = (0,-1,-1,-1,-1,0,0,1,1,1,1,0)^T.$$

If we reshuffle the vectors $\phi^r_{\rho,j}$'s as stated in Theorem 4.2.7, then

$$\Psi \coloneqq \begin{pmatrix} \phi^1_{i,1} & \phi^1_{2d,1} & \phi^2_{2d,1} & \phi^1_{3d-1,1} & \cdots & \phi^3_{3d-1,1} & \phi^1_{3d-2,1} & \cdots & \phi^3_{3d-2,1} & \phi^1_{3d-2,2} & \cdots & \phi^3_{3d-2,2} \end{pmatrix}$$

should block diagonalize M. For example,

$$\Psi^* M_{(12)} \Psi = \left(\begin{array}{cccccccccccc} \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \boxed{0} & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \boxed{1} & \boxed{0} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \boxed{0} & \boxed{1} & \boxed{0} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \boxed{1} & \boxed{0} & \boxed{0} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \boxed{0} & \boxed{0} & \boxed{-1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{-1} & \boxed{0} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \boxed{-1} & \boxed{0} & \boxed{0} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{0} & \boxed{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{-1} & \boxed{0} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{-1} & \boxed{0} & \boxed{0} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{0} & \boxed{0} & \boxed{1} \end{array}\right).$$

Furthermore, by listing the above vectors $\phi^r_{\rho,j}$'s one-by-one as stated in Theorem 4.2.8,

$$\Phi \coloneqq \begin{pmatrix} \phi^1_{i,1} & \phi^1_{2d,1} & \phi^2_{2d,1} & \phi^1_{3d-1} & \cdots & \phi^3_{3d-1,1} & \phi^1_{3d-2,1} & \phi^1_{3d-2,2} & \cdots & \phi^3_{3d-2,1} & \cdots & \phi^3_{3d-2,2} \end{pmatrix}$$

should block diagonalize $S(k)$. Indeed, we see that

$$\Phi^* S(k)\Phi = \begin{pmatrix} A^{S(k)}_{i,1\times 1} & 0 & 0 & 0 \\ 0 & B^{S(k)}_{2d,2\times 2} & 0 & 0 \\ 0 & 0 & C^{S(k)}_{3d-1,3\times 3} & 0 \\ 0 & 0 & 0 & D^{S(k)}_{3d-2,6\times 6} \end{pmatrix},$$

where

$$A^{S(k)}_{i,1\times 1} = e^{ibk}(1),$$
$$B^{S(k)}_{2d,2\times 2} = -e^{ibk}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$
$$C^{S(k)}_{3d-1,3\times 3} = e^{ibk}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

and

$$D^{S(k)}_{3d-2,6\times 6} = e^{ibk}/3\begin{pmatrix} -1 & -2\sqrt{2} & 0 & 0 & 0 & 0 \\ 2\sqrt{2} & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -2\sqrt{2} & 0 & 0 \\ 0 & 0 & 2\sqrt{2} & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & -2\sqrt{2} \\ 0 & 0 & 0 & 0 & 2\sqrt{2} & -1 \end{pmatrix}.$$

We represent the factorization of the determinants of $S(k)$'s for S_3 and S_4 graphically in Figure 4.3. Note that the top expression is the secular determinant of $S(k)$ for S_3 acting on K_4. It factorizes according to three irreps R_s, R_i and R_{2d}. If we set $a = b$, which means all edge lengths are equal in K_4, then each factor of $S(k)$

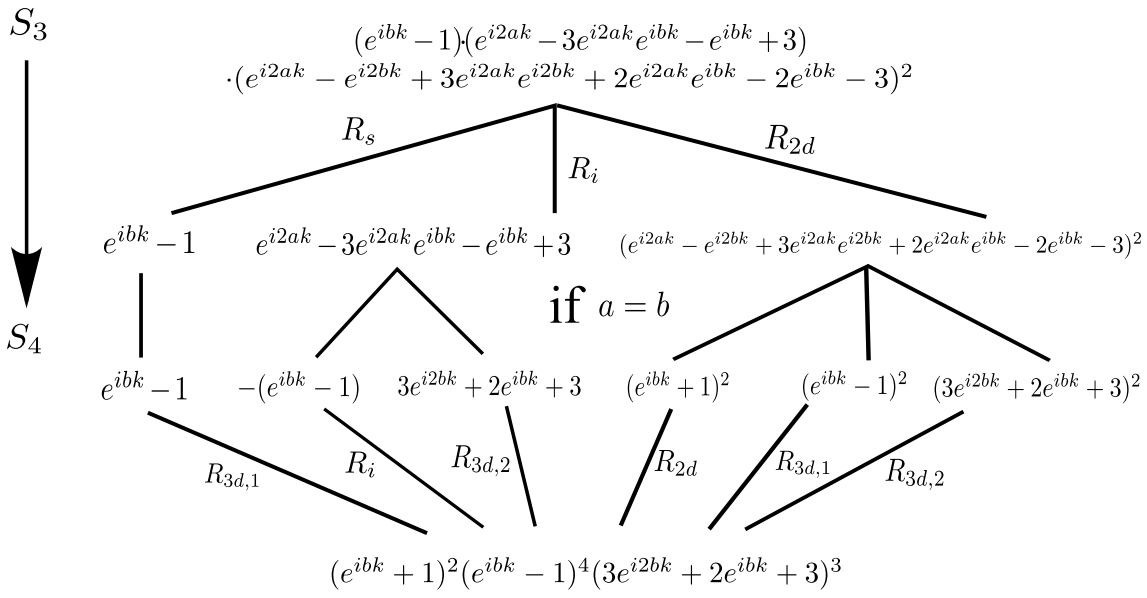

Figure 4.3: Factors of secular determinants of S_3 and S_4.

will factorizes further. The resulting factors are corresponding to irreps of the new secular determinant of $S(k)$ for S_4 acting on K_4. If we put all these factors together, that is exactly the new secular determinant of $S(k)$ for S_4, which is shown at the bottom.

4.4 Induced representations

There is another way to interpret Figure 4.3 using "induced representations". We introduce the definition first.

Let G be a finite group and H be a subgroup of G with a representation of R. Since the character completely identifies a representation, we may define $\mathrm{Ind}_H^G R$, the induction of the representation R from H to G, by

$$\chi_{\mathrm{Ind}_H^G R}(g) = \sum_{i=1}^{n} \chi_R\left(t_i^{-1} g t_i\right),$$

where $g \in G, n = |G : H|, \chi_R\left(t_i^{-1} g t_i\right) = 0$ for all $t_i^{-1} g t_i \notin H$, $\{t_i\}_1^n$ are the representatives for the left cosets of H in G. It can be shown that (see [12])

$$\text{dimInd}_H^G R = \text{dim} R \cdot |G : H|.$$

Consider the example of K_4, R_i, the identity representation of S_3, is viewed as a subgroup of S_4. We have

$$n = \text{dimInd}_{S_3}^{S_4} R_i = \text{dim} R_i \cdot |S_4 : S_3| = 1 \cdot 4 = 4.$$

Since S_4 does not have irreps of dimension 4, $\text{Ind}_{S_3}^{S_4} R_i$ is reducible. Choose the representatives

$$t_1 = (1), \quad t_2 = (14), \quad t_3 = (24), \quad t_4 = (34)$$

for the cosets of S_3 in S_4 so that

$$\{t_i S_3\}_{i=1}^4 = S_4.$$

The character of the induced representation is therefore

$$\begin{aligned}
\chi_{\text{Ind}_{S_3}^{S_4} R_i}(e) =& \sum_{i=1}^{4} \chi_{R_i}(e) = 4, \\
\chi_{\text{Ind}_{S_3}^{S_4} R_i}((12)) =& \chi_{R_i}((12)) + \chi_{R_i}((14)(12)(14)) + \chi_{R_i}((24)(12)(24)) \\
& + \chi_{R_i}((34)(12)(34)) \\
=& \chi_{R_i}((12)) + \chi_{R_i}((24)) + \chi_{R_i}((14)) + \chi_{R_i}((12)) \\
=& 1 + 0 + 0 + 1 \\
=& 2,
\end{aligned}$$

$$\begin{aligned}
\chi_{\mathrm{Ind}_{S_3}^{S_4} R_i}((123)) =& \chi_{R_i}((123)) + \chi_{R_i}((234)) + \chi_{R_i}((143)) + \chi_{R_i}((124)) \\
=& 1 + 0 + 0 + 0 \\
=& 1, \\
\chi_{\mathrm{Ind}_{S_3}^{S_4} R_i}((1234)) =& \chi_{R_i}((1234)) + \chi_{R_i}((1423)) + \chi_{R_i}((1432)) + \chi_{R_i}((1243)) \\
=& 0 + 0 + 0 + 0 \\
=& 0,
\end{aligned}$$

and

$$\begin{aligned}
\chi_{\mathrm{Ind}_{S_3}^{S_4} R_i}((12)(34)) =& \chi_{R_i}((12)(34)) + \chi_{R_i}((13)(24)) + \chi_{R_i}((14)(23)) + \chi_{R_i}((12)(34)) \\
=& 0 + 0 + 0 + 0 \\
=& 0.
\end{aligned}$$

Using character table of S_4, see Table 4.3, we know that

$$\mathrm{Ind}_{S_3}^{S_4} R_i = R_i^{S_4} \oplus R_{3d-2}^{S_4}. \tag{4.4.1}$$

Similar computations show that

$$\mathrm{Ind}_{S_3}^{S_4} R_s = R_s^{S_4} \oplus R_{3d-1}^{S_4}$$

and

$$\mathrm{Ind}_{S_3}^{S_4} R_{2d} = R_{2d}^{S_4} \oplus R_{3d-1}^{S_4} \oplus R_{3d-2}^{S_4}.$$

These computations provide an additional explanation for the factorizations in Figure 4.3. As we mentioned before, the secular determinant of the tetrahedron

graph with S_3 symmetry factorizes according to three irreps R_s, R_i, and R_{2d}. If we let $a = b$, each of these factors factorizes further. The factors occuring in the further factorization of the R_i term correspond to the irreps occurring in the induced representation of R_i, equation (4.4.1). The same rule applies to other factorizations. Note that the factor corresponding to $R_s^{S_4}$ is 1 and is not shown in the diagram.

5. SUMMARY

In Section 3, we proved that after a small modification of lengths of edges of a finite quantum graph, the spectrum can be made simple and each eigenfunction will never be zero on any vertex unless it is supported on a loop. Both of these results are important in applications, in particular all recent results on the number of zeros of graph eigenfunctions assume both the simplicity of eigenvalues and non-vanishing of eigenfunctions on vertices as a precondition, see [4, 8, 11, 15, 25].

In Section 4, we explicitly find a way to block diagonalize the scattering matrix of a symmetric graph and therefore to factorize the secular determinant. Our method of constructing vector spaces to block diagonalize the representation matrix is new. Current theorem states that the block diagonalization can be done, but there is no explicit way of saying how to do it. We found an explicit way to achieve this goal. The secular equation is an efficient way to find the spectrum of a quantum graph numerically. It is also very useful to study the spectral statistic analytically for some graphs. For example, Barra and Gaspard [13] introduced an interpretation of the secular determinant equation as an ergodic flow piercing a compact manifold (more precisely, an algebraic variety) on a torus. This interpretation leads to many surprising and very general results, including those of [5] and [9]. For more applications, see [17, 19, 20, 56].

In the work in process with Chris Joyner and Ram Band, we relate the blocks in the block-diagonal matrix $S(k)$ to the quotient graph construction of [12]. We also see accidental degeneracies in the graph with a large symmetry. We will construct more examples with persistent (accidental) degeneracies.

The following further questions can be asked. Suppose that we increase the

symmetries of the graph. The factors of the secular determinant will factorize further and possibly rearrange. Can we predict the way in which the rearrangement will happen? In an example we saw that it is connected with the notion of induced representations. Is this true in general? We also observed on several examples that the secular determinant of the scattering matrix $S(k)$ always has three factors for complete graphs with large symmetries. Why is it the case? What is the minimum size of symmetry group to achieve this?

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