Scattering Amplitudes in the Theory of Quantum Graphs

By

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Declaration and Approval

I the undersigned declare that this thesis is a presentation of my original research work. Wherever contributions of others are involved, every effort is made to indicate this clearly, with due reference to the literature, and acknowledgement of collaborative research and discussions. To the best of my knowledge, it has not been submitted in support of an application for another degree in any other university or any other institution of learning.

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In my capacity as advisor of the candidate's thesis, I certify that the above statements are true to the best of my knowledge and this thesis has my approval for submission.

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ABSTRACT

This study is about scattering matrices in the framework of quantum graphs. Such matrices describing equi-transmission are studied. The matrices are unitary Hermitian and therefore are independent of the energies of the associated system. In the absence of reflection, such matrices exist only in even dimensions. A complete description of reflectionless equi-transmitting matrices up to order six is given. In dimension six, 60 five-parameter families are obtained. The relation among the 60 matrices yield a combinatorial bipartite graph K_6^2.

When reflection is considered the standard matching condition matrix generates equi-transmitting matrices in dimensions $n \geq 3$. These are essentially the only equi-transmitting matrices when the order of the matrix is odd for $n \leq 5$. However when the order is even and the trace of the matrix is zero, there are other equi-transmitting matrices for $n \leq 6$. A complete description of these zero trace matrices up to order six is given.

Interplay between arbitrary phases appearing in vertex conditions and magnetic fluxes through the cycles in quantum graphs is discussed. It is shown that varying the vertex phases, one obtains at most g-dimensional family of unitary equivalent operators, where g is the genus of the graph.

PUBLICATIONS

The following publications are included in this thesis.

PAPER I: **On reflectionless equi-transmitting matrices**

P. Kurasov, R. Ogik and A. Rauf,

Opuscula Mathematica, **34** no. 3 (2014) 483-501.

PAPER II: **On equi-transmitting matrices**

P. Kurasov, and R. Ogik

Accepted for publication in Reports on Mathematical Physics

PAPER III: **Quantum graphs: magnetic fields, vertex conditions and unitary equivalence**,

P. Kurasov, R. Ogik

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Rao Wyclife Ogik

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This thesis is dedicated to my Dad and Mum.

Contents

INTRODUCTION

A quantum graph can be considered as one-dimensional simplical complex on which is defined a differential operator. This means that the edges are viewed as one-dimensional segments joining the vertices. The edges thus have a geometrical interpretation and could be regarded as physical wires for instance. The genesis of the field is attributed to the work done by Ruedenberg and Scherr [RS53] in 1953 in calculating the spectra of aromatic carbohydrate molecules following the suggestions given by L. Pauling in 1936. The concepts in quantum graph have been used to study and model propagation of waves at a nano-scale. In particular, they are used to give approximations of behaviour and gain insight of objects in mesoscopic physics and nanotechnology. This explains why the underlying mathematical concepts have become an important and interesting field in mathematics.

In scattering experiments, when waves propagated through a channel encounter a node there is a possibility of the occurrence of either their reflection or transition. The measure of transition and reflection probabilities are described in quantum physics by the square of the absolute values of the entries of the scattering matrix. This matrix was first introduced to quantum mechanics by John Archibald Wheerler [JA37]. In the 1940's Werner Heisenberg developed the theory independently and also introduced a unitary scattering matrix.

Part of this work focuses on cases of equi-transmission of waves through a vertex. In such cases it is assumed that the incoming waves are transmitted through a node into other channels with equal probability. We consider two different scenarios; namely, when there is no reflection (back scattering) of waves and when reflection is allowed. We will call the corresponding matrices reflectionless equi-transmitting and
equi-transmitting matrices respectively.

We also study the spectral theory of quantum graphs with regard to the unitary equivalence of the various operators acting on the functions defined on the metric graph. We analyse the dependence of the spectrum on the vertex phases introduced in the construction of equi-transmitting matrices as well as on the magnetic fluxes present in metric graphs with cycles.

The order of our discussion is as follows. Chapter one gives a brief survey of the field of quantum graphs with emphasis on the concepts deemed necessary in the subsequent chapters. Here we also give a literature review and state the problem. Chapter two is dedicated to the study of reflectionless equi-transmitting matrices while chapter three focuses on equi-transmitting matrices. The scattering matrices obtained contain several arbitrary phase parameters. The role of the so-called free parameters is in chapter four. In the conclusion we give a summary of the results obtained and suggestions for further research.

Chapter 1

QUANTUM GRAPHS

1.1 Introduction

In this chapter we give a brief survey of concepts of quantum graphs that are relevant to our study. The definition of a quantum graph is given in section 1.2. Discussion of parameterisation of self-adjoint vertex conditions is covered in section 1.3. In section 1.4 we study the spectrum of the Laplacian on the quantum graph. Here we consider both a compact graph and a star graph defined by a finite number of half lines. A survey of the concepts of both the vertex and edge scattering matrices are found in section 1.5. In section 1.6 we give a review of literature informing our research area. We also enumerate the specific objectives we set out to achieve.

1.2 Definition of a quantum graph

A quantum graph is a **metric graph** on which a **differential operator** is defined. Appropriate **vertex conditions** are introduced in order to make the differential operator self-adjoint. In what follows we give a description of each of the three components of a quantum graph.

1.2.1 Metric graph

A discrete or combinatorial graph is an ordered pair $(\mathbf{V}, \mathbf{E})$ of the set $\mathbf{V} = \{x_i\}$ of vertices and the set $\mathbf{E}$ of edges connecting the vertices. The set of edges can be viewed as the set of 2-element subsets of $\mathbf{V}$. In combinatorial graphs, the focus is on the vertices with edges serving the purpose of indicating connectivity. A metric graph is obtained by assigning positive length to the edges and the attention shifts to the edges. Consider N compact and semi-infinite edges E_n, each considered as a subset of an individual copy of $\mathbb{R}$

$$E_n = \begin{cases} [x_{2n-1}, x_{2n}]\,, & n = 1, \dots, N_c \\ [x_{2n-1}, \infty)\,, & n = N_c + 1, \dots, N_c + N_i = N, \end{cases}$$

where N_c (respectively N_i) denotes the number of compact (respectively semi-infinite) intervals. Let $\mathbf{V} = \{x_i\}$ be the set of all endpoints of the intervals E_n. On this set we define an equivalence relation as follows. Two end points x and y are equivalent if either of the following conditions hold

1. they are the end points of a loop, or,
2. they belong to two different edges and the two edges are coupled at the end points x and y.

It therefore follows that the set $\mathbf{V} = \{x_i\}$ can be partitioned into M equivalence classes V_m, $m = 1, \ldots, M$ which we call vertices.

Definition 1.2.1 *A metric graph Γ is the union of the edges E_n with the end points belonging to the same vertex identified*

$$\Gamma = \bigcup_{n=1}^{N} E_n/_{x\sim y},$$

The number d_m of elements in the class V_m is called the valence of V_m. Note that in a metric graph, intermediate points in an edge are also considered as points on the graph. The distance between any two points on the graph is therefore the shortest standard (usual) metric distance between them. This means that for any two points belonging to the same edge , the distance between them is the usual length of the corresponding interval induced.

Suppose the metric graph Γ has loops at some vertices and multiple edges joining some vertices. By introducing additional vertices on the loops and the multiple edges, we get a graph without the loops and multiple edges. But the new graph is completely equivalent to the original one. Thus where necessary in our discussion we will remove from the metric graph loops and multiple edges.

(a) (b)

FIGURE 1.1: Graph (b) is obtained from graph (a) by introducing additional vertices.

A finite graph is compact if $N_i = 0$. Each compact edge has the length $l_n = x_{2n} - x_{2n-1}$, and the total length of a compact (finite) metric graph is given as

$$\mathcal{L} = \sum_{n=1}^{N} l_n.$$

The inclusion of intermediate points on the edges enables one to define the Lebesgue measure on the graph. One can therefore define functions on Γ. Some function spaces that can be defined on metric graphs are the space of smooth functions with compact support $C_0^\infty(\Gamma \setminus \mathbf{V}) = \bigoplus_{E_n \in \mathbf{E}} C_0^\infty(E_n)$, the Hilbert space $L_2(\Gamma) = \bigoplus_{E_n \in \mathbf{E}} L_2(E_n)$ and the Sobolev space $W_2^2(\Gamma) = \bigoplus_{E_n \in \mathbf{E}} W_2^2(E_n)$. The boundary values of functions defined at the edge end point are given by

$$u(x_j) = \lim_{x \to x_j} u(x).$$

The boundary values of the normal derivatives are given by

$$\partial_n u(x_j) = \begin{cases} \lim\limits_{x \to x_j} \dfrac{d}{dx} u(x) & x_j \text{ is the left endpoint} \\ -\lim\limits_{x \to x_j} \dfrac{d}{dx} u(x) & x_j \text{ is the right endpoint,} \end{cases} \tag{1.2.1}$$

while that of the extended normal derivatives are given by

$$\partial u(x_j) = \begin{cases} \lim\limits_{x \to x_j} \left(\dfrac{d}{dx} u(x) - ia(x)\, u(x) \right) & x_j \text{ is the left endpoint} \\ -\lim\limits_{x \to x_j} \left(\dfrac{d}{dx} u(x) - ia(x)\, u(x) \right) & x_j \text{ is the right endpoint,} \end{cases}$$

where $a(x)$ is the magnetic potential of the magnetic Schrödinger operator (see the discussion on differential operators below). In all these limits, x approaches x_j from inside the corresponding edge. The normal and extended normal derivatives are independent of the direction in which the edge is parameterized.

1.2.2 Differential operators

Differential operators play the role of describing the wave dynamics along the edges in a metric graph. The differential operators usually used on quantum graphs are

- **Laplace** operator
$$L = -\frac{d^2}{dx^2};$$
- **Schrödinger** operator
$$L_q = -\frac{d^2}{dx^2} + q\left(x\right);$$
- **Magnetic Schrödinger** operator
$$L_{q,a} = \left(i\frac{d}{dx} + a\left(x\right)\right)^2 + q\left(x\right).$$

The functions $a\left(x\right)$ and $q\left(x\right)$ are the magnetic and electric potentials respectively both of which are real-valued. In addition the magnetic potential is continuously differentiable and the electric potential is locally square integrable and decays on infinite edges. Note that the differential operators described here are not self-adjoint unless appropriate vertex conditions at the vertices are introduced.

1.2.3 Vertex conditions

Vertices of valence one are called boundary vertices while those with valency greater than one are called internal vertices. Vertex conditions defined at boundary vertices are therefore called boundary conditions while those defined on internal vertices are called matching conditions.

Vertex conditions serve two main purposes. Firstly, for internal vertices, they indicate how the edges are coupled together thereby describing the topology of the metric graph. Secondly they are necessary to ensure that the differential operator is self-adjoint. The most commonly used matching/boundary conditions, called **standard** (**Neumann**, or **Kirchhoff**) **matching conditions** (SMC) are

$$\begin{cases} u \text{ is continuous at every vertex } V_m \\ \sum\limits_{x_j \in V_m} \partial_n u\left(x_j\right) = 0, \quad m = 1, 2, \ldots, M. \end{cases}$$

The derivatives are taken in the direction moving away from the vertex, i.e. they are normal derivatives (see (1.2.1)). One observes that in the case of a boundary vertex, that is a vertex with valence one, the conditions reduce to a single Neumann condition $\partial_n u\left(x_j\right) = 0$. For the vertex of valence two, the standard conditions imply that both the function and its derivatives are continuous at V_m. Hence the vertex can be removed and the two edges substituted with a single edge whose length is the sum of the of the lengths of the two original edges.

Some other examples of the matching conditions that appear in the literature are as follows.

1. $\delta-$**interaction:** This matching condition is described by the following equations

$$\begin{cases} u \text{ is continuous at every vertex } V_m \\ \displaystyle\sum_{x_j \in V_m} \partial_n u_j\left(V\right) = \alpha_m \cdot u\left(V\right), \quad \alpha_m \in \mathbb{R}. \end{cases}$$

If $\alpha_m = \infty$ then $u\left(V\right) = 0$ the vertex ceases to be a single vertex, but a collection of independent vertices of degree one.

2. $\delta'-$**interaction:** This is viewed as the dual of the $\delta-$interaction vertex condition. It is described by the following equations

$$\begin{cases} \partial_n u_i\left(V\right) = \partial_n u_j\left(V\right), \quad i \neq j \\ \displaystyle\sum_{x_j \in V_m} u_j\left(V\right) = \beta_m \cdot \partial_n u\left(V\right), \quad \beta_m \in \mathbb{R}. \end{cases}$$

If $\beta_m = \infty$ then $\partial_n u\left(V\right) = 0$ and from the first condition this matching condition becomes the Neumann condition.

Suppose vertex conditions at a vertex V can be partitioned into conditions connecting boundary values belonging to vertices V' and V'' such that $V = V' \cup V''$ and $V' \cap V'' = \varnothing$, then such vertex conditions are not properly connecting. If such a partitioning is not possible the vertex conditions are properly connecting. This study deals with properly connecting vertex conditions only.

We now give a formal definition of a quantum graph.

Definition 1.2.2 *A quantum graph is a metric graph furnished with a differential operator which acts on functions defined on the edges. The functions satisfy certain vertex conditions so as to make the differential operator self adjoint.*

1.3 Parametrization of Self-adjoint Vertex Conditions

In discussing various self-adjoint parametrization of vertex conditions we restrict ourselves to a star graph $\Gamma = \bigcup_{n=1}^{N}\left([0,\infty)\right)$ whose central vertex V has valence N. A number of such parametrization have emerged in the development of the field of quantum graphs and below we consider some of them. Suppose the domain of the Laplacian defined on Γ is the Hilbert space $L^2\left(\Gamma\right) = \bigoplus\limits_{E_n \in \mathbf{E}} L^2\left(E_n\right)$. Then the solution of the differential equation $-u''\left(x\right) = \lambda u\left(x\right)$, $\lambda = k^2$ is given by

$$u\left(x\right) = ae^{ikx} + be^{-ikx}, \quad x \in E_n.$$

Since the differential operator is of second order, it follows from the theory of ODE that two boundary conditions are necessary for each edge to obtain a solution.

In [KS99] Kostrykin and Schrader introduced the parameterization of vertex conditions at a vertex V with valence N as

$$\mathbf{Au}(V) + \mathbf{B}\partial\mathbf{u}(V) = 0, \tag{1.3.1}$$

where $\mathbf{u}(V)$ and $\partial\mathbf{u}(V)$ are the vectors of the limiting values at the vertex of the function, $\{u(x_j)\}_{x_j \in V}$, and its normal derivatives $\{\partial_n u(x_j)\}_{x_j \in V}$ while $\mathbf{A}$ and $\mathbf{B}$ are two $N \times N$ matrices. This parametrization results in a self-adjoint vertex conditions if and only if the $N \times 2N$ matrix $(\mathbf{A}, \mathbf{B})$ has maximal rank and the matrix $\mathbf{AB}^*$ is Hermitian – see [PK14, BK10] for a detailed account. However the parametrization fails to be unique, for suppose we multiply the above equation from the left by an invertible $N \times N$ matrix $\mathbf{C}$. Then we obtain the condition $\mathbf{CAu}(V) + \mathbf{CBu}'(V) = 0$ where the matrix $(\mathbf{CA}, \mathbf{CB})$ has maximal rank and the matrix $\mathbf{CA}(\mathbf{CB})^*$ is Hermitian.

To address the problem of uniqueness, Harmer in [H00] defined another self-adjoint boundary parametrization which can be formulated as follows. Consider the symmetric Laplace operator L in the Hilbert space $L^2(\Gamma) = \bigoplus_{E_n \in \mathbf{E}} L^2(E_n)$ whose domain is given by

$$\mathrm{Dom}(L) = \bigoplus_{E_n \in \mathbf{E}} C_0^\infty(E_n).$$

The self-adjoint extensions of L are the functions satisfying the boundary conditions

$$i(\mathbf{U}^* - \mathbf{I})\mathbf{u}(V) + (\mathbf{U}^* + \mathbf{I})\partial\mathbf{u}(V) = 0 \tag{1.3.2}$$

at the vertex V, where $\mathbf{U}$ is a unitary $N \times N$ matrix. Here $\mathbf{u}(V)$ and $\partial\mathbf{u}(V)$ are vectors of the boundary values of a function and its normal derivatives respectively at V.

In [KN10] Kurasov and Nowaczyk gave an equivalent parameterization described as follows. To the Laplace operator defined on Γ the corresponding maximal and minimal operators are given by the same formal expression as L but their domains are defined as $\mathrm{Dom}(L_{max}) = \bigoplus_{j=1}^{N} W_2^2((0,\infty))$ and $\mathrm{Dom}(L_{min}) = \bigoplus_{j=1}^{N} C_0^\infty((0,\infty))$ respectively. The following theorem gives the associated self adjoint extension.

Theorem 1.3.1 *The family of all self-adjoint extensions of the minimal operator L_{min} can be uniquely parameterized by an arbitrary $N \times N$ unitary matrix $\mathbf{S}$, so that the operator $L^{\mathbf{S}}$ is the restriction of $L_{max} = L_{min}^*$ to the set of functions satisfying the matching conditions*

$$i(\mathbf{S} - \mathbf{I})\mathbf{u}(V) = (\mathbf{S} + \mathbf{I})\partial\mathbf{u}(V). \tag{1.3.3}$$

This parameterization is identical to (1.3.2) provided $\mathbf{S} = \mathbf{U}^*$. As will be seen later, the parameterization (1.3.3) also has a clear physical interpretation, namely, for the value of the energy $k = 1$ the matrix $\mathbf{S}$ coincides with the vertex scattering matrix[1].

Now we establish the relation between the matching conditions (1.3.1) and (1.3.3). For matrices $\mathbf{A}$ and $\mathbf{B}$ satisfying the conditions prescribed in (1.3.1), define the matrices $\mathbf{A} - i\mathbf{B}$ and $\mathbf{A} + i\mathbf{B}$. We have that

$$\begin{aligned}(\mathbf{A} - i\mathbf{B})(\mathbf{A} - i\mathbf{B})^* &= \mathbf{A}\mathbf{A}^* + \mathbf{B}\mathbf{B}^* \\ &= (\mathbf{A} + i\mathbf{B})(\mathbf{A} + i\mathbf{B})^* = (\mathbf{A}, \mathbf{B})(\mathbf{A}, \mathbf{B})^*\end{aligned} \tag{1.3.4}$$

Next we observe that

$$\begin{aligned}\operatorname{rank}(\mathbf{A} - i\mathbf{B}) &= \operatorname{rank}\left((\mathbf{A} - i\mathbf{B})(\mathbf{A} - i\mathbf{B})^*\right) \\ &= \operatorname{rank}\left((\mathbf{A}, \mathbf{B})(\mathbf{A}, \mathbf{B})^*\right) = \operatorname{rank}((\mathbf{A}, \mathbf{B})) = N.\end{aligned}$$

Similarly $\operatorname{rank}(\mathbf{A} + i\mathbf{B}) = N$. Since the ranks are maximal, the matrices are invertible. Now define

$$\mathbf{S} = -(\mathbf{A} - i\mathbf{B})^{-1}(\mathbf{A} + i\mathbf{B}).$$

Then

$$\begin{aligned}\mathbf{S}\mathbf{S}^* &= \left((\mathbf{A} - i\mathbf{B})^{-1}(\mathbf{A} + i\mathbf{B})\right)\left((\mathbf{A} - i\mathbf{B})^{-1}(\mathbf{A} + i\mathbf{B})\right)^* \\ &= (\mathbf{A} - i\mathbf{B})^{-1}(\mathbf{A} + i\mathbf{B})(\mathbf{A} + i\mathbf{B})^*\left((\mathbf{A} - i\mathbf{B})^{-1}\right)^* \\ &= (\mathbf{A} - i\mathbf{B})^{-1}(\mathbf{A} - i\mathbf{B})(\mathbf{A} - i\mathbf{B})^*\left((\mathbf{A} - i\mathbf{B})^*\right)^{-1} = \mathbf{I}.\end{aligned}$$

Thus $\mathbf{S}$ is unitary. On the other hand if we choose $\mathbf{A}$ and $\mathbf{B}$ as

$$\mathbf{A} = i(\mathbf{S} - \mathbf{I}) \quad \text{and} \quad \mathbf{B} = \mathbf{S} + \mathbf{I},$$

we find that

$$\operatorname{rank}(\mathbf{A}, \mathbf{B}) = \operatorname{rank}(\mathbf{S} - \mathbf{I}, \mathbf{S} + \mathbf{I}) = N$$

and

$$\begin{aligned}\mathbf{B}\mathbf{A}^* &= (\mathbf{S} + \mathbf{I})(i(\mathbf{S} - \mathbf{I}))^* = -i(\mathbf{S} + \mathbf{I})(\mathbf{S}^* - \mathbf{I}) \\ &= i(\mathbf{S} - \mathbf{S}^*) = i(\mathbf{S} - \mathbf{I} + \mathbf{S}^*\mathbf{S} - \mathbf{S}^*) = i(\mathbf{S} - \mathbf{I})(\mathbf{S}^* + \mathbf{I}) = \mathbf{A}\mathbf{B}^*\end{aligned}$$

showing that $(\mathbf{A}, \mathbf{B})$ is of maximal rank and $\mathbf{B}\mathbf{A}^*$ is Hermitian.

[1]See definition 1.5.1

The parameterization (1.3.3) is equivalent to one involving a Hermitian matrix as shown in the following theorem[PK14].

Theorem 1.3.2 *The matching conditions* (1.3.3) *are equivalent to*

$$\begin{cases} \mathbf{P}_{-1}\mathbf{u} = \mathbf{0} \\ \mathbf{H}\left(\mathbf{I} - \mathbf{P}_{-1}\right)\mathbf{u} + \left(\mathbf{I} - \mathbf{P}_{-1}\right)\partial\mathbf{u} = \mathbf{0}, \end{cases} \tag{1.3.5}$$

where $\mathbf{P}_{-1}$ is the spectral projector for $\mathbf{S}$ corresponding to the eigenvalue -1,

$$\mathbf{H} = \left(\mathbf{I} - \mathbf{P}_{-1}\right) i \frac{\mathbf{I} - \mathbf{S}}{\mathbf{I} + \mathbf{S}} \left(\mathbf{I} - \mathbf{P}_{-1}\right)$$

is Hermitian. Note that the operator $\mathbf{I} + \mathbf{S}$ is invertible on the orthogonal complement to $\mathbf{P}_{-1}\mathbf{C}^N$.

From the equivalence established it follows that the matching conditions (1.3.3) can be considered as certain combination of Dirichlet and Robin type boundary conditions. Thus it is the most general vertex conditions for a star graph so that the associated Laplacian becomes self-adjoint. It also unique since there is a one-to-one correspondence between the set of self-adjoint extensions and the set of unitary matrices $\mathbf{S}$.

1.4 Spectrum of the Laplacian on the Metric Graphs

Consider first the simple example of a metric graph- a single interval.. Suppose the Dirichlet boundary conditions are imposed at each end point, then the eigenvalues of L are given by

$$\lambda_n = \frac{n^2\pi^2}{l^2}, \quad n = 1, 2, \ldots,$$

where l is the length of the interval. The corresponding eigenfunctions are

$$u_n\left(x\right) = \sin\left(\frac{n\pi x}{l}\right), \quad n = 1, 2, \ldots.$$

On the other hand when we impose Neumann boundary conditions at each end point, the eigenvalues of L on the compact edge are

$$\lambda_n = \frac{n^2\pi^2}{l^2}, \quad n = 0, 1, 2, \ldots,$$

while the corresponding eigenfunctions are

$$u_n(x) = \cos\left(\frac{n\pi x}{l}\right), \quad n = 0, 1, 2, \ldots.$$

If on the other hand the compact edge is replaced by the whole real line, then the operator L will have the continuous spectrum $[0, \infty)$. In this case the operator does not have eigenvalues and eigenfunctions in the classical sense. The solutions of $Lu = \lambda u$ are linear combinations of $e^{\pm i\sqrt{\lambda}x}$. These oscillate if $\lambda > 0$, they are constant if $\lambda = 0$ and grow in either direction if $\lambda \in \mathbb{C} \setminus [0, \infty)$. Instead, the Laplacian has generalised eigenfunctions

$$u(x) = e^{ikx}, \qquad k \in \mathbb{R}$$

with generalized eigenvalues $\lambda = k^2$. Suppose the Laplacian is considered on the domain $\left\{u(x) \in W_2^2([0, \infty)) : u'(0) = hu(0), h \in \mathbb{R}\right\}$. The spectrum may have some negative eigenvalues besides the continuous spectrum (if $h < 0$).

We now discuss the spectrum of a star graph formed by N semi-infinite edges connected to one vertex V. The Laplace operator $L = -\frac{d^2}{dx^2}$ is defined on the set of functions from $W_2^2(\Gamma \setminus V)$ satisfying the matching conditions (1.3.3).

The spectrum of the Laplace operator consists of absolutely continuous spectrum $[0, \infty)$ of multiplicity N and may be a finite number of negative eigenvalues. The absolutely continuous spectrum is the same for the Laplacian defined on the functions satisfying the Dirichlet and Neumann conditions at the vertex, but the generalised eigenfunctions are different.

The Laplacian with the matching conditions determined by (1.3.3) is a finite rank perturbation (in the resolvent sense) of the Dirichlet Laplacian and therefore the absolutely continuous spectrum is preserved. This means that the difference between the resolvents $(L_S - \lambda)^{-1}$ and $(L_D - \lambda)^{-1}$ is a finite rank operator. Here L_D and L_S are the Laplacian with Dirichlet and standard matching conditions described by (1.3.3) respectively. Moreover the Laplacian on a star graph can have at most N negative eigenvalues.

The number of negative eigenvalues is determined as follows. Every eigenfunction is of the form

$$\mathbf{u}(x) = e^{-\chi x}\mathbf{a}, \qquad \chi > 0,$$

where we use vector notations. The functions satisfy the equation

$$-\frac{d^2}{dx^2}\mathbf{u} = -\chi^2\mathbf{u}.$$

The corresponding possible eigenvalue is $\lambda = -\chi^2$. The function $\mathbf{u}$ is an eigenfucntion only if it satisfies the matching conditions

$$i\left(\mathbf{S}-\mathbf{I}\right)\mathbf{a}=-\chi\left(\mathbf{S}+\mathbf{I}\right)\partial\mathbf{a}. \tag{1.4.1}$$

Recall that the map

$$z\mapsto i\frac{1-z}{1+z}$$

maps the unit disc on to the upper half-plane. The lower unit semicircle is mapped onto the negative semi axis and the upper unit semicircle is mapped onto the positive semi axis. Let us write the vector $\mathbf{a}$ using the eigenvalues of $\mathbf{e}_j$ of the unitary matrix $\mathbf{S}$; $\mathbf{a}=\sum a_j\mathbf{e}_j$. Then (1.4.1) can be written as

$$i\left(e^{i\theta_j}-1\right)a_j=-\chi\left(e^{i\theta_j}+1\right)a_j.$$

It therefore follows that when $\theta_j=0$ and $\theta_j=\pi$, the corresponding a_j are equal to zero. In all cases we have

$$\chi_j=i\frac{1-e^{i\theta_j}}{1+e^{i\theta_j}}=\frac{\sin\left(\theta_j/2\right)}{\cos\left(\theta_j/2\right)}.$$

All such χ_j are real numbers, but only positive χ_j lead to eigenvalues; with the corresponding eigenfunctions being square integrable. Therefore every $\theta_j\in(0,\pi)$ determines an eigenvalue of the Laplace operator with matching conditions (1.3.3). This therefore means that the spectrum of the Laplacian on the star graph with N semi-infinite edges determined by the matching conditions (1.3.3) is given by

1. the absolutely continuous spectrum $[0,\infty)$ of multiplicity N.
2. finite number of negative eigenvalues $\lambda_j^2=-\left(\frac{\sin(\theta_j/2)}{\cos(\theta_j/2)}\right)^2$, where $e^{i\theta_j}$ are the eigenvalues of $\mathbf{S}$ lying on the upper unit semicircle.

The following theorem [PK14] characterises the spectrum of the Laplacian on a quantum graph with the boundary conditions defined by the standard matching conditions.

Theorem 1.4.1 *The spectrum of the standard Laplacian on the quantum graph Γ contains the branch of absolutely continuous spectrum $[0,\infty)$ with multiplicity equal to the number N_i of infinite edges in Γ. The negative spectrum consists of a finite number of eigenvalues. If Γ is compact, then the spectrum is pure discrete with unique accumaltion point $+\infty$, satisfying the Weyl's asymptotic law*

$$\lambda_n\sim\frac{\pi^2}{\mathcal{L}^2}n^2,\quad n\to\infty$$

where $\mathcal{L}$ is the total length of the compact graph.

1.5 Scattering Matrices

1.5.1 Vertex Conditions and Vertex Scattering Matrix

Related to the study of coupling of edges at a vertex is the concept of scattering of waves. The scattering of waves at a vertex is described by means of the vertex scattering matrix. The study of scattering of waves in a quantum graph requires the analysis of scattering at a vertex. It thus suffices in such studies to consider a star graph. For such a graph whose central vertex V has valence N, consider arbitrary solution to the equation $-u'' = k^2 u$ given by

$$u(x) = a_j e^{ik(x-x_j)} + b_j e^{-ik(x-x_j)}, \quad x \in E_j. \tag{1.5.1}$$

Let the amplitude of the incomming wave along edge E_j be b_j while that of the outgoing wave along edge E_i be a_i with the corresponding vectors given by $\mathbf{b}$ and $\mathbf{a}$ respectively. The amplitudes a_j and b_j are not independent since u in (1.5.1) should satisfy the vertex conditions. The relation between $\mathbf{a}$ and $\mathbf{b}$ is described by the vertex scattering matrix.

Definition 1.5.1 *The $d_m \times d_m$ unitary matrix $\mathbf{S}_V(k)$ such that*

$$\mathbf{a} = \mathbf{S}_V(k)\,\mathbf{b}, \tag{1.5.2}$$

is the vertex scattering matrix.

We now discuss the relation between the scattering matrix and the self-adjoint vertex conditions parameterization (1.3.3). The vertex value of the solution (1.5.1) at the vertex V in the star graph $\Gamma = \bigcup_{j=1}^{d_m} [0,\infty)$ is $\mathbf{u}(0) = \mathbf{a} + \mathbf{b}$. The value of the normal derivatives at the vertex is $\partial_n \mathbf{u}(0) = ik(\mathbf{a} - \mathbf{b})$. Substituting these values into equation (1.3.3) we obtain that

$$(\mathbf{S} - \mathbf{I})(\mathbf{a} + \mathbf{b}) = k(\mathbf{S} + \mathbf{I})(\mathbf{a} - \mathbf{b}).$$

Substituting the value of $\mathbf{a}$ from (1.5.2) into this equation and simplifying one obtains

$$\mathbf{S}_V(k) = \frac{(k+1)\,\mathbf{S} + (k-1)\,\mathbf{I}}{(k-1)\,\mathbf{S} + (k+1)\,\mathbf{I}}, \quad k \neq 0. \tag{1.5.3}$$

It can be observed that for $k = 1$, the unitary matrix $\mathbf{S}$ parameterizing matching conditions is precisely the vertex scattering matrix, that is $\mathbf{S}_V(1) = \mathbf{S}$. This makes the parameterization (1.3.3) special in that it has relevant interpretation, namely, the matrix $\mathbf{S}$ can be considered as the scattering matrix.

Plugging the orthogonal decomposition of $\mathbf{S}$ given by

$$\mathbf{S} = \sum_{n=1}^{d_m} e^{i\theta_n} \langle , \mathbf{e}_n \rangle \, \mathbf{e}_n$$

into (1.5.3) we obtain

$$\mathbf{S}_V(k) = \sum_{n=1}^{d_m} \frac{k\left(e^{i\theta_n}+1\right)+\left(e^{i\theta_n}-1\right)}{k\left(e^{i\theta_n}+1\right)-\left(e^{i\theta_n}-1\right)} \langle \cdot, \, \mathbf{e}_n \rangle \mathbf{e}_n.$$

From this equation it can be seen that both $\mathbf{S}$ and $\mathbf{S}_V(k)$ have the same eigenvectors. The eigenvalues of $\mathbf{S}_V(k)$ may depend on the energy k. For the eigenvalues $e^{i\theta_n} = 1$ and $e^{i\theta_n} = -1$ of $\mathbf{S}$, the corresponding eigenvalues of $\mathbf{S}_V(k)$ are also 1 and -1 respectively and for those values of k, the quotient $\frac{k\left(e^{i\theta_n}+1\right)+\left(e^{i\theta_n}-1\right)}{k\left(e^{i\theta_n}+1\right)-\left(e^{i\theta_n}-1\right)}$ is independent of k. All the other eigenvalues tend to 1 as $k \to \infty$. The high energy limit of $\mathbf{S}_V(k)$ exists [PK14] and is given by

$$\mathbf{S}_V(\infty) = \lim_{k\to\infty} \mathbf{S}_V(k) = -\mathbf{P}_{-1} + (\mathbf{I} - \mathbf{P}_{-1}) = \mathbf{I} - 2\mathbf{P}_{-1}.$$

It follows that if S is chosen such that the spectrum $\sigma(\mathbf{S}) = \{\pm 1\}$, then the corresponding vertex scattering matrix is independent of the energy. For this to happen it is necessary that $\mathbf{S}$ should not only be unitary, but also Hermitian.

1.5.2 Edge Scattering Matrix

We now discuss the edge scattering matrix. Consider the edge $E = [x_1, x_2]$ which is embedded in the real line $\mathbb{R}$. The solution of the differential equation

$$-\frac{d^2u(x)}{dx^2} = \lambda u(x), \qquad \lambda = k^2, \tag{1.5.4}$$

on $\mathbb{R}$ are generalized eigenfunctions which describe scattered waves along $\mathbb{R}$ and we write as follows

$$u(x) = \begin{cases} a_1 e^{-ik|x-x_1|} + b_1 e^{ik|x-x_1|} & x < x_1, \\ a_2 e^{-ik|x-x_2|} + b_2 e^{ik|x-x_2|} & x > x_2. \end{cases}$$

In this representation, $e^{-ik|x-x_j|}$, $j = 1, 2$ are waves coming into the edge E through the vertices x_1 and x_2, while $e^{ik|x-x_j|}$ getting out of the edge through the same vertices. It follows that

$$\partial_n u(x) = \begin{cases} a_1 ike^{-ik|x-x_1|} - b_1 ike^{ik|x-x_1|} & x < x_1, \\ -a_2 ike^{-ik|x-x_2|} + b_2 ike^{ik|x-x_2|} & x > x_2. \end{cases}$$

At the vertices x_1 and x_2, the solution and its derivative have the following data.

$$\begin{pmatrix} u(x_1) \\ \partial_n u(x_1) \end{pmatrix} = \begin{pmatrix} a_1 + b_1 \\ a_1 ik - b_1 ik \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} u(x_2) \\ \partial_n u(x_2) \end{pmatrix} = \begin{pmatrix} a_2 + b_2 \\ -a_2 ik + b_2 ik \end{pmatrix}.$$

We introduce a mapping of the data at x_1 to x_2 called a transfer matrix

$$\mathbf{T}(k) : \begin{pmatrix} u(x_1) \\ \partial_n u(x_1) \end{pmatrix} \to \begin{pmatrix} u(x_2) \\ \partial_n u(x_2) \end{pmatrix}$$

leading to

$$\mathbf{T} \begin{pmatrix} a_1 + b_1 \\ a_1 ik - b_1 ik \end{pmatrix} = \begin{pmatrix} a_2 + b_2 \\ -a_2 ik + b_2 ik \end{pmatrix}$$

where u is any solution to the differential equation on the interval $[x_1, x_2]$. We then determine a relation between the amplitudes of the incoming and outgoing waves given by

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \mathbf{S}_E \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}.$$

The matrix $\mathbf{S}_E$ is called the edge scattering matrix. It is clear that this matrix does not formally come from scattering problems in the sense of Definition 1.5.1.

Example 1.5.1 *Consider the following metric graph consisting of the edges* $E_n = [x_{2n-1}, x_{2n}]$, $n = 1, 2, 3, 4, 5, 6$ *and vertices* $V_1 = \{x_1, x_6, x_7\}$, $V_2 = \{x_2, x_3, x_9\}$, $V_3 = \{x_4, x_5, x_{11}\}$, $V_4 = \{x_8\}$, $V_5 = \{x_{10}\}$ *and* $V_6 = \{x_{12}\}$.

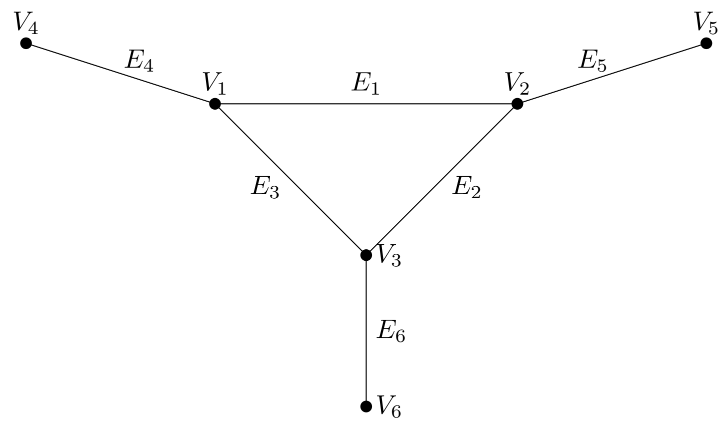

FIGURE 1.2

Let the vertex conditions be defined by (1.3.3) *where*

$$\mathbf{S} = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}.$$

for internal vertices. Observe that $\mathbf{S}$ *is irreducible, hence properly connecting. Further* $\sigma(\mathbf{S}) = \{\pm 1\}$ *so that* $\mathbf{S}_{V_n}(k)$ *is independent of* k *and in particular* $\mathbf{S}_{V_n}(k) = \mathbf{S}$, $n = 1, 2, 3$. *For external vertices* $\mathbf{S} = (1)$. *Then* $\mathbf{S}_{V_n}(k) = (1)$, $n = 4, 5, 6$. *The global vertex scattering matrix can be written as*

$$\mathbf{S}_V = \mathrm{diag}(\mathbf{S}, \mathbf{S}, \mathbf{S}, 1, 1, 1).$$

We now determine the edge scattering matrix. Consider the edge $E_1 = [x_1, x_2]$ *and let the associated transfer matrix be given by* $\mathbf{T}^1(k) = \left(t^1_{ij}\right)$, $i, j = 1, 2$. *By direct computations one obtains that*

$$\mathbf{S}_{E_1}(k) = \begin{pmatrix} \frac{k^2 t^1_{12} + t^1_{21} - ik\left(t^1_{11} - t^1_{22}\right)}{k^2 t^1_{12} - t^1_{21} + ik\left(t^1_{11} + t^1_{22}\right)} & \frac{2ik}{k^2 t^1_{12} - t^1_{21} + ik\left(t^1_{11} + t^1_{22}\right)} \\ \frac{2ik}{k^2 t^1_{12} - t^1_{21} + ik\left(t^1_{11} + t^1_{22}\right)} & \frac{k^2 t^1_{12} + t^1_{21} + ik\left(t^1_{11} - t^1_{22}\right)}{k^2 t^1_{12} - t^1_{21} + ik\left(t^1_{11} + t^1_{22}\right)} \end{pmatrix}.$$

In the computations we have used the fact that $\det\left(\mathbf{T}^1(k)\right) = 1$ *for all energies [PK14]. It has also been shown [PK14] that* $k^2 t^1 12 + t^1_{21} + ik\left(t^1_{11} - t^1_{22}\right) \neq 0$ *for* $\Im(k) \geq 0$ *and* $\Re(k) \neq 0$. *When the potentials are zero as in* (1.5.4) *then*

$$t_{11} = \cos kl_1, \quad t_{12} = \frac{1}{k}\sin kl_1, \quad t_{21} = -k\sin kl_1, \quad t_{22} = \cos kl_1$$

where $l_1 = x_2 - x_1$. The above matrix then simplifies to

$$\mathbf{S}_{E_1} = \begin{pmatrix} 0 & e^{ikl_1} \\ e^{ikl_1} & 0 \end{pmatrix}.$$

Consequently the global edge scattering matrix is

$$\mathbf{S}_E(k) = \operatorname{diag}\left(\mathbf{S}_{E_1}, \mathbf{S}_{E_2}, \mathbf{S}_{E_3}, \mathbf{S}_{E_4}, \mathbf{S}_{E_5}, \mathbf{S}_{E_6}\right).$$

1.6 Literature Review and Statement of the Problem

1.6.1 Equi-transmitting matrices

The vertex scattering matrix can be seen as the unitary matrix which describes the probabilities that the waves penetrate the vertex from one edge to another. In quantum mechanics such probabilities are given by the squared absolute values of the corresponding matrix entries $|s_{ij}|^2$. One may say that all edges are equivalent if and only if

$$\begin{cases} |s_{ij}|^2 = |s_{lm}|^2, & \text{for all } i \neq j, l \neq m \\ |s_{ii}|^2 = |s_{jj}|^2 & \text{for all } i, j. \end{cases}$$

Initial studies of equally transmitting scattering matrices are due to the work of Harrison et el in 2007 in [HSW07]. They studied such matrices only in the case where back scattering is not allowed. They defined such matrices to be unitary and whose off-diagonal entries have equal amplitudes given by $(d_m - 1)^{-1/2}$, where d_m is the valency of the corresponding vertex.

Their construction of the matrices involved the use of the Hadamard matrices and Diriclet characters. The Hadamard conjecture proposes that a Hadamard matrix of order $4k$ exists for every positive integer k. However existence problem is an open question in the theory of Hadamard matrices. This implies that the matrices constructed in [HSW07] only exist for the cases where the associated Hadamard matrix exists. The construction using the Dirichlet characters guarantees that this class of equally transmitting matrices exists when the order is $P + 1$ where P is an odd prime number. They note that the only equally transmitting matrix without reflection of odd order that they managed to construct is

$$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & w & w^2 \\ 1 & 1 & 0 & w^2 & w \\ 1 & w & w^2 & 0 & 1 \\ 1 & w^2 & w & 1 & 0 \end{pmatrix}, \qquad w = e^{\frac{2}{3}\pi i}.$$

They indicated that it is not known whether there exists any other such equally transmitting matrix without reflection of odd order. Note that this matrix is not Hermitian and therefore the vertex scattering matrix depends on the energy. Such a matrix is equi-transmitting just for one value of the energy parameter.

Turek and Cheon [TC112] studied equally transmitting matrices where back scattering is allowed. They gave various cases for which Hermitian unitary equally transmitting exist. The cases are given in terms of the ratio $d := |s_{jj}| / |s_{jk}|$ where $\mathbf{S}_V \in \mathbb{C}^{d_m, d_m}$ is unitary and $|s_{lm}| = |s_{jk}|$ for all $l \neq m$, $j \neq k$. Here d_m is the order of the matrix $\mathbf{S}_V$. For some of the cases they considered, the construction involved the use of Hadamard and conference matrices.

In [TC11] they studied energy dependent equally transmitting matrices that incorporated the δ and δ' couplings.

In this thesis we study equally transmitting matrices that are independent of the energy. We are going to call such matrices equi-transmitting. Below we give the definition of the equi-transmitting matrices we have studied.

Definition 1.6.1 *An $d_m \times d_m$ matrix $\mathbf{S}_V$ is equi-transmitting (ET-matrix) if the following hold*

1. $\mathbf{S}_V = \mathbf{S}_V^* = \mathbf{S}_V^{-1}$,
2. $|s_{ii}| = r$,
3. $|s_{ij}| = |s_{lm}|, \qquad i \neq j, l \neq m.$

Let us denote the moduli of the reflection and transmission coefficients respectively as follows

$$|s_{ii}| = r \text{ for all } i \text{ and } |s_{ij}| = t, \quad \text{for all } i \neq j.$$

The ET-matrices can be represented as $\mathbf{S}_V = \mathbf{D}_\theta^* \hat{\mathbf{C}} \mathbf{D}_\theta$ where

$$\hat{\mathbf{C}} = \begin{pmatrix} \pm r & t & t & \cdots & t \\ t & \pm r & ta_{23} & \cdots & ta_{2d_m} \\ t & t\bar{a}_{23} & \pm r & & ta_{3d_m} \\ \vdots & \vdots & & \ddots & \vdots \\ t & t\bar{a}_{2d_m} & t\bar{a}_{3d_m} & \cdots & \pm r \end{pmatrix}, \tag{1.6.1}$$

$$\mathbf{D}_\theta = \operatorname{diag}\left(e^{i\theta_1}, e^{i\theta_2}, \ldots, e^{i\theta_{d_m}}\right), \quad \theta_i \in [-\pi, \pi), \quad i = 1, 2, \ldots, d_m,$$

$$a_{ij} \in \mathbb{C} \text{ such that } |a_{ij}| = 1 \quad \text{for all } i = 2, \ldots, d_m - 1, j = 3, \ldots, d_m.$$

The matrices $\mathbf{S}_V$ and $\hat{\mathbf{C}}$ are equal up to the phases defined by $\mathbf{D}_\theta$ and the equi-transmission properties of $\mathbf{S}_V$ are preserved in $\hat{\mathbf{C}}$. We therefore narrow down our study of ET-matrices to matrix $\hat{\mathbf{C}}$ and in particular describe the results in terms of matrix $\hat{\mathbf{C}}$. When $r = 0$ in $\mathbf{S}_V$ (or $\hat{\mathbf{C}}$) the corresponding matrix is a reflectionless equi-transmitting matrix (RET-matrix).

1.6.2 Magnetic fluxes and vertex phases

Kostrykin and Schrader in [KS03] have studied the dependence of the spectrum of the magnetic Laplacian on the magnetic flux. They gave a complete description of the set of all magnetic Laplacians on a metric graph which can be obtained from a given self-adjoint Laplacian by perturbing it by magnetic fields.

In [KA15] Kurasov and Serio showed that if the matching conditions for the only vertex of the eight shaped graph is parameterised by

$$\mathbf{S} = \begin{pmatrix} 0 & 0 & \alpha & \beta \\ 0 & 0 & -\beta & \alpha \\ \alpha & -\beta & 0 & 0 \\ \beta & \alpha & 0 & 0 \end{pmatrix}, \quad \alpha, \beta \in \mathbb{R}, \quad \alpha^2 + \beta^2 = 1$$

then the spectrum of the magnetic operator is independent of the flux through one of the loops, provided the flux through the other loop is zero. They also showed dependence of the spectrum on magnetic fluxes may vanish.

Now consider the magnetic Schrödinger operator

$$L_{q,a} = \left(i\frac{d}{dx} + a\left(x\right) \right)^2 + q\left(x\right)$$

where $a \in C\left(\Gamma\right)$ and $q \in L_2\left(x\right)$ are the magnetic and electric potentials respectively both of which are real-valued. Consider the unitary transformation

$$U_a : u\left(x\right) \mapsto e^{i\theta_n(x)} u\left(x\right), \quad x \in E_n = \left[x_{2n-1}, x_{2n}\right]. \tag{1.6.2}$$

If

$$\theta_n\left(x\right) = \int_{x_{2n-1}}^{x} a\left(y\right) dy, \quad x \in E_n$$

then it follows that

$$U_a L_{q,a} U_a^{-1} = L_{q,0}, \tag{1.6.3}$$

that is, the magnetic potential has been eliminated.

Suppose the vertex conditions are defined by (1.3.3) where

$$\mathbf{S} = \operatorname{diag}(\mathbf{S}_1, \mathbf{S}_2, \ldots, \mathbf{S}_M)$$

with $\mathbf{S}_m$ being the corresponding unitary matrix parameterising the vertex condition at vertex V_m with valency d_m. The spectral properties of $L_{q,a}(\mathbf{S})$ does not depend on the particular form of the magnetic potential, since it can be eliminated. However the transformation (1.6.3) leads to different matching condions as explained below.

Consider the diagonal unitary matrix $\mathbf{U}_m$ given by

$$\mathbf{U}_m = \operatorname{diag}\left(e^{i\theta_1}, e^{i\theta_2}, \ldots, e^{i\theta_{d_m}}\right),$$

where θ_n are real parameters in (1.6.2). Associated to each $\mathbf{U}_m$ we define a unitary diagonal matrix

$$\mathbf{D}_m = \operatorname{diag}\left(e^{i\varphi_1}, e^{i\varphi_2}, \ldots, e^{i\varphi_{d_m}}\right), \quad \varphi_n \in \mathbb{R},$$

where φ_n are chosen equal to the values of θ_n at the corresponding end points. Note that the operator $L_{q,a}(\mathbf{S})$ is unitarily equivalent to $L_{q,0}\left(\mathbf{D}^{-1}\mathbf{S}\mathbf{D}\right)$, where $\mathbf{D} = \operatorname{diag}(\mathbf{D}_1, \mathbf{D}_2, \ldots, \mathbf{D}_M)$. Thus the new vertex conditions are defined by the matrix

$$\tilde{\mathbf{S}} = \mathbf{D}^{-1}\mathbf{S}\mathbf{D}.$$

Now suppose that the magnetic and electric potentials are fixed for a magnetic Shrödinger operator, while the vertex conditions are determined up to vertex phases. We seek to determine the maximal number of independent parameters that describe such operators up to unitary equivalence.

In summary our objectives are

1. give a simple criteria for determining the existence of both the RET and ET matrices. Our construction and analysis depend only on the unitary and Hermitian properties of matrices.
2. give a complete description of all RET and ET matrices up to order six.
3. determine the influence of the phases in the matrix $\mathbf{D}_\theta$ on the spectral properties of the quantum graphs.

Chapter 2

REFLECTIONLESS EQUI-TRANSMITTING MATRICES

2.1 Introduction

This chapter is devoted to the discussion reflectionless equi-transmitting (RET) matrices. In Section 2.2 we determine the order for which RET-matrices exist. It is shown that when reflection is prohibited, then such matrices exist only in even dimension. In Section 2.3 we give a complete description of reflectionless equi-transmitting matrices of sizes 2, 4 and 6. We observe that the parameter-free RET-matrices of order six form a combinatorial bipartite graph K_6^2.

2.2 Existence of Reflectionless Equi-transmitting Matrices

Assume that the $d_m \times d_m$ matrix $\mathbf{S}_V$ is reflectionless, unitary and Hermitian. Then its trace is zero and is equal to the sum of eigenvalues, which are equal to ± 1. Hence the dimension d_m has to be an even number. In fact it is enough to require that $\mathbf{S}_V$ is unitary and reflectionless for all energies. In the following theorem we show that RET-matrices only exist in even dimensions.

Theorem 2.2.1 *Suppose $\mathbf{S}_V$ is an $d_m \times d_m$ unitary matrix and let $(\mathbf{S}_V(k))_{jj} = 0$, $j = 1, \ldots, d_m$ and for any k. Then d_m is even and $\mathbf{S}_V$ is Hermitian.*

Let the eigenvalues of $\mathbf{S}_V$ be denoted by λ_n and the corresponding eigenvectors by $\vec{e}_n = (z_1^n, z_2^n, \ldots, z_{d_m}^n)$ which are chosen orthonormal, for for $j = 1, \ldots, d_m$, we have

$$(\mathbf{S}_V(k))_{jj} = \sum_{n=1}^{d_m} \frac{k(\lambda_n + 1) + (\lambda_n - 1)}{k(\lambda_n + 1) - (\lambda_n - 1)} \left|z_j^n\right|^2 = 0.$$

This gives us an $d_m \times d_m$ system of equations. For brevity let's introduce the notation $a_n = \lambda_n + 1$ and $b_n = \lambda_n - 1$. Then for $j = 1, \ldots, d_m$ the system of equations becomes

$$\sum_{n=1}^{d_m} \frac{ka_n + b_n}{ka_n - b_n} \left|z_j^n\right|^2 = 0.$$

Since the eigenvectors $\{\vec{e}_n\}$ form an orthonormal basis, we have $|z_1^n|^2 + \cdots + \left|z_{d_m}^n\right|^2 = 1$, $n = 1, \ldots, d_m$. So summing all the equations in the system we end up with the single equation

$$\sum_{n=1}^{d_m} \frac{ka_n + b_n}{ka_n - b_n} = 0. \tag{2.2.1}$$

It follows that

$$\sum_{n=1}^{d_m} \left\{ (ka_n + b_n) \prod_{\substack{m=1 \\ m \neq n}}^{N} (ka_m - b_m) \right\} = 0.$$

Assume first that d_m is **odd**. The function in the above equation can be seen as a polynomial in k and it is identically zero only if all coefficients at different powers are zero. In particular, the coefficient of k^{d_m} gives us

$$d_m \prod_{n=1}^{d_m} a_n = 0.$$

Without loss of generality we take $a_{d_m} = 0$ which yields $\lambda_{d_m} = -1$. Substituting this into equation (2.2.1), the last term in that sum equals -1. Hence we obtain

$$\sum_{n=1}^{d_m-1} \frac{ka_n + b_n}{ka_n - b_n} = 1.$$

Simplifying this equation we have

$$\sum_{n=1}^{d_m-1} \left\{ (ka_n + b_n) \prod_{\substack{m=1 \\ m \neq n}}^{d_m-1} (ka_m - b_m) \right\} = \prod_{n=1}^{d_m-1} (ka_n - b_n).$$

Proceeding as before and comparing the coefficients of the highest power of k we see that

$$(d_m - 1) \prod_{n=1}^{d_m-1} a_n = \prod_{n=1}^{v-1} a_n \qquad \Rightarrow \qquad (d_m - 2) \prod_{n=1}^{d_m-1} a_n = 0. \tag{2.2.2}$$

Since d_m is odd, it follows that $d_m - 2 \neq 0$ and so without loss of generality we assume, in the second equation in (2.2.2), that $a_{d_m-1} = 0$. This implies that $\lambda_{d_m-1} = -1$. Continuing in a similar manner, we observe that at every step, the coefficient $(d_m - \alpha)$ in the second equation in (2.2.2) is such that $\alpha \in 2_{\geqslant}$. Therefore $d_m - \alpha \neq 0$ for all applicable α. This has the consequence that $a_n = 0$ for all $n = 1, \ldots, d_m$ so that $\lambda_n = -1$ for all $n = 1, \ldots, d_m$. But that is impossible since the trace of S is zero. Hence d_m is **even**.

For convenience of manipulation, we set $d_m = 2\beta$, $\beta \in {}_{\geqslant}$. By the preceding calculations we see that $a_{2\beta} = a_{2\beta-1} = \cdots = a_{\beta+1} = 0$ which implies that $\lambda_n = -1$, $n = \beta+1, \ldots, 2\beta$. Taking into account that the trace of $\mathbf{S}_V$ is zero we get:

$$\mathrm{Tr}\mathbf{S}_V = \sum_{n=1}^{2\beta} \lambda_n = \sum_{n=1}^{\beta} \lambda_n + (-1)\,\beta = 0 \quad \Rightarrow \quad \sum_{n=1}^{\beta} \lambda_n = \beta.$$

Since $|\lambda_n| = 1$ for all $n = 1, \ldots, 2\beta$ we obtain that $\lambda_n = 1$, $n = 1, \ldots, \beta$. Therefore all the eigenvalues of $\mathbf{S}_V$ are not only on the unit circle but are also real and precisely are -1 and 1. Hence $\mathbf{S}_V$ is also Hermitian.

2.3 Reflectionless Equi-transmitting Matrices of Sizes 2, 4 and 6

In (1.6.1) when $r = 0$, t must be equal to $\frac{1}{\sqrt{d_m - 1}}$ and can be can be factored out so that $\hat{\mathbf{C}}$ has the representation

$$\hat{\mathbf{C}} = t \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & a_{23} & \cdots & a_{2d_m} \\ 1 & \overline{a}_{23} & 0 & & a_{3d_m} \\ \vdots & \vdots & & \ddots & \vdots \\ 1 & \overline{a}_{2d_m} & \overline{a}_{3d_m} & \cdots & 0 \end{pmatrix} = \frac{1}{\sqrt{d_m - 1}} \mathbf{C}$$

In what follows we determine RET-matrices when $d_m = 2$, $d_m = 4$ and $d_m = 6$.

When $d_m = 2$ it is clear that the associated RET-matrices have the form

$$\mathbf{S}_V = \begin{pmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{pmatrix} = \mathrm{diag}\left(1, e^{-i\theta}\right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathrm{diag}\left(1, e^{i\theta}\right),$$

where $\theta \in [-\pi, \pi]$. We have just a single one-parameter family.

Every RET-matrix in dimension four possesses the representation

$$\mathbf{S}_V = \operatorname{diag}\left(1, e^{-i\theta_1}, e^{-i\theta_2}, e^{-i\theta_3}\right) \frac{1}{\sqrt{3}} \, \mathbf{C} \, \operatorname{diag}\left(1, e^{i\theta_1}, e^{i\theta_2}, e^{i\theta_3}\right),$$

where $\theta_n \in [-\pi, \pi]$ and

$$\mathbf{C} = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & a & b \\ 1 & \bar{a} & 0 & c \\ 1 & \bar{b} & \bar{c} & 0 \end{pmatrix}.$$

The numbers $a, b, c \in \mathbb{C}$ have absolute value one and are chosen such that the rows (and columns) are orthogonal. It should be observed that the rows (and columns) of $\mathbf{C}$ are already normalized. Using the orthogonality conditions of the rows of $\mathbf{C}$ and solving for a, b and c we obtain $a = \pm i$, $b = -a$ and $c = -\bar{a}$. From these values of the parameters we obtain the following two matrices, which are complex conjugate or transpose of each other:

$$\mathbf{C}_1 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & i & -i \\ 1 & -i & 0 & i \\ 1 & i & -i & 0 \end{pmatrix} \qquad \mathbf{C}_2 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & -i & i \\ 1 & i & 0 & -i \\ 1 & -i & i & 0 \end{pmatrix}.$$

Hence the set of all RET-matrices in dimension four consists of two $3-$parameter nonintersecting families.

In our discussion of RET-matrices as well as ET-matrices of order six we will need to use the following lemma.

Lemma 1 *The sum of four complex numbers z_1, z_2, z_3, z_4 of equal magnitude equals zero if and only if at least one of the following cases occur:*

$$(z_3 = -z_1 \wedge z_4 = -z_2) \vee (z_4 = -z_1 \wedge z_3 = -z_2) \vee (z_2 = -z_1 \wedge z_4 = -z_3).$$

This is illustrated in the following figure.

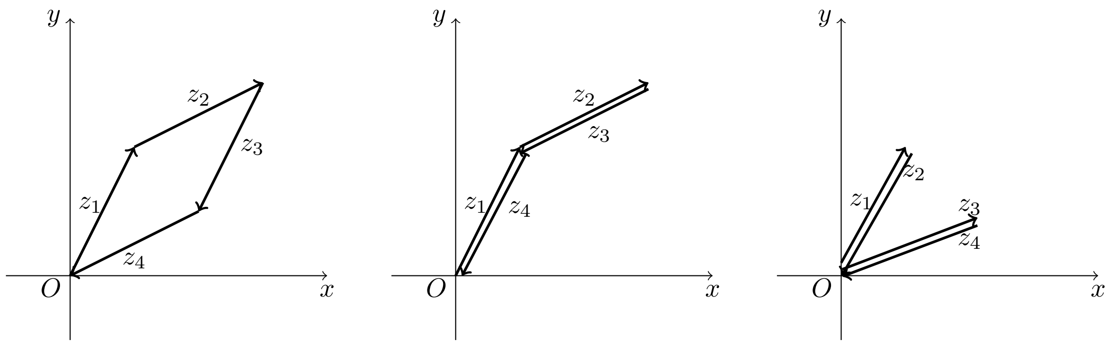

FIGURE 2.1: Illustration of Lemma 1

Remark 1 *Basically the Lemma is used to reduce the number of parameters in a given system. It is applied successively to subsequent systems until all the parameters are determined or some parameters are expressed in terms of irreducible parameters.*

Equi-transmitting matrices in dimension six take the form

$$\mathbf{S}_V = \mathbf{D}_\theta^{-1} \frac{1}{\sqrt{5}} \, \mathbf{C} \, \mathbf{D}_\theta, \tag{2.3.1}$$

where $\mathbf{D}_\theta = \text{diag}\left(1, e^{i\theta_1}, e^{i\theta_2}, e^{i\theta_3}, e^{i\theta_4}, e^{i\theta_5}\right)$, $\theta_n \in [-\pi, \pi)$ and

$$\mathbf{C} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & a & b & c & d \\ 1 & \overline{a} & 0 & e & f & g \\ 1 & \overline{b} & \overline{e} & 0 & h & l \\ 1 & \overline{c} & \overline{f} & \overline{h} & 0 & m \\ 1 & \overline{d} & \overline{g} & \overline{l} & \overline{m} & 0 \end{pmatrix}.$$

The parameters $a, b, c, d, e, f, g, h, l, m \in \mathbb{C}$ have absolute value one and are chosen so that the rows (columns) of $\mathbf{S}_V$ are orthogonal. The orthogonality conditions yield the following 15 equations in 10 unknowns:

$$\begin{cases} a+b+c+d=0 & (1)\\ \overline{a}+e+f+g=0 & (2)\\ \overline{b}+\overline{e}+h+l=0 & (3)\\ \overline{c}+\overline{f}+\overline{h}+m=0 & (4)\\ \overline{d}+\overline{g}+\overline{l}+\overline{m}=0 & (5)\end{cases} \qquad \begin{cases} 1+b\overline{e}+c\overline{f}+d\overline{g}=0 & (6)\\ 1+ae+c\overline{h}+d\overline{l}=0 & (7)\\ 1+af+bh+d\overline{m}=0 & (8)\\ 1+ag+bl+cm=0 & (9)\end{cases} \tag{2.3.2}$$

$$\begin{cases} 1+\overline{a}b+f\overline{h}+g\overline{l}=0 & (10)\\ 1+\overline{a}c+eh+g\overline{m}=0 & (11)\\ 1+\overline{a}d+el+fm=0 & (12)\end{cases} \qquad \begin{cases} 1+\overline{b}c+\overline{e}f+l\overline{m}=0 & (13)\\ 1+\overline{b}d+\overline{e}g+hm=0 & (14)\end{cases} \quad \begin{cases}1+\overline{c}d+\overline{f}g+\overline{h}l=0 & (15).\end{cases}$$

Below we give two examples illustrating how all RET-matrices of size 6 can be obtained.

Example 2.3.1 (Case 1.1) *We recall that the parameters in the matrix* $\mathbf{C}$ *are complex numbers of absolute value one. Therefore for any of these parameters* x *we have that* $x\overline{x} = |x|^2 = 1$. *Applying Lemma 1 to equation (1) in the system* (2.3.2) *we end up with the following three cases:*

$$\begin{aligned} &\textit{Case } 1: \quad b=-a, \quad d=-c,\\ &\textit{Case } 2: \quad c=-a, \quad d=-b,\\ &\textit{Case } 3: \quad d=-a, \quad c=-b. \end{aligned} \tag{2.3.3}$$

Let us consider the first possibility (cases 2 and 3 can be treated in a similar way). Substituting the values of b and d into (2.3.2)*, we obtain the following system:*

$$\begin{cases} \overline{a}+e+f+g=0 & (2)\\ -\overline{a}+\overline{e}+h+l=0 & (3)\\ \overline{c}+\overline{f}+\overline{h}+m=0 & (4)\\ -\overline{c}+\overline{g}+\overline{l}+\overline{m}=0 & (5)\end{cases} \qquad \begin{cases} 1-a\overline{e}+c\overline{f}-c\overline{g}=0 & (6)\\ 1+ae+c\overline{h}-c\overline{l}=0 & (7)\\ 1+af-ah-c\overline{m}=0 & (8)\\ 1+ag-al+cm=0 & (9)\end{cases}$$

$$\begin{cases} f\overline{h}+g\overline{l}=0 & (10)\\ 1+\overline{a}c+eh+g\overline{m}=0 & (11)\\ 1-\overline{a}c+el+fm=0 & (12)\end{cases} \qquad \begin{cases} 1-\overline{a}c+\overline{e}f+l\overline{m}=0 & (13)\\ 1+\overline{a}c+\overline{e}g+hm=0 & (14)\end{cases} \quad \begin{cases}\overline{f}g+\overline{h}l=0 & (15).\end{cases} \tag{2.3.4}$$

Equation (15) can be eliminated since it is a multiple of equation (10). Application of Lemma 1 to equation (2) in (2.3.4) *yields the following cases:*

$$\begin{aligned}
&\textit{Case } 1.1: \quad e = -\bar{a}, \quad g = -f,\\
&\textit{Case } 1.2: \quad f = -\bar{a}, \quad g = -e,\\
&\textit{Case } 1.3: \quad g = -\bar{a}, \quad f = -e.
\end{aligned}$$

We pick the first case again, and substitute the corresponding values of e and g into (2.3.4) *and obtain the following system:*

$$\begin{cases} -\overline{a} - a + h + l = 0 & (3)\\ \overline{c} + \overline{f} + \overline{h} + m = 0 & (4)\\ -\overline{c} - \overline{f} + \overline{l} + \overline{m} = 0 & (5) \end{cases} \qquad \begin{cases} 1 + a^2 + c\overline{f} + c\overline{f} = 0 & (6)\\ c\overline{h} - c\overline{l} = 0 & (7)\\ 1 + af - ah - c\overline{m} = 0 & (8)\\ 1 - af - al + cm = 0 & (9) \end{cases}$$

$$\begin{cases} f\overline{h} - f\overline{l} = 0 & (10)\\ 1 + \overline{a}c - \overline{a}h - f\overline{m} = 0 & (11)\\ 1 - \overline{a}c - \overline{a}l + fm = 0 & (12) \end{cases} \qquad \begin{cases} 1 - \overline{a}c - af + l\overline{m} = 0 & (13)\\ 1 + \overline{a}c + af + hm = 0 & (14) \end{cases}$$

From equation (7) in the above system we have that $l = h$. Substituting this value of l into equation (3) of the same system, we have that $\Re(a) = h$. This means that $h \in \mathbb{R}$ and since it has absolute value one it follows that $h = \pm 1$. This in turn implies that $l = \pm 1$ and $a = \pm 1$. Adding equations (4) and (5) and then substituting the values of l and h, we obtain $m = \mp 1$. Substituting $a = \pm 1$ into equation (6) yields $c\bar{f} = -1 \Rightarrow f = -c$. The parameter c can be chosen arbitrary leading to the following matrices:

$$\mathbf{C}_{1.1} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1\\ 1 & 0 & \pm 1 & \mp 1 & c & -c\\ 1 & \pm 1 & 0 & \mp 1 & -c & c\\ 1 & \mp 1 & \mp 1 & 0 & \pm 1 & \pm\\ 1 & \overline{c} & -\overline{c} & \pm 1 & 0 & \mp 1\\ 1 & -\overline{c} & \overline{c} & \pm 1 & \mp 1 & 0 \end{pmatrix}.$$

Remark 2 *The case we have considered will be numbered **Case 1.1**. This means that we have applied Lemma 1 twice and that in each case we have chosen the first option. The first application is to equation (1) of the initial system which yields three possibilities. We choose the first option from the three possibilities with the corresponding substitution giving us the second system. This system now has at most fourteen equations, equation (1) having been eliminated by the above substitution. The second application of Lemma 1 is now to equation (2) of the second system which also yields three possibilities. The second index in the notation means that we have chosen the first option again from the second three possibilities in order to determine the matrix.*

Example 2.3.2 (Case 3.1.1) *Suppose that now we consider the third case in* (2.3.3)*. Substituting the values of $d = -a$ and $c = -b$ into the system* (2.3.2) *we obtain the following system:*

$$\begin{cases} \overline{a}+e+f+g=0 & (2) \\ \overline{b}+\overline{e}+h+l=0 & (3) \\ -\overline{b}+\overline{f}+\overline{h}+m=0 & (4) \\ -\overline{a}+\overline{g}+\overline{l}+\overline{m}=0 & (5) \end{cases} \qquad \begin{cases} 1+b\overline{e}-b\overline{f}-a\overline{g}=0 & (6) \\ 1+ae-b\overline{h}-a\overline{l}=0 & (7) \\ 1+af+bh-a\overline{m}=0 & (8) \\ 1+ag+bl-bm=0 & (9) \end{cases}$$

$$\begin{cases} 1+\overline{a}b+f\overline{h}+g\overline{l}=0 & (10) \\ 1-\overline{a}b+eh+g\overline{m}=0 & (11) \\ el+fm=0 & (12) \end{cases} \qquad \begin{cases} \overline{e}f+l\overline{m}=0 & (13) \\ 1-a\overline{b}+\overline{e}g+hm=0 & (14) \end{cases} \quad \begin{cases} 1+a\overline{b}+\overline{f}g+\overline{h}l=0 & (15). \end{cases} \tag{2.3.5}$$

From this system, we see that equation (13) is a multiple of equation (12) and so can be discarded. Applying Lemma 1 to equation (2) of this system we obtain the following three cases:

$$\begin{aligned} &\textit{Case } 3.1: \quad e=-\bar{a}, \quad g=-f, \\ &\textit{Case } 3.2: \quad f=-\bar{a}, \quad g=-e, \\ &\textit{Case } 3.3: \quad g=-\bar{a}, \quad f=-e. \end{aligned}$$

We pick the case 3.1 and substitute the corresponding values of e and g into the system (2.3.5) *and thus obtain the following system:*

$$\begin{cases} \overline{b}-a+h+l=0 & (3) \\ -\overline{b}+\overline{f}+\overline{h}+m=0 & (4) \\ -\overline{a}-\overline{f}+\overline{l}+\overline{m}=0 & (5) \end{cases} \qquad \begin{cases} 1-ab-b\overline{f}+a\overline{f}=0 & (6) \\ -b\overline{h}-a\overline{l}=0 & (7) \\ 1+af+bh-a\overline{m}=0 & (8) \\ 1-af+bl-bm=0 & (9) \end{cases}$$

$$\begin{cases} 1+\overline{a}b+f\overline{h}-f\overline{l}=0 & (10) \\ 1-\overline{a}b-\overline{a}h-f\overline{m}=0 & (11) \\ -\overline{a}l+fm=0 & (12) \end{cases} \qquad \begin{cases} 1-a\overline{b}+af+hm=0 & (14) \\ a\overline{b}+\overline{h}l=0 & (15). \end{cases} \tag{2.3.6}$$

We discard equation (15) because it is a multiple of equation(7). Here we need to apply Lemma 1 once more, this time to equation (3) of the system (2.3.6).

$$\begin{aligned} &\textit{Case } 3.1.1: \quad b=\bar{a}, \quad l=-h \\ &\textit{Case } 3.1.2: \quad h=a, \quad l=-\bar{b} \\ &\textit{Case } 3.1.3: \quad l=a, \quad h=-\bar{b}. \end{aligned}$$

We then pick the first case. Substituting the corresponding values of b and l into the system (2.3.6) *gives us the following system:*

$$\begin{cases} -a+\overline{f}+\overline{h}+m=0 & (4)\\ -\overline{a}-\overline{f}-\overline{h}+\overline{m}=0 & (5)\end{cases} \qquad \begin{cases} -\overline{a}\overline{f}+a\overline{f}=0 & (6)\\ -\overline{a}\overline{h}+a\overline{h}=0 & (7)\\ 1+af+\overline{a}h-a\overline{m}=0 & (8)\\ 1-af-\overline{a}h-\overline{a}m=0 & (9)\end{cases}$$

$$\begin{cases} 1+\overline{a}^2+f\overline{h}+f\overline{h}=0 & (10)\\ 1-\overline{a}^2-\overline{a}h-f\overline{m}=0 & (11)\\ \overline{a}h+fm=0 & (12)\end{cases} \qquad \begin{cases} 1-a^2+af+hm=0 \quad (14).\end{cases}$$

From equation (7) we see that $a\in\mathbb{R}$, $\Rightarrow a=\pm1$. Adding equations (4) and (5) and then substituting the values of a we have that $\Re(m)=\pm1\Rightarrow m=\pm1$. Substituting the values of a into equation (10) we obtain that $f\overline{h}=-1$, which implies that $h=-f$. From these we see that the corresponding matrix is

$$\mathbf{C}_{3.1.1}=\begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1\\ 1 & 0 & \pm1 & \pm & \mp1 & \mp1\\ 1 & \pm1 & 0 & \mp1 & f & -f\\ 1 & \pm1 & \mp1 & 0 & -f & f\\ 1 & \mp1 & \overline{f} & -\overline{f} & 0 & \pm1\\ 1 & \mp1 & -\overline{f} & \overline{f} & \pm1 & 0\end{pmatrix}.$$

Continuing as in the above examples in all cases we obtain 30 (different) one-parameter families of matrices. A summary of all the cases can be seen in Table 2.1. Below we list all the 30 different parameter dependent matrices where the subscript denotes the row (and column) which does not contain a parameter.

$$\mathbf{A}_2=\begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1\\ 1 & 0 & \pm1 & \pm1 & \mp1 & \mp1\\ 1 & \pm1 & 0 & \mp1 & \alpha & -\alpha\\ 1 & \pm1 & \mp1 & 0 & -\alpha & \alpha\\ 1 & \mp1 & \overline{\alpha} & -\overline{\alpha} & 0 & \pm1\\ 1 & \mp1 & -\overline{\alpha} & \overline{\alpha} & \pm1 & 0\end{pmatrix}, \mathbf{B}_2=\begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1\\ 1 & 0 & \pm1 & \mp1 & \pm1 & \mp1\\ 1 & \pm1 & 0 & \beta & \mp1 & -\beta\\ 1 & \mp1 & \overline{\beta} & 0 & -\overline{\beta} & \pm1\\ 1 & \pm1 & \mp1 & -\beta & 0 & \beta\\ 1 & \mp1 & -\overline{\beta} & \pm1 & \overline{\beta} & 0\end{pmatrix},$$

$$\mathbf{C}_2=\begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1\\ 1 & 0 & \pm1 & \mp1 & \mp1 & \pm1\\ 1 & \pm1 & 0 & \gamma & -\gamma & \mp1\\ 1 & \mp1 & \overline{\gamma} & 0 & \pm1 & -\overline{\gamma}\\ 1 & \mp1 & -\overline{\gamma} & \pm1 & 0 & \overline{\gamma}\\ 1 & \pm1 & \mp1 & -\gamma & \gamma & 0\end{pmatrix},$$

$$\mathbf{A}_3 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \mp1 & \alpha & -\alpha \\ 1 & \pm1 & 0 & \pm1 & \mp1 & \mp1 \\ 1 & \mp1 & \pm1 & 0 & -\alpha & \alpha \\ 1 & \overline{\alpha} & \mp1 & -\overline{\alpha} & 0 & \pm1 \\ 1 & -\overline{\alpha} & \mp1 & \overline{\alpha} & \pm1 & 0 \end{pmatrix}, \mathbf{B}_3 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \beta & \mp1 & -\beta \\ 1 & \pm1 & 0 & \mp1 & \pm1 & \mp1 \\ 1 & \overline{\beta} & \mp1 & 0 & -\overline{\beta} & \pm1 \\ 1 & \mp1 & \pm1 & -\beta & 0 & \beta \\ 1 & -\overline{\beta} & \mp1 & \pm1 & \overline{\beta} & 0 \end{pmatrix},$$

$$\mathbf{C}_3 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \gamma & -\gamma & \mp1 \\ 1 & \pm1 & 0 & \mp1 & \mp1 & \pm1 \\ 1 & \overline{\gamma} & \mp1 & 0 & \pm1 & -\overline{\gamma} \\ 1 & -\overline{\gamma} & \mp1 & \pm1 & 0 & \overline{\gamma} \\ 1 & \mp & \pm1 & -\gamma & \gamma & 0 \end{pmatrix},$$

$$\mathbf{A}_4 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \mp1 & \alpha & -\alpha \\ 1 & \pm1 & 0 & \mp1 & -\alpha & \alpha \\ 1 & \mp1 & \mp1 & 0 & \pm1 & \pm1 \\ 1 & \overline{\alpha} & -\overline{\alpha} & \mp1 & 0 & \mp1 \\ 1 & -\overline{\alpha} & \overline{\alpha} & \pm1 & \mp1 & 0 \end{pmatrix}, \mathbf{B}_4 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \beta & \pm1 & \mp1 & -\beta \\ 1 & \overline{\beta} & 0 & \mp1 & -\overline{\beta} & \pm1 \\ 1 & \pm1 & \mp1 & 0 & \pm1 & \mp1 \\ 1 & \mp1 & -\beta & \pm1 & 0 & \beta \\ 1 & -\overline{\beta} & \pm1 & \mp1 & \overline{\beta} & 0 \end{pmatrix},$$

$$\mathbf{C}_4 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \gamma & \pm1 & -\gamma & \mp1 \\ 1 & \overline{\gamma} & 0 & \mp1 & \pm1 & -\overline{\gamma} \\ 1 & \pm1 & \mp1 & 0 & \mp1 & \pm1 \\ 1 & -\overline{\gamma} & \pm1 & \mp1 & 0 & \overline{\gamma} \\ 1 & \mp1 & -\gamma & \pm1 & \gamma & 0 \end{pmatrix},$$

$$\mathbf{A}_5 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \alpha & -\alpha & \pm1 & \mp1 \\ 1 & \overline{\alpha} & 0 & \pm & \mp1 & -\overline{\alpha} \\ 1 & -\overline{\alpha} & \pm1 & 0 & \mp1 & \overline{\alpha} \\ 1 & \pm1 & \mp1 & \mp1 & 0 & \pm1 \\ 1 & \mp1 & \alpha & \alpha & \pm1 & 0 \end{pmatrix}, \mathbf{B}_5 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \beta & \mp1 & -\beta \\ 1 & \pm1 & 0 & -\beta & \mp1 & \beta \\ 1 & \overline{\beta} & -\overline{\beta} & 0 & \pm1 & \mp1 \\ 1 & \mp1 & \mp1 & \pm1 & 0 & \pm1 \\ 1 & -\overline{\beta} & \overline{\beta} & \mp1 & \pm1 & 0 \end{pmatrix},$$

$$\mathbf{C}_5 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \gamma & \pm 1 & \mp 1 & -\gamma \\ 1 & \overline{\gamma} & 0 & -\overline{\gamma} & \pm 1 & \mp 1 \\ 1 & \pm 1 & -\gamma & 0 & \mp 1 & \gamma \\ 1 & \mp 1 & \pm 1 & \mp 1 & 0 & \pm 1 \\ 1 & -\overline{\gamma} & \mp 1 & \overline{\gamma} & \pm 1 & 0 \end{pmatrix},$$

$$\mathbf{A}_6 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \alpha & -\alpha & \pm 1 & \mp 1 \\ 1 & \overline{\alpha} & 0 & \mp 1 & -\overline{\alpha} & \pm 1 \\ 1 & -\overline{\alpha} & \mp 1 & 0 & \overline{\alpha} & \pm 1 \\ 1 & \pm 1 & -\alpha & \alpha & 0 & \mp 1 \\ 1 & \mp 1 & \pm 1 & \pm 1 & \mp 1 & 0 \end{pmatrix}, \mathbf{B}_6 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \beta & \pm 1 & -\beta & \mp 1 \\ 1 & \overline{\beta} & 0 & -\overline{\beta} & \mp 1 & \pm 1 \\ 1 & \pm 1 & -\beta & 0 & \beta & \mp 1 \\ 1 & -\overline{\beta} & \mp & \overline{\beta} & 0 & \pm 1 \\ 1 & \mp 1 & \pm 1 & \mp 1 & \pm 1 & 0 \end{pmatrix},$$

$$\mathbf{C}_6 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm 1 & \gamma & -\gamma & \mp 1 \\ 1 & \pm 1 & 0 & -\gamma & \gamma & \mp 1 \\ 1 & \overline{\gamma} & -\overline{\gamma} & 0 & \mp 1 & \pm 1 \\ 1 & -\overline{\gamma} & \overline{\gamma} & \mp 1 & 0 & \pm 1 \\ 1 & \mp 1 & \mp 1 & \pm 1 & \pm 1 & 0 \end{pmatrix}.$$

The parameter dependent matrices are such that one row and one column with the same indexing are without the parameter. The parameter occurs twice in each of the remaining four rows and columns. Since the first row and column are fixed, there remains only four possibilities for taking up the two positions to be occupied by the parameter. This gives 6 matrices. Since there are five different ways in which the parameter free row (and column) can be taken up, we obtain the $6 \times 5 = 30$ matrices in agreement with the results obtained.

It is natural to classify the above one-parameter matrices according to which row (and column) is parameter free. This gives us five families of one-parameter matrices which we denote as follows:

$$\{\mathbf{A}_i, \mathbf{B}_i, \mathbf{C}_i\} \quad i = 2, 3, 4, 5, 6. \tag{2.3.7}$$

It is possible to obtain one matrix from another within a given family by matrix permutations.

Assigning the values ± 1 to the parameters yields 60 parameter free matrices. We observe that there are only 12 distinct such matrices obtained from the 60. Each of these 12 is an intersection of certain five (out of the 60) families of matrices. Equation (2.3.8) illustrates how the intersections are obtained. Below we also list the parameter free matrices.

$$\mathbf{D}_1 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \pm1 & \mp1 & \mp1 \\ 1 & \pm1 & 0 & \mp1 & \pm1 & \mp1 \\ 1 & \pm1 & \mp1 & 0 & \mp1 & \pm1 \\ 1 & \mp1 & \pm1 & \mp1 & 0 & \pm1 \\ 1 & \mp1 & \mp1 & \pm1 & \pm1 & 0 \end{pmatrix}, \mathbf{D}_2 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \pm1 & \mp1 & \mp1 \\ 1 & \pm1 & 0 & \mp1 & \mp1 & \pm1 \\ 1 & \pm1 & \mp1 & 0 & \pm1 & \mp1 \\ 1 & \mp1 & \mp1 & \pm1 & 0 & \pm1 \\ 1 & \mp1 & \pm1 & \mp1 & \pm1 & 0 \end{pmatrix},$$

$$\mathbf{D}_3 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \mp1 & \pm1 & \mp1 \\ 1 & \pm1 & 0 & \pm1 & \mp1 & \mp1 \\ 1 & \mp1 & \pm1 & 0 & \mp1 & \pm1 \\ 1 & \pm1 & \mp1 & \mp1 & 0 & \pm1 \\ 1 & \mp1 & \mp1 & \pm1 & \pm1 & 0 \end{pmatrix},$$

$$\mathbf{D}_4 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \mp1 & \mp1 & \pm1 \\ 1 & \pm1 & 0 & \mp1 & \pm1 & \mp1 \\ 1 & \mp1 & \mp1 & 0 & \pm1 & \pm1 \\ 1 & \mp1 & \pm1 & \pm1 & 0 & \mp1 \\ 1 & \pm1 & \mp1 & \pm1 & \mp1 & 0 \end{pmatrix}, \mathbf{D}_5 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \mp1 & \mp1 & \pm1 \\ 1 & \pm1 & 0 & \pm1 & \mp1 & \mp1 \\ 1 & \mp1 & \pm1 & 0 & \pm1 & \mp1 \\ 1 & \mp1 & \mp1 & \pm1 & 0 & \pm1 \\ 1 & \pm1 & \mp1 & \mp1 & \pm1 & 0 \end{pmatrix},$$

$$\mathbf{D}_6 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & \pm1 & \mp1 & \pm1 & \mp1 \\ 1 & \pm1 & 0 & \mp1 & \mp1 & \pm1 \\ 1 & \mp1 & \mp1 & 0 & \pm1 & \pm1 \\ 1 & \pm1 & \mp1 & \pm1 & 0 & \mp1 \\ 1 & \mp1 & \pm1 & \pm1 & \mp1 & 0 \end{pmatrix}.$$

n_1		n_2		n_3		n_4		Matrix
1	$b=-a, d=-c$	1	$e=-\overline{a}, g=-f$					$\mathbf{A}_4$
		2	$f=-\overline{a}, g=-e$	1	$e=a, l=-h$			$\mathbf{A}_3$
				2	$h=\overline{a}, l=-\overline{e}$			$\mathbf{A}_6$
				3	$l=\overline{a}, h=-\overline{e}$			$\mathbf{B}_2$
		3	$g=-\overline{a}, f=-e$	1	$e=a, l=-h$			$\mathbf{A}_3$
				2	$h=\overline{a}, l=-\overline{e}$			$\mathbf{C}_2$
				3	$l=\overline{a}, h=-\overline{e}$			$\mathbf{A}_5$
2	$c=-a, d=-b$	1	$e=-\overline{a}, g=-f$	1	$b=\overline{a}, l=-h$			$\mathbf{A}_2$
				2	$h=a, l=-\overline{b}$			$\mathbf{B}_6$
				3	$l=a, h=-\overline{b}$			$\mathbf{B}_3$
		2	$f=-\overline{a}, g=-e$					$\mathbf{B}_5$
		3	$g=-\overline{a}, f=-e$	1	$e=-b, l=-h$			$\mathbf{C}_4$
				2	$h=-\overline{b}, l=-\overline{e}$			$\mathbf{D}_1$
				3	$l=-\overline{b}, h=-\overline{e}$			$\mathbf{D}_4$
3	$d=-a, c=-b$	1	$e=-\overline{a}, g=-f$	1	$b=\overline{a}, l=-h$			$\mathbf{A}_2$
				2	$h=a, l=-\overline{b}$			$\mathbf{C}_3$
				3	$l=a, h=-\overline{b}$			$\mathbf{C}_5$
		2	$f=-\overline{a}, g=-e$	1	$e=-b, l=-h$			$\mathbf{B}_4$
				2	$h=-\overline{b}, l=-\overline{e}$			$\mathbf{D}_6$
				3	$l=-\overline{b}, h=-\overline{e}$	1	$b=-\overline{a}, m=e$	$\mathbf{B}_2$
						2	$e=-a, m=\overline{b}$	$\mathbf{C}_3$
						3	$m=a, e=-\overline{b}$	$\mathbf{B}_4$
		3	$g=-\overline{a}, f=-e$					$\mathbf{C}_6$

TABLE 2.1: Summary of substitutions made to obtain various cases.

The 12 parameter free matrices are in fact integer conference matrices.[1] There exist complex conference matrices as well. The intersections are formed by picking one and only one matrix from each family. We list below the twelve intersections. In the notation used to denote the intersections, the superscript indicates the choice made. For instance, $\mathbf{D}_1^u$ means that we have chosen the matrix corresponding to the *upper* sign in matrix $\mathbf{D}_1$. In a similar manner, $\mathbf{D}_1^l$ means that we have chosen the matrix in $\mathbf{D}_1$ corresponding to the *lower* sign.

[1] A conference matrix is an $n \times n$ matrix $\mathbf{C}$ with diagonal entries 0 and off diagonal entries ± 1 which satisfies $\mathbf{C}\mathbf{C}^t = (n-1)\,I$.

$$
\begin{aligned}
\mathbf{D}_1^u &= \mathbf{A}_2^u(1) = \mathbf{B}_3^u(1) = \mathbf{C}_4^u(1) = \mathbf{C}_5^u(1) = \mathbf{C}_6^u(1)\,,\\
\mathbf{D}_1^l &= \mathbf{A}_2^l(-1) = \mathbf{B}_3^l(-1) = \mathbf{C}_4^l(-1) = \mathbf{C}_5^l(-1) = \mathbf{C}_6^l(-1)\,,\\
\mathbf{D}_2^l &= \mathbf{A}_2^l(1) = \mathbf{C}_3^l(-1) = \mathbf{B}_4^l(-1) = \mathbf{B}_5^l(-1) = \mathbf{B}_6^l(-1)\,,\\
\mathbf{D}_2^u &= \mathbf{A}_2^u(-1) = \mathbf{C}_3^u(1) = \mathbf{B}_4^u(1) = \mathbf{B}_5^u(1) = \mathbf{B}_6^u(1)\,,\\
\mathbf{D}_3^l &= \mathbf{B}_2^l(-1) = \mathbf{A}_3^l(-1) = \mathbf{B}_4^u(-1) = \mathbf{A}_5^l(-1) = \mathbf{C}_6^l(1)\,,\\
\mathbf{D}_3^u &= \mathbf{B}_2^u(1) = \mathbf{A}_3^u(1) = \mathbf{B}_4^l(1) = \mathbf{A}_5^u(1) = \mathbf{C}_6^u(-1)\,,\\
\mathbf{D}_4^l &= \mathbf{C}_2^l(1) = \mathbf{B}_3^l(1) = \mathbf{A}_4^l(1) = \mathbf{A}_5^u(-1) = \mathbf{B}_6^u(-1)\,,\\
\mathbf{D}_4^u &= \mathbf{C}_2^u(-1) = \mathbf{B}_3^u(-1) = \mathbf{A}_4^u(-1) = \mathbf{A}_5^l(1) = \mathbf{B}_6^l(1)\,,\\
\mathbf{D}_5^u &= \mathbf{C}_2^u(1) = \mathbf{A}_3^u(-1) = \mathbf{C}_4^l(1) = \mathbf{B}_5^u(-1) = \mathbf{A}_6^l(1)\,,\\
\mathbf{D}_5^l &= \mathbf{C}_2^l(-1) = \mathbf{A}_3^l(1) = \mathbf{C}_4^u(-1) = \mathbf{B}_5^l(1) = \mathbf{A}_6^u(-1)\,,\\
\mathbf{D}_6^u &= \mathbf{B}_2^u(-1) = \mathbf{C}_3^u(-1) = \mathbf{A}_4^u(1) = \mathbf{C}_5^l(1) = \mathbf{A}_6^u(1)\,,\\
\mathbf{D}_6^l &= \mathbf{B}_2^1(1) = \mathbf{C}_3^l(1) = \mathbf{A}_4^l(-1) = \mathbf{C}_5^u(-1) = \mathbf{A}_6^l(-1)\,.
\end{aligned}
\tag{2.3.8}
$$

Combinatorial bipartite regular graph K_6^2

We now discuss the observations made from the twelve intersections. If we consider these intersections as vertices of a discrete graph then graph obtained is bipartite and 5-regular. In the figure below each edge represents a one-parameter family (a loop). In fact each family is described by 6 parameters if one take into account the parameters $\theta_1, \ldots, \theta_5$ appearing in equation (2.3.1). The corresponding intersection are therefore 5-parameter families corresponding to six-dimensional conference matrices.

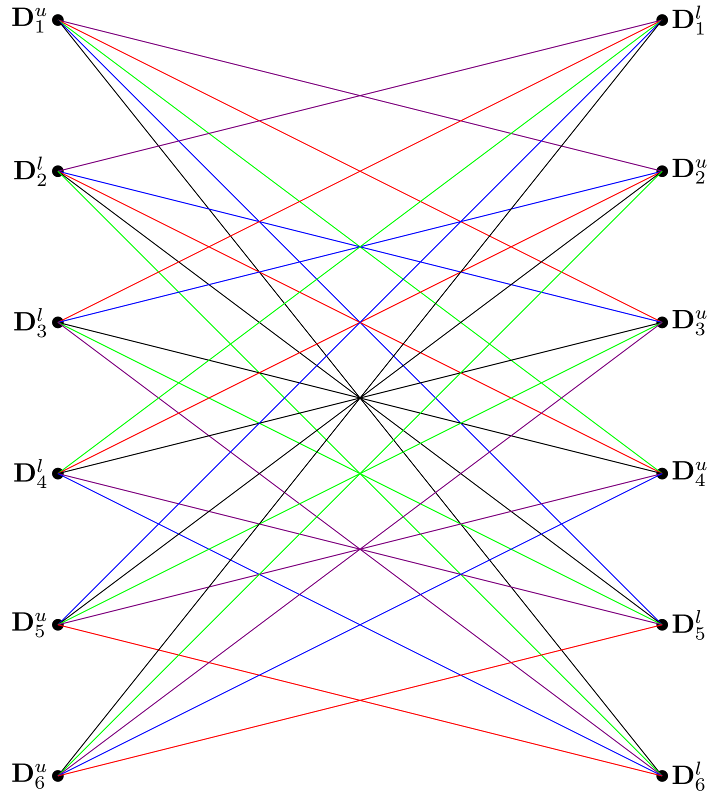

FIGURE 2.2: Five- and six-parameter families of 6×6 RET-matrices

An edge connecting any of the vertices is one and only one of the thirty one-parameter family of matrices where one vertex corresponds to the matrix obtained by assigning the value $+1$ to the parameter, while the other vertex is obtained by assigning the value -1 to the parameter. For example the edge connecting the vertices $\mathbf{D}_1^u$ and $\mathbf{D}_2^u$ is a loop determined by the matrix $\mathbf{A}_2(\alpha)$, where α is a complex number on the unit circle. In particular $\mathbf{D}_1^u = \mathbf{C}_5^u(1)$ and $\mathbf{D}_2^u = \mathbf{C}_5^u(-1)$. Figure 2.2 is the graph obtained where we have assigned a distinct colour to each family according to the classification in the notation (2.3.7).

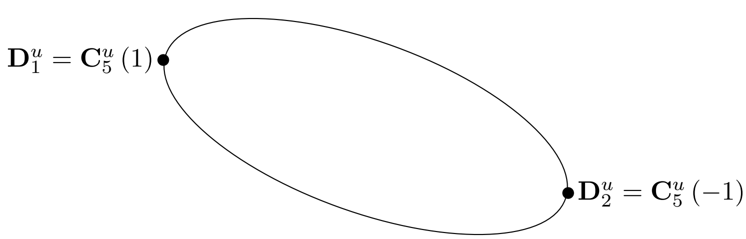

FIGURE 2.3: Edge connecting the vertices $\mathbf{D}_1^u$ and $\mathbf{D}_2^u$

Chapter 3

EQUI-TRANSMITTING MATRICES

3.1 Introduction

The gist of this chapter is the study of equi-transmitting (ET) matrices. In section 3.2 we describe the various transformations by which other ET-matrices can be generated from a given ET-matrix. Certain bounds on r are covered in section 3.3 where we also introduce the notation used to represent various cases discussed in subsequent sections. In section 3.4 we give examples of general ET-matrices. In section 3.5 we discuss cases in which no ET-matrix of order five exists. A complete description of ET-matrices of even orders up to order six when the trace is zero is given in section 3.6.

3.2 Transformations

Recall that ET-matrices have the representation given by

$$\mathbf{S}_V = \mathbf{D}_\theta^* \hat{\mathbf{C}} \mathbf{D}_\theta, \tag{3.2.1}$$

where

$$\hat{\mathbf{C}} = \begin{pmatrix} \pm r & t & t & \cdots & t \\ t & \pm r & ta_{23} & \cdots & ta_{2d_m} \\ t & t\overline{a}_{23} & \pm r & & ta_{3d_m} \\ \vdots & \vdots & & \ddots & \vdots \\ t & t\overline{a}_{2d_m} & t\overline{a}_{3d_m} & \cdots & \pm r \end{pmatrix},$$

$$\mathbf{D}_\theta = \operatorname{diag}\left(e^{i\theta_1}, \ldots, e^{i\theta_{d_m}}\right), \quad \theta_i \in [-\pi, \pi), \quad i = 1, 2, \ldots, d_m,$$

$$a_{ij} \in \mathbb{C} \text{ such that } |a_{ij}| = 1 \quad \text{for all } i = 2, \ldots, d_m - 1, j = 3, \ldots, d_m, i < j.$$

As pointed out in Section 1.6, the focus is on matrix $\hat{\mathbf{C}}$ since $|\hat{c}_{ij}| = |s_{ij}|$, $i, j = 1, 2, \ldots, d_m$. Note that for a given $\hat{\mathbf{C}}$ the family $\mathbf{S}$ is described by adding just $d_m - 1$ independent parameters, since the transformation $\theta_1 \mapsto 0$, $\theta_2 \mapsto \theta_2 - \theta_1$, $\cdots$, $\theta_{d_m} \mapsto \theta_{d_m} - \theta_1$ does not change the matrix $\mathbf{S}_V$.

Having an ET-matrix $\mathbf{S}$ one can obtain another ET-matrix by means of appropriate matrix transformation. Below we discuss such transformations

1. Let $\mathbf{D}$ be a diagonal matrix whose diagonal entries comprise ± 1. The transformation

$$(\mathbf{S}_V)_{\mathbf{D}} = \mathbf{D}^{-1}\mathbf{S}_V\mathbf{D}$$

   has the effect that certain entries of $\mathbf{S}_V$ have their signs reversed. However signs of the diagonal entries remain unchanged because the reversal of their signs is done twice. Such a transformation yields yet another ET-matrix since $\left|((\mathbf{S}_V)_{\mathbf{D}})_{ij}\right| = \left|(\mathbf{S}_V)_{ij}\right|$, $i, j = 1, 2, \ldots, N$.

2. The transformation $\mathbf{S}_V \mapsto -\mathbf{S}_V$ has the effect of reversing the signs of all the entries of $\mathbf{S}$. It is clear that the resulting matrix is again an ET-matrix.

3. Let $\mathbf{P}_{lm}$ be a permutation matrix. The matrix

$$(\mathbf{S}_V)_{\mathbf{P}} = \mathbf{P}_{lm}\mathbf{S}_V\mathbf{P}_{lm}$$

   is obtained by interchanging in $\mathbf{S}_V$ rows (and columns) l and m. Therefore $\left|((\mathbf{S}_V)_{\mathbf{P}})_{ij}\right| = \left|(\mathbf{S}_V)_{ij}\right|$, $i, j = 1, 2, \ldots, d_m$ meaning that $(\mathbf{S}_V)_{\mathbf{P}}$ is also an ET-matrix.

From the foregoing it follows that the study of ET-matrices can be done up to the above transformations.

3.3 Possible Values of r and t

It should be observed that the ET-matrix is defined in such a way that $r \geq 0$ and $t \geq 0$. Let the order of the matrix be d_m. Since the matrix $\hat{\mathbf{C}}$ is unitary, the rows are normalised and so row 1 of matrix $\mathbb{C}$ yields the equation

$$r^2 + (d_m - 1)\, t^2 = 1 \tag{3.3.1}$$

From the equation and the constraints on r and t, it follows that $r, t \in [0, 1]$.

When $r = 1$, then $t = 0$ and the corresponding matrix $\mathbf{C}$ (see equation (3.2.1)) is a diagonal matrix whose diagonal entries comprises ± 1. This is a trivial class of ET-matrices. It is the case where there is total reflection, i.e. no waves are transmitted. On the other hand when $r = 0$

then $t = \frac{1}{\sqrt{d_m - 1}}$ and one obtains an RET-matrix. These have been discussed up to order six in Chapter 2. We exclude these two cases, $r = 1$ and $r = 0$, from our further investigations.

Since $\mathbf{S}_V$ is Hermitian and unitary its spectrum consists of ± 1. Let n^+ be the multiplicity of $+1$ in the spectrum of $\mathbf{S}_V$. Let ν^+ be the number of positive diagonal entries of the matrix $\mathbf{S}_V$. If the order of $\mathbf{S}_V$ is N, then the numbers n^+ and ν^+ can assume any value in the set $\{0, 1, \ldots, d_m\}$. Determining the trace of S_V from its eigenvalues one obtains $\mathrm{Tr}\left(\mathbf{S}_V\right) = n^+ + (-1)\left(d_m - n^+\right) = 2n^+ - d_m$. On the other hand if it is determined from the diagonal entries then $\mathrm{Tr}\left(\mathbf{S}_V\right) = r\nu^+ + (-r)\left(d_m - \nu^+\right) = r\left(2\nu^+ - d_m\right)$. From these two equations possible value of r is determined by

$$r = \frac{2n^+ - d_m}{2\nu^+ - d_m}. \tag{3.3.2}$$

This formula is applicable only when $2\nu^+ - d_m \neq 0$. Therefore $r = 1$ only if $n^+ = \nu^+$, while $r = 0$ only if $n^+ = \frac{1}{2}d_m$.

It should be noted that when n is even and $n^+ = \nu^+ = \frac{1}{2}n$, formula (3.3.2) does not determine r. To determine r in this case we need to carry out further study. This case has turned out to be significant despite our initial skepticism of what could be obtained from it. It is only in this case that an ET-matrix other than those generated by the SMC-matrix can be constructed for $n \leq 6$. ET-matrices for $r, t \in (0, 1)$ will be referred to as nontrivial ET-matrices while those corresponding to $r = 1$ will be called trivial ET-matrices.

The diagrams in Figure 3.1 give a graphical depiction of the possible values of r. The first figure is for the case when n is odd, while the second figure is for the case when n is even.

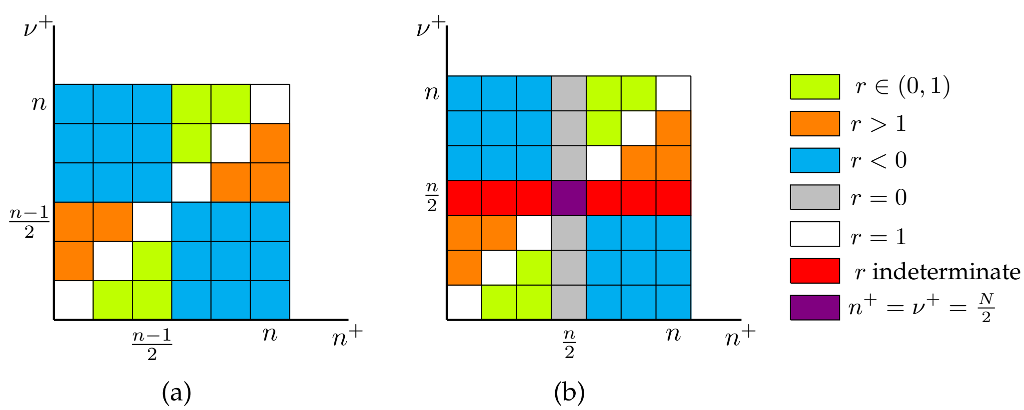

FIGURE 3.1: Possible values of r; (a) when n is odd and (b) when n is even

The diagonal white cells represent the trivial cases where $r = 1$ and for which the corresponding ET-matrix is a diagonal matrix. The orange cells represent cases where $r > 1$ while the blue cells represent cases where $r < 0$. Both of these cases are excluded since applicable values of r should be in the interval $(0, 1)$. The lime cells represent cases where $r \in (0, 1)$ and where there is a possibility of obtaining an ET-matrix. We have the following additional cases in figure (b). The light gray cells represent cases where $r = 0$ and where the corresponding ET-matrices are reflectionless. The red cells represent cases where r is infinite so that no ET-matrix can be constructed. The middle violet cell represent the cases where r is indeterminate from formula (3.3.2) but where it might be possible to construct ET-matrices from the definition of $\mathbf{S}_V$.

The various cases to be considered when investigating the existence of ET-matrices will be denoted by the ordered pair (n^+, ν^+). It should be noted that the cases (n^+, ν^+) and $(d_m - n^+, d_m - \nu^+)$ yield the same values of r and t.

We now discuss the viable cases for the existence of an ET-matrix when $r, t \in (0, 1)$. The cases where $n^+ = \nu^+$ are excluded since they give rise to $r = 1$. The exception to this is the case $(n^+, \nu^+) = \left(\frac{d_m}{2}, \frac{d_m}{2}\right)$ with n even, when (3.3.2) does not determine r. In the description below, we note that $n^+ > \nu^+$.

When d_m is odd then cases for which $r, t \in (0, 1)$ are given by

$$(n^+, \nu^+) \text{ and } (d_m - n^+, d_m - \nu^+)\,, \qquad \text{where} \quad \begin{cases} n^+ \in \left\{1, 2, \ldots, \frac{d_m - 1}{2}\right\} \\ \nu^+ \in \left\{0, 1 \ldots, \frac{d_m - 3}{2}\right\}. \end{cases} \tag{3.3.3}$$

On the other hand when d_m is even then such cases are given by

$$(n^+, \nu^+)\,, (d_m - n^+, d_m - \nu^+) \text{ and } \left(\tfrac{d_m}{2}, \tfrac{d_m}{2}\right)\,, \text{ where } \begin{cases} n^+ \in \left\{1, 2, \ldots, \frac{d_m}{2} - 1\right\} \\ \nu^+ \in \left\{0, 1 \ldots, \frac{d_m}{2} - 2\right\}. \end{cases} \tag{3.3.4}$$

3.4 General Examples

3.4.1 Diagonal matrices

For all n, whenever $r = 1$, there exists an equi-transmitting diagonal matrix. This matrix is not interesting in the framework of quantum graphs since it describes completely independent (not connected) edges.

3.4.2 Reflectionless equi-transmitting matrices

These are obtained when $r = 0$. We have discussed these matrices in Chapter 2 where it has been proved that such matrices exist only when n is even.

3.4.3 Standard matching conditions equi-transmitting matrices

For every incoming wave along a given edge, say E_j, in a star graph with n infinite edges there are both reflected waves along the same edge and transmitted waves along the other $d_m - 1$ edges E_l. This condition is described by the equation

$$u(x) = \begin{cases} e^{-ikx} + R_j e^{ikx}, x \in E_j \\ T_{lj} e^{ikx}, x \in E_l \end{cases} \tag{3.4.1}$$

where R_j is the reflection coefficient along edge E_j and T_{lj} is the transmission coefficient of waves transmitted from edge E_j into edge E_l. Recall that under standard matching conditions (SMC) coupling, a function defined on a quantum graph Γ satisfies the following conditions at a vertex

$$\begin{cases} u \text{ is continuous} \\ \sum u'(x) = 0. \end{cases} \tag{3.4.2}$$

Suppose the coupling of edges at the central vertex V with valency d_m is given by the SMC. Suppose also that the edges are parameterised as $E_j = [0, \infty)$, $j = 1, \ldots, n$. Conditions (3.4.2) are obviously invariant under edge permutation. Therefore the corresponding scattering matrix is not only equitransmiiting but all reflection (R_j) and all transition (T_{lj}) coefficients are identical. Continuity at $x = 0$ is therefore described by

$$1 + R = T. \tag{3.4.3}$$

The normal derivative is given by

$$u'(x) = \begin{cases} -ike^{-ikx} + ikR_i e^{ikx}, & x \in E_j \\ ikT_{lj} e^{ikx}, & x \in E_l \end{cases}$$

Applying the conditions on normal derivatives for SMC we have that

$$-(1 - R) + (d_m - 1) T = 0. \tag{3.4.4}$$

Solving for R and T in (3.4.3) and (3.4.4) we obtain that

$$T = \frac{2}{d_m} \quad \text{and} \quad R = -1 + \frac{2}{d_m}.$$

Thus the matrix S arising from the SMC is given by

$$s_{jl} = \begin{cases} -1 + \frac{2}{d_m}, & j = l \\ \frac{2}{d_m}, & j \neq l. \end{cases} \tag{3.4.5}$$

It is easy to see that this matrix is Hermitian (symmetric in this case since all the entries are real). It is also easy to see that $\mathbf{S}_V^t \mathbf{S}_V = \mathbf{S}_V \mathbf{S}_V^t = \mathbf{I}$, i.e. S is orthogonal. Thus $\mathbf{S}$ is Hermitian, unitary and equi-transmitting for all $n \geq 2$. Using the notations introduced in section 1.6, we see that

$$|s_{jl}| = \begin{cases} r = \frac{d_m - 2}{d_m}, & j = l \\ t = \frac{2}{d_m}, & j \neq l \end{cases}, \qquad d_m \geq 2. \tag{3.4.6}$$

Note that $r \in (0, 1)$, and when $d_m = 2$, the matrix is RET. We will refer to this matrix as the SMC-matrix.

3.4.4 Cases $(1, 0)$ and $(d_m - 1, d_m)$

For any given d_m the case (n^+, ν^+)=$(1, 0)$ yields the equation $-d_m r = -(d_m - 2)$ which implies that $r = 1 - \frac{2}{d_m}$. When this value of r is substituted into the equation $r^2 + (d_m - 1) t^2 = 1$ the positive value of t is obtained as $t = \frac{2}{d_m}$. Since in this case all the diagonal entries are negative, the associated matrix $\hat{\mathbf{C}}$ has the representation

$$\hat{\mathbf{C}}_{1,0} = \begin{pmatrix} -1 + \frac{2}{d_m} & \frac{2}{d_m} & \frac{2}{d_m} & \cdots & \frac{2}{d_m} \\ \frac{2}{d_m} & -1 + \frac{2}{d_m} & \frac{2}{d_m} a_{23} & \cdots & \frac{2}{d_m} a_{2d_m} \\ \frac{2}{d_m} & \frac{2}{d_m} \overline{a}_{23} & -1 + \frac{2}{d_m} & & \frac{2}{d_m} a_{3d_m} \\ \vdots & \vdots & & \ddots & \\ \frac{2}{d_m} & \frac{2}{d_m} \overline{a}_{2d_m} & \frac{2}{d_m} \overline{a}_{3d_m} & \cdots & -1 + \frac{2}{d_m} \end{pmatrix},$$

where $a_{ij} \in \{z \in \mathbb{C} : |z| = 1\}$ $i = 2, \ldots, d_m - 1, j = 3, \ldots, d_m, i < j$. Thus there are $\frac{1}{2}(d_m - 1)$ $(d_m - 2)$ such parameters. The inner products of the rows yield certain $\frac{1}{2} d_m (d_m - 1)$ equations. The orthogonality between the first row and all the other rows give the following $d_m - 1$ equations

$$
\begin{aligned}
-\alpha + a_{23} + a_{24} + \cdots + a_{2,d_m-1} + a_{2d_m} &= 0 \\
-\alpha + \overline{a}_{23} + a_{34} + \cdots + a_{3,d_m-1} + a_{3d_m} &= 0 \\
&\vdots \\
-\alpha + \overline{a}_{2,d_m-1} + \overline{a}_{3,d_m-1} + \cdots + \overline{a}_{d_m-2,d_m-1} + a_{d_m-1,d_m} &= 0 \\
-\alpha + \overline{a}_{2d_m} + \overline{a}_{3d_m} + \cdots + \overline{a}_{d_m-2,d_m} + \overline{a}_{d_m-1,d_m} &= 0
\end{aligned}
\tag{3.4.7}
$$

where $\alpha = \frac{2r}{t} = 2\left(1 - \frac{2}{d_m}\right)\frac{d_m}{2} = (d_m - 2)$. On the other hand, each of the above equations contain $d_m - 2$ unknowns. Since each parameter is unimodular, all the equations are satisfied if and only if each of the unknowns is unity, i.e. $a_{ij} = 1$, $i = 2, \ldots, d_m - 1$, $j = 3, \ldots, d_m$, $i < j$. All the other $\frac{1}{2}(d_m - 2)(d_m - 1)$ equations are of the form

$$
\begin{aligned}
&-\alpha\overline{a}_{ij} + 1 + \textstyle\sum_{l=3}^{d_m} a_{il}a_{jl} = 0, \\
&\text{for all } i = 2, \ldots, d_m - 1, j = 3, \ldots, d_m, i \neq l \neq j, i < j.
\end{aligned}
\tag{3.4.8}
$$

All these equations are also satisfied when all the parameters are unity. It follows that the matrix determined has the same transition probabilities as the SMC matrix and is given as follows

$$
\mathbf{C}_{1,0} = \begin{pmatrix}
-1 + \frac{2}{d_m} & \frac{2}{d_m} & \frac{2}{d_m} & \cdots & \frac{2}{d_m} \\
\frac{2}{d_m} & -1 + \frac{2}{d_m} & \frac{2}{d_m} & \cdots & \frac{2}{d_m} \\
\frac{2}{d_m} & \frac{2}{d_m} & -1 + \frac{2}{d_m} & & \frac{2}{d_m} \\
\vdots & \vdots & & \ddots & \vdots \\
\frac{2}{d_m} & \frac{2}{d_m} & \frac{2}{d_m} & \cdots & -1 + \frac{2}{d_m}
\end{pmatrix}. \tag{3.4.9}
$$

The case $(n^+, \nu^+) = (d_m - 1, d_m)$ can be analysed in a similar way leading to the matrix

$$
\hat{\mathbf{C}}_{d_m-1,d_m} = \begin{pmatrix}
1 - \frac{2}{d_m} & \frac{2}{d_m} & \frac{2}{d_m} & \cdots & \frac{2}{d_m} \\
\frac{2}{d_m} & 1 - \frac{2}{d_m} & -\frac{2}{d_m} & \cdots & -\frac{2}{d_m} \\
\frac{2}{d_m} & -\frac{2}{d_m} & 1 - \frac{2}{d_m} & & -\frac{2}{d_m} \\
\vdots & \vdots & & \ddots & \vdots \\
\frac{2}{d_m} & -\frac{2}{d_m} & -\frac{2}{d_m} & \cdots & 1 - \frac{2}{d_m}
\end{pmatrix}. \tag{3.4.10}
$$

The relation between the two matrices is given by

$$
\hat{\hat{\mathbf{C}}}_{d_m-1,d_m} = -\mathbf{D}\hat{\mathbf{C}}_{1,0}\mathbf{D}
$$

where $\mathbf{D}$ is an $d_m \times d_m$ diagonal matrix given by $\mathbf{D} = \operatorname{diag}(-1, 1, \ldots, 1)$. This means that for all $d_m \geq 2$, the cases $(1, 0)$ and $(d_m - 1, d_m)$ give the same transition probabilities as the SMC.

Observation 1 *From the above discussion we observe that ET-matrices which have the same transition probabilities as (generated by) SMC-matrix and their various transformations exist for all $n \geq 2$. In our notation they correspond to $(n^+, \nu^+) = (1, 0)$ and $(n^+, \nu^+) = (d_m - 1, d_m)$. The associated matrices are* (3.4.9) *and* (3.4.10) *respectively. We point out that the cases $(1, 0)$ and $(d_m - 1, d_m)$ determine the non trivial ET-matrices for $n \geq 3$.*

3.5 Nonzero trace, no ET-matrix

In this section we discuss cases (n^+, ν^+) for which there is a possibility of obtaining an ET-matrix according to equations (3.3.3) and (3.3.4) but for which no ET-matrix exists. We consider $n = 5$ since the described set is empty when $n = 3, 4$. Thus the cases to be discussed are $(2, 0)$, $(2, 1)$, $(3, 4)$ and $(3, 5)$. In what follows we give the details of the analysis of the case $(2, 0)$. The other cases are covered in the Appendix.

Case $(2, 0)$. In this case all diagonal entries are negative and two eigenvalues are positive. The values of r and t are $\frac{1}{5}$ and $\frac{\sqrt{6}}{5}$ respectively. The corresponding matrix $\hat{\mathbf{C}}$ is represented as follows

$$\hat{\mathbf{C}} = \begin{pmatrix} -r & t & t & t & t \\ t & -r & at & bt & ct \\ t & \overline{a}t & -r & dt & et \\ t & \overline{b}t & \overline{d}t & -r & ft \\ t & \overline{c}t & \overline{e}t & \overline{f}t & -r \end{pmatrix},$$

where $a, \ldots, f \in \{z \in \mathbb{C} : |z| = 1\}$. Since the rows of C are orthogonal, their inner products yield the following system of equations

$$\begin{cases} -2r + t\,(a + b + c) = 0 & (1) \\ -2r + t\,(\overline{a} + d + e) = 0 & (2) \\ -2r + t\left(\overline{b} + \overline{d} + f\right) = 0 & (3) \\ -2r + t\left(\overline{c} + \overline{e} + \overline{f}\right) = 0 & (4) \end{cases} \qquad \begin{cases} -2\overline{a}r + t\left(1 + \overline{b}d + \overline{c}e\right) = 0 & (5) \\ -2\overline{b}r + t\left(1 + \overline{a}\overline{d} + \overline{c}f\right) = 0 & (6) \\ -2\overline{c}r + t\left(1 + \overline{a}\overline{e} + \overline{b}\overline{f}\right) = 0 & (7) \end{cases} \tag{3.5.1}$$

$$\begin{cases} -2\overline{d}r + t\left(1 + a\overline{b} + \overline{e}f\right) = 0 & (8) \\ -2\overline{e}r + t\left(1 + a\overline{c} + \overline{d}\overline{f}\right) = 0 & (9) \end{cases} \qquad \left\{ -2\overline{f}r + t\,(1 + b\overline{c} + d\overline{e}) = 0 \quad (10). \right.$$

In what follows we determine the characteristic polynomial of matrix $\hat{\mathbf{C}}$ from its spectrum and by direct computation from the entries of C. Since $\sigma\left(\hat{\mathbf{C}}\right) = \{1, 1, -1, -1, -1\}$ we have

$$\Delta_{\hat{\mathbf{C}}}(\lambda) = -(\lambda - 1)^2 (\lambda + 1)^3 = -\left(\lambda^5 + \lambda^4 - 2\lambda^3 - 2\lambda^2 + \lambda + 1\right). \tag{3.5.2}$$

On the other hand by direct computation

$$\Delta_{\hat{\mathbf{C}}}(\lambda) = -\lambda^5 - 5r\lambda^4 + 10\left(t^2 - r^2\right)\lambda^3 + \tag{3.5.3}$$

where $\alpha = 2\frac{r}{t} = \frac{\sqrt{6}}{3}$. Thus we rewrite the polynomial as

$$\Delta_{\hat{\mathbf{C}}}(\lambda) = -\lambda^5 - 5r\lambda^4 + 10\left(t^2 - r^2\right)\lambda^3 + \left(30rt^2 - 10r^3 + t^3\left[6\alpha + a + \overline{a}\right]\right)\lambda^2 + \cdots \tag{3.5.4}$$

Substituting the values of r and t and comparing the corresponding coefficients in (3.5.2) and (3.5.4) we readily see that the coefficients of λ^5 and λ^4 are equal. Simplifying the coefficient of λ^3 in (3.5.4) we obtain that

$$10\left(\frac{6}{25} - \frac{1}{25}\right) = 2$$

in agreement with the value in (3.5.2). Equating the coefficients of λ^2 we obtain

$$30rt^2 - 10r^3 + t^3\left(6\alpha + a + \overline{a}\right) = 2$$

which when simplified we obtain

$$\Re(a) = \frac{\alpha}{3}.$$

By making appropriate combinations in the coefficient of t^3 in (3.5.3) one can show that

$$\Re(a) = \Re(b) = \Re(c) = \frac{\alpha}{3}.$$

Consequently imaginary parts of a, b and c may coincide or differ by a sign. Hence it is impossible that (eq(1))

$$a + b + c = \alpha.$$

This contradiction implies that no ET-matrix can be obtained in this case.

3.6 Trace zero; characterization of ET-matrices.

As already discussed in Section 3.4 there are ET-matrices generated by the SMC-matrix for all $n \geq 3$. In Section 3.5 we have shown that for all $\frac{n}{2} \neq n^+ \neq \nu^+$, $n = 5$ no ET-matrix can be obtained. When $n = 2$ and $n = 3$, the only case viable for the existence of an ET-matrix according to equations (3.3.3) and (3.3.4) is $(n^+, \nu^+) = (2, 1)$. When $n = 2$ this case yields an RET-matrix. When $n = 3$ the corresponding matrix has the same transition probabilities as the SMC-matrix. It therefore follows that when $n \leq 5$ is odd, the only ET-matrices that can be constructed are those generated by the SMC-matrix. In this section we have constructed ET-matrices up to order six when the trace of the matrix is zero.

3.6.1 Order 2

The case leading to the trace of the matrix equal to zero is given by $(n^+, \nu^+) = (1, 1)$. The corresponding representation of matrix $\hat{\mathbf{C}}$ is

$$\hat{\mathbf{C}} = \begin{pmatrix} r & t \\ t & -r \end{pmatrix}.$$

Normalisation of the rows yield the relation $t = \sqrt{1 - r^2}$ where $r \in (0, 1)$. The corresponding ET-matrices $\hat{\mathbf{C}}$ are a one-parameter family given as follows

$$\hat{\mathbf{C}}_{1,1} = \begin{pmatrix} r & \sqrt{1-r^2} \\ \sqrt{1-r^2} & -r \end{pmatrix}, \quad r \in (0, 1).$$

3.6.2 Order 4

The case represented by $n^+ = \frac{n}{2} = \nu^+$ for $n = 4$ is $(2, 2)$. Below we give a theorem characterising nontrivial zero trace ET-matrices of order 4.

Theorem 3.6.1 *All zero trace ET-matrices $\hat{\mathbf{C}}$ of order 4 for which $\left|\left(\hat{\mathbf{C}}\right)_{ii}\right| \neq 1$ and $\left|\left(\hat{\mathbf{C}}\right)_{ii}\right| \neq 0$ are*

$$\hat{\mathbf{C}} = \frac{1}{\sqrt{3 + \Re(\vartheta)^2}} \begin{pmatrix} -\Re(\vartheta) & 1 & 1 & 1 \\ 1 & -\Re(\vartheta) & \vartheta & \overline{\vartheta} \\ 1 & \overline{\vartheta} & \Re(\vartheta) & -\overline{\vartheta} \\ 1 & \vartheta & -\vartheta & \Re(\vartheta) \end{pmatrix}, \quad \vartheta \in \{z \in \mathbb{C} : |z| = 1\}.$$

or any matrix obtained from $\hat{\mathbf{C}}$ by the permutation $\mathbf{D}_\theta^* \hat{\mathbf{C}} \mathbf{D}_\theta$, where
$\mathbf{D}_\theta = \mathrm{diag}\left(e^{i\theta_1}, e^{i\theta_2}, e^{i\theta_3}, e^{i\theta_4}\right)$, $\theta_i \in [-\pi, \pi)$, $i = 1, 2, 3, 4$.

The number of positive and negative diagonal entries are equal and the corresponding matrix $\hat{\mathbf{C}}$ can be represented by

$$\hat{\mathbf{C}} = \begin{pmatrix} r & t & t & t \\ t & r & at & bt \\ t & \overline{a}t & -r & ct \\ t & \overline{b}t & \overline{c}t & -r \end{pmatrix},$$

where $a, b, c \in \{z \in \mathbb{C} : |z| = 1\}$. Using the orthogonality of the rows we have the following system of equations

$$\begin{aligned} 2r + t\,(a+b) &= 0 \quad (1) & 1 + \overline{b}c &= 0 \quad (4) \\ \overline{a} + c &= 0 \quad (2) & 1 + \overline{ac} &= 0 \quad (5) \\ \overline{b} + \overline{c} &= 0 \quad (3) & -2r\overline{c} + t\left(1 + a\overline{b}\right) &= 0 \quad (6). \end{aligned}$$

Solving for the parameters a, b, c, it is obtained that a can be chosen arbitrary, in which case $b = \overline{a}$ and $c = -\overline{a}$. A relation between r and t based on the system is obtained as $r + t\Re(a) = 0$. Using this relation between r and t and that in (3.3.1) one obtains that $t = \frac{1}{\sqrt{3+\Re(a)^2}}$ and $r = \frac{-\Re(a)}{\sqrt{3+\Re(a)^2}}$. The parameter a is chosen such that $\Re(a) < 0$ because $r > 0$. Therefore the matrix $\hat{\mathbf{C}}$ is given by

$$\hat{\mathbf{C}}_{2,2} = \frac{1}{\sqrt{3 + \Re(a)^2}} \begin{pmatrix} -\Re(a) & 1 & 1 & 1 \\ 1 & -\Re(a) & a & \overline{a} \\ 1 & \overline{a} & \Re(a) & -\overline{a} \\ 1 & a & -a & \Re(a) \end{pmatrix}, \quad |a| = 1, \Re(a) < 0.$$

For example, suppose $a = -e^{i\theta}$, then the appropriate values of θ are in the interval $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$. The corresponding matrix $\hat{\mathbf{C}}$ is given as follows

$$\hat{\mathbf{C}}_{2,2} = \frac{1}{\sqrt{3 + \cos^2\theta}} \begin{pmatrix} \cos\theta & 1 & 1 & 1 \\ 1 & \cos\theta & -e^{i\theta} & -e^{-i\theta} \\ 1 & -e^{-i\theta} & -\cos\theta & e^{-i\theta} \\ 1 & -e^{i\theta} & e^{i\theta} & -\cos\theta \end{pmatrix}, \quad \theta \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right).$$

It is therefore observed that when $N = 4$, all nontrivial ET-matrices (that are not reflectionless) obtained can be put into the following two categories

1. Matrices generated by the SMC-matrix.
2. One-parameter family matrices $\hat{\mathbf{C}}_{2,2}$ with zero trace.

3.6.3 Order 6

Now we characterise nontrivial zero trace matrices of order 6. The case $n^+ = \frac{n}{2} = \nu^+$ when $n = 6$ is denoted by $(3,3)$.

Theorem 3.6.2 *Let* $\mathbf{D}_\theta = \operatorname{diag}\left(e^{i\theta_1}, \ldots, e^{i\theta_6}\right), \quad \theta_i \in [-\pi, \pi), \quad i = 1, 2, \ldots, 6.$ *All zero trace ET-matrices* $\hat{\mathbf{C}}$ *of order* 6 *for which* $\left|\left(\hat{\mathbf{C}}\right)_{ii}\right| \neq 1$ *and* $\left|\left(\hat{\mathbf{C}}\right)_{ii}\right| \neq 0$ *exist as stated below or any matrix obtained from* $\hat{\mathbf{C}}$ *by the permutation* $\mathbf{D}_\theta^* \hat{\mathbf{C}} \mathbf{D}_\theta$.

(a) $\hat{\mathbf{C}}$ *is a two-parameters family of matrices given by*

$$\hat{\mathbf{C}} = \frac{1}{\sqrt{20+\xi^2}} \begin{pmatrix} -\xi & 2 & 2 & 2 & 2 & 2 \\ 2 & -\xi & 2a & 2b & 2c & 2d \\ 2 & 2\overline{a} & -\xi & -2c & 2\overline{b} & -2d \\ 2 & 2\overline{b} & -2\overline{c} & \xi & -2\overline{b} & 2\overline{c} \\ 2 & 2\overline{c} & 2b & -2b & \xi & -2\overline{c} \\ 2 & 2\overline{d} & -2\overline{d} & 2c & -2c & \xi \end{pmatrix}, \quad b, c \in \{z \in \mathbb{C} : |z| = 1\}$$

$$\xi = -\Re(b+c) \pm \sqrt{\left(\Re(b+c)\right)^2 - 4\Im(b)\Im(c)}, \quad a = \frac{bc(-\xi-b-c)}{1+bc}, \quad d = \frac{-\xi-b-c}{1+bc}.$$

(b) $\hat{\mathbf{C}}$ *is a one-parameter family of matrices given by*

$$\hat{\mathbf{C}} = \frac{1}{\sqrt{5+(1-\Re(b))^2}} \begin{pmatrix} 1-\Re(b) & 1 & 1 & 1 & 1 & 1 \\ 1 & 1-\Re(b) & -1 & b & \overline{b} & -1 \\ 1 & -1 & 1-\Re(b) & -1 & \overline{b} & b \\ 1 & \overline{b} & -1 & -1+\Re(b) & -\overline{b} & 1 \\ 1 & b & b & -b & -1+\Re(b) & -b \\ 1 & -1 & \overline{b} & 1 & -\overline{b} & -1+\Re(b) \end{pmatrix},$$

$b \in \{z \in \mathbb{C} : |z| = 1\}, b \neq 1$

(c) $\hat{\mathbf{C}}$ *is a unique real matrix given by*

$$\hat{\mathbf{C}} = \frac{1}{3} \begin{pmatrix} 2 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & -1 & -1 & -1 & -1 \\ 1 & -1 & 2 & -1 & -1 & -1 \\ 1 & -1 & -1 & -2 & 1 & 1 \\ 1 & -1 & -1 & 1 & -2 & 1 \\ 1 & -1 & -1 & 1 & 1 & -2 \end{pmatrix}$$

The number of positive and negative diagonal entries are equal, and so the corresponding matrix $\hat{\mathbf{C}}$ can be represented as

$$\hat{\mathbf{C}} = \begin{pmatrix} r & t & t & t & t & t \\ t & r & at & bt & ct & dt \\ t & \overline{a}t & r & et & ft & gt \\ t & \overline{b}t & \overline{e}t & -r & ht & lt \\ t & \overline{c}t & \overline{f}t & \overline{h}t & -r & mt \\ t & \overline{d}t & \overline{g}t & \overline{l}t & \overline{m}t & -r \end{pmatrix},$$

where

$$a, b, c, d, e, f, g, h, l, m \in \{z \in \mathbb{C} : |z| = 1\}.$$

From the orthogonality of the rows of $\hat{\mathbf{C}}$ we obtain the following system of equations

$$\begin{cases} 2r + t\,(a + b + c + d) = 0 & (1) \\ 2r + t\,(\overline{a} + e + f + g) = 0 & (2) \\ \overline{b} + \overline{e} + h + l = 0 & (3) \\ \overline{c} + \overline{f} + \overline{h} + m = 0 & (4) \\ \overline{d} + \overline{g} + \overline{l} + \overline{m} = 0 & (5) \end{cases} \qquad \begin{cases} 2\overline{a}r + t\left(1 + \overline{b}e + \overline{c}f + \overline{d}g\right) = 0 & (6) \\ 1 + \overline{ae} + \overline{c}h + \overline{d}l = 0 & (7) \\ 1 + \overline{a}\overline{f} + \overline{bh} + \overline{d}m = 0 & (8) \\ 1 + \overline{ag} + \overline{bl} + \overline{cm} = 0 & (9) \end{cases} \tag{3.6.1}$$

$$\begin{cases} 1 + a\overline{b} + \overline{f}h + \overline{g}l = 0 & (10) \\ 1 + a\overline{c} + \overline{e}\overline{h} + \overline{g}m = 0 & (11) \\ 1 + a\overline{d} + \overline{e}\overline{l} + \overline{f}\overline{m} = 0 & (12) \end{cases} \qquad \begin{cases} -2\overline{h}r + t\left(1 + b\overline{c} + e\overline{f} + \overline{l}m\right) = 0 & (13) \\ -2\overline{l}r + t\left(1 + b\overline{d} + e\overline{g} + \overline{h}\overline{m}\right) = 0 & (14) \end{cases} \quad \begin{cases} -2\overline{m}r + t\left(1 + c\overline{d} + f\overline{g} + h\overline{l}\right) = 0 & (15). \end{cases}$$

In this system there are nine equations to which Lemma 1 can be applied directly: equations (3), (4), (5), (7), (8), (9), (10), (11) and (12) (refer to Remark 1).

(a) **Two-parameters family of matrices.**

Here the choices made when Lemma 1 is applied to equation (3), (4) and (5) respectively of the system (3.6.1) are

$$\begin{cases} h = -\overline{b} \\ l = -\overline{e} \end{cases}, \qquad \begin{cases} f = -h \\ m = -\overline{c} \end{cases} \qquad \text{and} \qquad \begin{cases} g = -m \\ l = -d \end{cases}.$$

The following relations immediately emerge; $e = \overline{d}$, $f = \overline{b}$ and $g = \overline{c}$. With these relations the system (3.6.1) reduces to the following

$$\begin{cases} 2r + t\,(a + b + c + d) = 0 \\ \overline{a}d - \overline{b}\overline{c} = 0. \end{cases} \tag{3.6.2}$$

From the first equation in (3.6.2) and from equation (3.3.1), the values of r and t in terms of a, b, c, d are

$$r = \frac{\xi}{\sqrt{20+\xi^2}}, \qquad t = \frac{2}{\sqrt{20+\xi^2}},$$

where $\xi = -(a+b+c+d)$. Since r and t are real and nonnegative, ξ has to be chosen real and positive, that is, $a+b+c+d<0$. Remembering that the parameters are unimodular, the system (3.6.2) can now be written as

$$\begin{cases} a+b+c+d = -\xi \in \mathbb{R}_+ \\ a = bcd, \end{cases}$$

where $\mathbb{R}_+ = (0,\infty)$. These equations can be written as a linear system on a and d as follows

$$\begin{cases} a+d = -\xi - b - c \\ a - bcd = 0. \end{cases} \tag{3.6.3}$$

The system yields values of a and d if and only if the determinant of the coefficients matrix does not vanish. Thus we require that $bc \neq -1$. It follows that obtained as

$$a = \frac{bc\,(-\xi-b-c)}{1+bc}, \qquad d = \frac{-\xi-b-c}{1+bc}. \tag{3.6.4}$$

So far the solution depends on the parameters b, c and ξ. But the parameters are not free since a and d obtained in (3.6.4) should be unimodular. This requirement allows us to determine ξ from b and c. Substituting the value of d above into the equation $d\overline{d} = 1$ and simplifying one obtains that

$$\xi^2 + 2\xi\Re(b+c) + 4\Im(b)\Im(c) = 0$$

from which it follows that

$$\xi = -\Re(b+c) \pm \sqrt{(\Re(b+c))^2 - 4\Im(b)\Im(c)}. \tag{3.6.5}$$

The value $\xi \in \mathbb{R}_+$ is obtained in any of the following cases

1. $(\Re(b+c))^2 - 4\Im(b)\Im(c) > 0$ and $\Im(b)\Im(c) < 0$. Here there exists a unique $\xi \in \mathbb{R}_+$.
2. $(\Re(b+c))^2 - 4\Im(b)\Im(c) > 0$, $\Im(b)\Im(c) > 0$ and $\Re(b+c) < 0$. There exists two $\xi \in \mathbb{R}_+$.
3. $(\Re(b+c))^2 - 4\Im(b)\Im(c) = 0$, $\Im(b)\Im(c) > 0$ and $\Re(b+c) < 0$. There exists a unique $\xi \in \mathbb{R}_+$.
4. $\Im(b)\Im(c) = 0$ and $\Re(b+c) < 0$. There exists a unique $\xi \in \mathbb{R}_+$ since $\xi = 0$ is excluded.

The corresponding matrix $\hat{\mathbf{C}}$ can now be written as follows

$$\hat{\mathbf{C}} = \frac{1}{\sqrt{20+\xi^2}} \begin{pmatrix} -\xi & 2 & 2 & 2 & 2 & 2 \\ 2 & -\xi & 2a & 2b & 2c & 2d \\ 2 & 2\overline{a} & -\xi & -2c & 2\overline{b} & -2d \\ 2 & 2\overline{b} & -2\overline{c} & \xi & -2\overline{b} & 2\overline{c} \\ 2 & 2\overline{c} & 2b & -2b & \xi & -2\overline{c} \\ 2 & 2\overline{d} & -2\overline{d} & 2c & -2c & \xi \end{pmatrix}.$$

Here b and c are arbitrary parameters subject to $bc \neq -1$, (3.6.5) gives the value of ξ in terms of b and c, while a and d by the equations (3.6.4), again in terms of b and c.

Now suppose that $bc = -1$ is allowed. Then $c = -\overline{b}$ and the system (3.6.3) now becomes

$$\begin{cases} a + d = -\xi - b + \overline{b} \\ a + d = 0. \end{cases}$$

This implies that $\xi = -b + \overline{b}$. This is a contradiction since $\xi \in \mathbb{R}_+$ while $-b + \overline{b}$ is pure imaginary.

(b) **One-parameter family of matrices**

This result is obtained by making the following choices when Lemma 1 is applied to equations (3), (4) and (5) respectively of the system (3.6.1).

$$\begin{cases} h = -\overline{b} \\ l = -\overline{e} \end{cases}, \qquad \begin{cases} c = -h \\ m = -\overline{f} \end{cases} \qquad \text{and} \qquad \begin{cases} l = -d \\ m = -g. \end{cases}$$

With these substitutions, the equations (3), (4), and (5) are satisfied and can be deleted from the system. It can also be seen that $c = \overline{b}$, $e = \overline{d}$ and $g = \overline{f}$. Equation (7) can now be written as $\overline{a}d - 1 = 0$ which implies that $d = a$. Consequently we have $e = \overline{a}$ and $l = -a$. Equations (1) and (2) of the system (3.6.1) now become

$$2r + t\left(2a + b + \overline{b}\right) = 0 \quad (1) \qquad 2r + t\left(2\overline{a} + f + \overline{f}\right) = 0 \quad (2).$$

Evaluating the difference of equation (1) and the conjugate of equation (2) yields that $\Re(f) = \Re(b)$ which means that either $f = b$ or $f = \overline{b}$

Choosing $f = \overline{b}$ [1], one obtains that a and b are arbitrary and equations (1), (13) and (15) of the system (3.6.1) can be written as follows

$$2r + t\left(2a + b + \overline{b}\right) = 0 \quad (1)$$

$$2br + t\left(1 + b^2 + 2\overline{a}b\right) = 0 \quad (13)$$

$$2\overline{b}r + t\left(1 + 2\overline{a}\overline{b} + \overline{b}^2\right) = 0 \quad (15).$$

[1]Of course the possibility $f = \overline{b}$ should also be considered when obtaining all possible matrices C (see Part (b))

Equation (1) then takes the form $r + t\left(a + \Re\left(b\right)\right) = 0$. Since r and t are real, a is also real meaning that $a = \pm 1$. The resulting relation between r and t and equation (3.3.1) yield that

$$t = \frac{1}{\sqrt{5+\beta^2}} \quad \text{and} \quad r = \frac{-\beta}{\sqrt{5+\beta^2}},$$

where $\beta = a + \Re\left(b\right) = \pm 1 + \Re\left(b\right)$.

Since $r > 0$, β should be chosen negative and this is obtained when $a = -1$. The sign of $\Re\left(b\right)$ does not determine the sign of β because $\left|\Re\left(b\right)\right| \leq 1$. In particular the value $b = 1$ is not allowed because it leads to $r = 0$ which is excluded. Thus $\beta = -1 + \Re\left(b\right)$, $b \neq 1$. The ET-matrix $\hat{\mathbf{C}}$ is fully determined and is given in terms of b as seen below

$$\hat{\mathbf{C}} = \frac{1}{\sqrt{5+\left(1-\Re\left(b\right)\right)^2}} \begin{pmatrix} 1-\Re\left(b\right) & 1 & 1 & 1 & 1 & 1 \\ 1 & 1-\Re\left(b\right) & -1 & b & \overline{b} & -1 \\ 1 & -1 & 1-\Re\left(b\right) & -1 & \overline{b} & b \\ 1 & \overline{b} & -1 & -1+\Re\left(b\right) & -\overline{b} & 1 \\ 1 & b & b & -b & -1+\Re\left(b\right) & -b \\ 1 & -1 & \overline{b} & 1 & -\overline{b} & -1+\Re\left(b\right) \end{pmatrix},$$

$|b| = 1, b \neq 1.$

This family is described by one real parameter.

(c) **Unique real matrix**

Suppose in part (b) the relation $f = b$ is chosen instead of $f = \overline{b}$, while other relations are retained, then equations (6) and (13) of the system (3.6.1) now become

$$2\overline{a}r + t\left(1 + 2\overline{a}\overline{b} + b^2\right) = 0 \quad (6) \qquad 2br + t\left(1 + b^2 + 2\overline{a}\overline{b}\right) = 0 \quad (13).$$

The difference of these two equations shows that $b = \overline{a}$. With this value of b, equation (1) can now be written as $r + t\left(a + \Re\left(a\right)\right) = 0$. This is a relation between r and t which together with equation (3.3.1) give us

$$t = \frac{1}{\sqrt{5+\left(a+\Re\left(a\right)\right)^2}} \quad \text{and} \quad r = \frac{-\left(a+\Re\left(a\right)\right)}{\sqrt{5+\left(a+\Re\left(a\right)\right)^2}}.$$

Since r is real, a is also necessarily real implying that $a = \pm 1$. The appropriate choice of a so that r is nonnegative is $a = -1$. Thus the matrix C is fully determined and is real

$$\hat{\mathbf{C}} = \frac{1}{3} \begin{pmatrix} 2 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & -1 & -1 & -1 & -1 \\ 1 & -1 & 2 & -1 & -1 & -1 \\ 1 & -1 & -1 & -2 & 1 & 1 \\ 1 & -1 & -1 & 1 & -2 & 1 \\ 1 & -1 & -1 & 1 & 1 & -2 \end{pmatrix}.$$

The obtained matrix gives the same transition probabilities as the SMC-matrix.

Chapter 4

Magnetic Fields, Vertex Conditions and Unitary Equivalence

In this chapter we discuss the unitary equivalence of the spectrum of quantum graphs. The layout of the chapter is as follows: In Section 4.1 we describe in details unitary multiplication transformations and their effect on quantum graphs. The subsequent section is devoted to vertex phases and their connection to equi-transmitting matrices. Section 4.3 entails the analysis where we determine the maximal number of parameters that describe the Shrödinger operators that are unitarily equivalent when vertex phases are varied. The last section is devoted to an explicit example.

4.1 Unitary transformations and magnetic Schrödinger operators

Models leading to unitary equivalent operators are usually identified in quantum mechanics since the corresponding processes are identical. An important class of unitary transformations is that of multiplication factors that are unimodular. This is because they preserve the probability density determined by the absolute value of the wave function. They also preserve the class of magnetic Schrödinger differential expressions.

Consider the magnetic Schrödinger equation formally given by the differential expression

$$L_{q,a} = \left(i \frac{d}{dx} + a(x) \right)^2 + q(x), \tag{4.1.1}$$

where $a \in C(\Gamma), q \in L_2(\Gamma)$ are real magnetic and electric potentials respectively. Suppose the vertex conditions are defined by

$$i \left(\mathbf{S}_m - \mathbf{I} \right) \vec{\psi}_m = \left(\mathbf{S}_m + \mathbf{I} \right) \partial \vec{\psi}_m, \tag{4.1.2}$$

where $\vec{\psi}_m$ and $\partial\vec{\psi}_m$ are the respective vectors of the limiting values of the function $\vec{\psi}$ and its extended normal derivative at V_m. Note that

$$\partial\psi(x_j) = (-1)^{j+1} \left(\psi'(x) - ia(x)\psi(x)\right)|_{x=x_j}. \tag{4.1.3}$$

Each vector in (4.1.2) has dimension equal to d_m- the number of end-points joined at V_m. The $d_m \times d_m$ matrix $\mathbf{S}_m$ should be unitary and irreducible.

Since the probability density is given by the absolute value of the wave function squared $\rho(x) = |\psi(x)|^2$, if the phase space is fixed, then it is natural to identify operators $\tilde{H}$ and H. They are connected by the unitary transformation via multiplication by a unimodular function $\mathbf{U}(x) = \exp i\Theta(x),\ \Theta(x) \in \mathbb{R}$:

$$\tilde{H} = \mathbf{U}^{-1}H\mathbf{U} = e^{-i\Theta(x)}He^{i\Theta(x)}. \tag{4.1.4}$$

Let us consider two special cases.

Special case 1. If the function $\Theta(x)$ is chosen to be equal to a real constant $\Theta_0(x) \equiv \theta,\ \theta \in \mathbb{R}$, then the operator of multiplication $\mathbf{U}$ commutes with any H and therefore $\tilde{H} = H$.

Special case 2. Another example of the function Θ is when it is chosen equal to a constant on each edge of Γ

$$\Theta_e(x) = \theta_n,\ \ x \in E_n, \tag{4.1.5}$$

where θ_n are certain real parameters. With this choice of Θ the differential operators $\tilde{H}$ and H coincide on every edge E_n, but they may be different, since the vertex conditions at a vertex V_m are affected if the phases associated with the edges joined at V_m are different.

More precisely, assume without loss of generality that the edges joined together at the vertex V_m are enumerated as $E_1, E_2, \ldots, E_{d_m}$ and that the functions from the domain of H satisfy vertex conditions (4.1.2). Consider the diagonal unitary matrix $\mathbf{U}_m$ given by

$$\mathbf{U}_m = \mathrm{diag}\ \left(e^{i\theta_1}, e^{i\theta_2}, \ldots, e^{i\theta_{d_m}}\right),$$

where θ_n were used in (4.1.5) to define Θ_e. Then the unitary matrices $\tilde{\mathbf{S}}_m$ and $\mathbf{S}_m$ associated with the operators $\tilde{H}$ and H respectively are connected via

$$\tilde{\mathbf{S}}_m = \mathbf{U}_m^{-1}\mathbf{S}_m\mathbf{U}_m. \tag{4.1.6}$$

To prove this assume that $\psi \in \mathrm{Dom}\,(\tilde{H})$. Every such function after the transformation $\mathbf{U}$ is mapped to a function from the domain of H and therefore satisfies condition (4.1.2)

$$i(\mathbf{S}_m - \mathbf{I})\mathbf{U}_m\vec{\psi}_m = (\mathbf{S}_m + \mathbf{I})\mathbf{U}_m\partial\vec{\psi}. \tag{4.1.7}$$

Multiplying both sides by $\mathbf{U}_m^{-1}$ we arrive at

$$i(\tilde{\mathbf{S}}_m - \mathbf{I})\vec{\psi}_m = (\tilde{\mathbf{S}}_m + \mathbf{I})\partial\vec{\psi}. \tag{4.1.8}$$

Considering transformations given by functions Θ_e (4.1.5) we obtain self-adjoint operators $\tilde{H}$ given by the same differential expression as H, but where vertex conditions are defined by matrices $\tilde{\mathbf{S}}_m$ instead of $\mathbf{S}_m$. The relation between these matrices is described by (4.1.6).

The general case. We now discuss the relation between $\tilde{H}$ and H in the case of general $\Theta(x)$, and as can be seen below, we require that this function is continuously differentiable. Moreover we assume that the operator H is a magnetic Schrödinger operator given by (4.1.1). Our assumption on Θ implies that $\tilde{H}$ is again a magnetic Schrödinger operator. It will be convenient to denote by $\tilde{}$ the parameters corresponding to $\tilde{H}$. Applying formula

$$\left(i\frac{d}{dx} + a(x)\right)e^{i\Theta(x)}\psi(x) = e^{i\Theta(x)}\left(i\frac{d}{dx} + a(x) - \Theta'(x)\right)\psi(x)$$

twice we obtain the following formula for the transformed operator

$$\begin{aligned} \tilde{H}\psi &= e^{-i\Theta(x)}\left[\left(i\frac{d}{dx} + a(x)\right)^2 + q(x)\right]e^{i\Theta(x)}\psi \\ &= \left(i\frac{d}{dx} + a(x) - \Theta'(x)\right)^2\psi + q(x)\psi. \end{aligned} \tag{4.1.9}$$

It follows that

$$\tilde{q}(x) = q(x), \text{ and } \tilde{a}(x) = a(x) - \Theta'(x), \tag{4.1.10}$$

i.e. the electric potential q is invariant under the similarity transformation (4.1.4), while the magnetic potential changes.

The transformation of the vertex conditions is the same as the one discussed in the second special case. The only difference is that the values θ_n are the limiting values of the function $\Theta(x)$ at the end points x_n joined in the vertex V_m. Note that the extended normal derivatives given by (4.1.3) are changed accordingly, since their definition depends on the value of the magnetic potential.

In particular, the magnetic potential on every edge can be eliminated if one choses:

$$\Theta(x) = \int_{x_0}^{x} a(y)dy.$$

Observe that eliminating magnetic potential one introduces new phases in vertex conditions as given by (4.1.6). Hence in order to study spectral properties of magnetic Schrödinger operators on metric graphs it is enough to consider Schrödinger operators with zero magnetic potentials, but with different extra phases in vertex conditions. We are going to call these phases **vertex**

phases and will in particular study the dependence of the spectrum upon these phases.

Special case 3. If the graph Γ is a tree, then the function Θ eliminating magnetic potential can be chosen as

$$\Theta(x) = \int_{x_0}^{x} a(y)dy, \tag{4.1.11}$$

where the point $x_0 \in \Gamma$ is arbitrary and integration is along the shortest path on Γ connecting x_0 and x. Note that the function Θ is continuous. Also observe that integration along the edges forming the path should be carried out respecting their orientation: if the path goes along an edge in the positive direction, then the corresponding contribution should be taken with $+$ve sign, otherwise with $-$ve sign. It follows that magnetic potential on a tree can be eliminated without changing the vertex conditions, *i.e.* the spectrum of a magnetic Schrödinger operator on a tree coincides with the spectrum of the operator with zero magnetic potential and precisely the same electric potential and the same vertex conditions.

Assume now that Γ is not a tree, but contains cycles. Consider then any spanning tree T on Γ obtained by chopping precisely $g = N - M + 1$ vertices - one on each independent cycle in Γ where N is the number of edges while M is the number of vertices in Γ. Then magnetic potential on T can be eliminated as described above. Using the same function Θ to eliminate magnetic potential on Γ leads to introducing at most g vertex phases, since the values of Θ at different parts of the chopped vertices may be different. Assume that a vertex V_m was divided into two vertices V_m' and V_m''. If $\Theta(V_m') \neq \Theta(V_m'')$ then the matrix $\mathbf{S}_m$ describing vertex conditions on Γ is transformed by (4.1.6). The matrix $\mathbf{U}_m$ contains factors $e^{i\Theta(V_m')}$ and $e^{i\Theta(V_m'')}$, but one common factor in the similarity transformation can be cancelled. Hence the matrix $\tilde{\mathbf{S}}_m$ depends on the difference $\Theta(V_m') - \Theta(V_m'')$ which is in fact equal to the integral of the magnetic potential over the independent cycle to which V_m belongs. We conclude that elimination of the magnetic potential on a graph with g cycles leads to an operator with zero magnetic potential, the same electric potential and new vertex conditions containing at most g phases equal to

$$\Phi_j = \int_{C_j} a(y)dy, \quad j = 1, 2, \dots, g. \tag{4.1.12}$$

These phases can be interpreted as the fluxes of the magnetic field through the independent cycles C_j.

4.2 Vertex phases and transition probabilities

The vertex phases described above appear not only as a result of the elimination of the magnetic potential on a metric graph. Such phases appear naturally when one tries to reconstruct a unitary matrix from the absolute values of the entries. The transition probabilities corresponding to such unitary scattering matrix S_m are given by $\rho_{ij} = |(\mathbf{S}_m)_{ij}|^2$. Therefore matrices with the same absolute values of entries describe essentially the same physics.

Consider the similarity transformation

$$\mathbf{S}_m \mapsto \hat{\mathbf{S}}_m = \mathbf{D}_m^{-1}\mathbf{S}_m\mathbf{D}_m, \tag{4.2.1}$$

where D_m is a diagonal unitary matrix

$$\mathbf{D}_m = \text{diag}\ \left(e^{i\varphi_1}, e^{i\varphi_2}, \ldots, e^{i\varphi_{d_m}}\right),\ \ \varphi_j \in \mathbb{R}. \tag{4.2.2}$$

Note that this transformation coincides with (4.1.6) if all phases φ_j are chosen equal to the values of $\Theta(x)$ at the corresponding end points.

The transformation (4.2.1) does not change the transition probabilities, hence knowing the transition probabilities ρ_{ij} the matrix $\mathbf{S}_m$ can be determined up to the vertex phases φ_j only. The transformation can be used to make one of the rows or one of the columns in $\mathbf{S}_m$ real, or if $\mathbf{S}_m$ in addition is Hermitian then one may make real simultaneously one row and one column with the same number. The difference between the matrices $\mathbf{S}_m$ and $\tilde{\mathbf{S}}_m$ lies in phase factors that the waves acquire while penetrating through the vertex. These phases can be completely ignored if the graph Γ has no cycles (tree), but should be taken into account when the cycles are present. For every vertex V_m in Γ and any $\mathbf{S}_m$ there is a $d_m - 1$ – parameter family of unitary matrices $\mathbf{D}^{-1}\mathbf{S}_m\mathbf{D}$ leading to the same scattering amplitudes. Any two members from such a family are connected via transformation (4.2.1), which contains $d_m - 1$ **vertex phases**.

It is natural to ask the following question: is it possible to reconstruct the scattering matrix from the scattering amplitudes up to the vertex phases? It appears that the answer in general is negative, in particular if several of the entries in **S** have the same absolute value. Here is one example of a one parameter family of reflectionless equitransmitting matrices of order 6 [**?**]

$$\hat{\mathbf{C}}_{1,1,1} = \frac{1}{\sqrt{5}} \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & -1 & -1 \\ 1 & 1 & 0 & -1 & f & -f \\ 1 & 1 & -1 & 0 & -f & f \\ 1 & -1 & \overline{f} & -\overline{f} & 0 & 1 \\ 1 & -1 & -\overline{f} & \overline{f} & 1 & 0 \end{pmatrix},$$

where f is any unimodular complex number. All matrices from this family have the same reflection probability $|\,(\mathbf{S}_V)_{jj}\,|^2 = 0$ (reflectionless) and the same transition probabilities (equitransmitting) $|\,(\mathbf{S}_V)_{ij}\,|^2 = \frac{1}{5}$, $i \neq j$. Of course, the considered example is very special, since many of the entries in $\hat{\mathbf{C}}_{1,1,1}$ have the same absolute value. Applying the similarity transformation (4.2.1) one obtains a 6-parameter family of matrices with the same transition probabilities.

4.3 The main result

Note that the total number of arbitrary vertex phases is equal to $\sum_{m=1}^{M}(d_m - 1) = \sum_{m=1}^{M} d_m - \sum_{m=1}^{M} 1 = 2N - M$ and could be rather large. On the other hand the transformation (4.1.5) leaves the differential operator unchanged. This transformation contains $N-1$ independent parameters, since one common factor can be removed from the similarity transformation. Hence it seems that the family of different operators (not unitary equivalent) can be described by at most

$$2N - M - (N-1) = N - M + 1 = g$$

independent parameters. Our goal is to prove this result. Our previous discussions imply that it is enough to prove the result of the case of zero magnetic potential. On the other hand despite the magnetic potential being eliminated from our discussion, the easiest way to describe the independent parameters is via fluxes introduced in (4.1.12).

Theorem 4.3.1 *The spectrum of the Schrödinger operator $L_{q,a}(\mathbf{S})$ on a metric graph Γ with zero magnetic potential $a(x) \equiv 0$, fixed electric potential q and vertex conditions given by (4.1.2) with the unitary matrices $\hat{\mathbf{S}}_m = \mathbf{D}_m^{-1}\mathbf{S}_m\mathbf{D}_m$ containing arbitrary vertex phases is described by at most $g = N - M + 1$ parameters, where g is the genus of Γ.*

Let $\mathbf{U}$ be the unitarily transformation defined by (4.1.5). Let us denote by $\tilde{L}$ the transformed Schrödinger operator

$$\tilde{L} = \mathbf{U}^{-1} L \mathbf{U}. \tag{4.3.1}$$

The operators $\tilde{L}$ and L are unitarily equivalent. Moreover the corresponding differential expressions coincide, since on every edge $\mathbf{U}$ acts as a multiplication by a constant; $\tilde{a}(x) \equiv 0, \tilde{q}(x) = q(x)$. The difference lies in the vertex conditions, since generally $\tilde{\mathbf{S}}_m \neq \mathbf{S}_m$ (see (4.1.6)).

Formula (4.1.6) shows that the transformation $\mathbf{U}$ can be chosen so that all free phases in any particular $\mathbf{S}_m$ disappear. More precisely, let the vertex conditions be described by the vertex scattering matrix $\mathbf{D}_m^{-1}\mathbf{S}_m\mathbf{D}_m$, where the diagonal matrix $\mathbf{D}_m$ is the diagonal matrix containing free phases at V_m. We see that the vertex conditions for $\tilde{L}$ are described by $\mathbf{S}_m$ alone if and only if the matrix $\mathbf{U}_m$ is chosen so that $\mathbf{D}_m\mathbf{U}_m$ is a scalar, *i.e.* proportional to the unit matrix. This can always be done if the phases θ_n can be chosen freely. Moreover this can always be done if just one of the phases θ_n is fixed. This observation will be important for our future considerations.

Note that we considered just one particular vertex. If the graph Γ contains cycles, then there appear certain restrictions on how the phases on any cycle can be chosen. Therefore assume first that Γ contains no cycles, *i.e.* it is a tree and that vertex conditions are given by the matrices $\mathbf{D}_m^{-1}\mathbf{S}\mathbf{D}_m$. Let us show that the unitary transformation $\mathbf{U}$ can be chosen so that all phases are eliminated, *i.e.* the vertex conditions are given by $\mathbf{S}_m$ alone at all vertices V_m. Obviously such transformation $\mathbf{U}$ can be defined up to a general phase factor, since if $\mathbf{U}$ is the desired transformation, then $e^{i\theta}\mathbf{U},\ \theta \in \mathbb{R}$ solves the problem as well. Consider any root edge denoted without loss of generality by E_1 and define $\theta_1 = 0.$, *i.e.* $\mathbf{U}$ restricted to E_1 is the identity transformation. The root edge connects two vertices: one of degree one and one of arbitrary degree. Let us denote these vertices by V_1 and V_2 respectively. Then define $\mathbf{U}$ on all edges joined together at V_2 so that the matrix $\tilde{\mathbf{S}}_2$ contains zero free phases. This can always be done, since only one of the phases associated with V_2 - the phase θ_1, - is fixed. This process can be continued to define $\mathbf{U}$ on the whole tree, since moving from the root to the periphery of Γ on each step we need to define $\mathbf{U}$ on all except one edges joined at a vertex ($\mathbf{U}$ is already defined on the edge nearest to the root). Hence for trees the unitary transformation $\mathbf{U}$ can be defined so that all vertex phases are eliminated. It follows that the spectrum of a Schrödinger operator on a tree does not depend on the free phases in vertex conditions. This statement is similar to the fact that the spectrum of a *magnetic* Schrödinger operator on a tree is independent of the magnetic potential.

Consider now any connected graph Γ and choose an arbitrary spanning tree T obtained from Γ by chopping precisely $g = M - N + 1$ edges in the middle. These edges can be chosen so that every independent cycle contains just one of the chosen edges. Let us denote the chopped edges by $E_1, E_2, \ldots, E_g$ and by $E_n^{\pm}$ the corresponding smaller edges obtained after chopping.

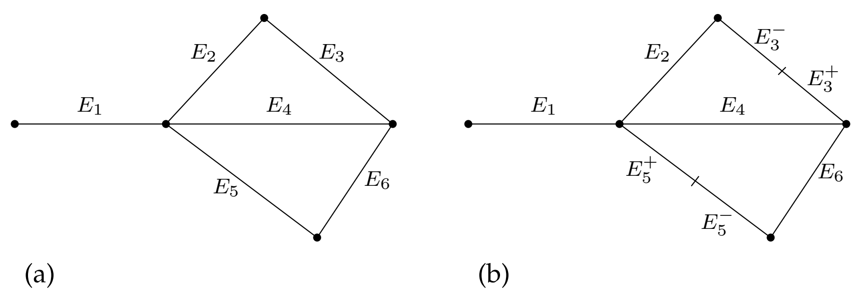

FIGURE 4.1: (a) Graph Γ with cycles and (b) graph T obtained from Γ by chopping edges corresponding to independent cycles

In what follows we are going to identify the Hilbert spaces $L_2(E_n)$ and $L_2(E_n^-) \oplus L_2(E_n^+)$. As before all vertex phases on T can be eliminated by a unitary transformation $\mathbf{U}$. If ψ is an eigenfunction on the original graph Γ, then $\mathbf{U}^{-1}\psi$ is not necessarily an eigenfunction on T, since the transformation $\mathbf{U}$ restricted to E_n^- and E_n^+ may be different - the function $\mathbf{U}^{-1}\psi$ may be discontinuous as a function on E_n. It follows that the operator $\tilde{L} = \mathbf{U}^{-1} L \mathbf{U}$ can be considered as a Schrödinger operator on the original graph Γ (without any additional matching conditions at the middle points of $E_n, n = 1, 2, \ldots, g$) only if all the phases $\theta_n^{\pm}$ coincide pairwise

$$\theta_n^- = \theta_n^+, \;\; n = 1, 2, \ldots, g. \tag{4.3.2}$$

One may always achieve (4.3.2) by choosing appropriately one of the two free phases associated with the edge E_n on the cycle. Since the edges E_n belong to different independent cycles, identifying unitary equivalent operators gives a g-parameter family. In other words the spectrum of L depends not on all free phases, but on the g phases described above. Each of these phases is associated with one of the independent cycles in Γ.

The parameters describing not unitary equivalent operators will be interpreted as fluxes of the magnetic field through the independent cycles.

Theorem 4.3.2 *For any Schrödinger operator on a graph Γ with electric potential q and defined on functions satisfying (4.1.2) with $d_m - 1$ arbitrary vertex phases at each vertex V_m there exists a unitary* *equivalent magnetic Schrödinger operator on Γ with the same electric potential and zero phases in vertex conditions.*

For our purposes it will be enough to consider magnetic Schrödinger operators with magnetic potential supported by the left subedges of chopped edges:

$$\mathrm{supp}\ a \subset \cup_{n=1}^{g} E_n^- .$$

Consider the spanning tree T constructed during the proof of the previous theorem as well as the unitary transformation $\mathbf{U}$ on T leading to may be different phases θ_n^- and θ_n^+. If all $\theta_n^{\pm}$ are pairwise equal then the Schrödinger operator with zero magnetic potential $\mathbf{U}^{-1} L_q \mathbf{U}$ solves the task. If some of $\theta_n^{\pm}$ are pairwise different, let us choose magnetic potential a so that

$$\int_{x_{2n-1}}^{(x_{2n}+x_{2n-1})/2} a(x)dx = \theta_n^- - \theta_n^+ . \tag{4.3.3}$$

Remember that the edge $E_n = [x_{2n-1}, x_{2n}]$ has been divided into two edges: $E_n^- = [x_{2n-1}, (x_{2n} + x_{2n-1})/2]$ and $E_n^+ = [(x_{2n} + x_{2n-1})/2, x_{2n}]$, so that $(x_{2n} + x_{2n-1})/2$ is nothing else than the middle point of E_n. Then the unitary transformation $\mathbf{V}_a$ of multiplication by the function $V_a(x)$

$$V_a(x) = \begin{cases} e^{i\int_{x_{2n-1}}^{x} a(y)dy}, & x \in E_n^- = [x_{2n-1}, \frac{x_{2n}+x_{2n-1}}{2}], n = 1, 2, \dots, g, \\ 1, & \text{otherwise}, \end{cases} \tag{4.3.4}$$

determines the magnetic Schrödinger operator on Γ with vertex conditions including zero free phases

$$\hat{L} = \mathbf{V}_a \mathbf{U}^{-1} L_q \mathbf{U} \mathbf{V}_a^{-1}. \tag{4.3.5}$$

We first note that the operator $\mathbf{V}_a \mathbf{U}^{-1} L_q \mathbf{U} \mathbf{V}_a$ is defined by a magnetic Schrödinger differential expression on each interval E_n. This follows directly from formula (4.1.9). Moreover the function V_a is identically equal to one in a neighborhood of every vertex, since $\mathrm{supp}\ a$ is separated from the end points of the interval. Therefore if the functions from the domain of $\mathbf{U}^{-1} L_q \mathbf{U}$ satisfy vertex conditions with zero free phases, then the same property holds for the functions from the domain of $\mathbf{V}_a \mathbf{U}^{-1} L_q \mathbf{U} \mathbf{V}_a$. It remains to show that the functions from the domain of this operator are continuous and have continuous derivatives at the middle points of chopped edges $E_n, n = 1, 2, \dots, g$, *i.e.* that the defect introduced by tranformation $\mathbf{U}$ is "repaired".

The functions from the domain of $\mathbf{U}^{-1} L_q \mathbf{U}$ as well as their first derivatives satisfy the following conditions at the middle points of chopped edges:

$$e^{i\varphi_n^-} f\left(\frac{x_{2n} + x_{2n-1}}{2} - 0\right) = e^{i\varphi_n^+} f\left(\frac{x_{2n} + x_{2n-1}}{2} + 0\right). \tag{4.3.6}$$

The function V_a is constant close to the middle points in E_n

$$V_a\left(\frac{x_{2n} + x_{2n-1}}{2} - 0\right) = e^{i(\varphi_n^- - \varphi_n^+)}, \quad V_a\left(\frac{x_{2n} + x_{2n-1}}{2} + 0\right) = 1.$$

Hence the functions from the domain of $\mathbf{V}_a\mathbf{U}^{-1}L_q\mathbf{U}\mathbf{V}_a^{-1}$ satisfy

$$e^{-i(\varphi_n^- - \varphi_n^+)}e^{i\varphi_n^-}f\left(\frac{x_{2n}+x_{2n-1}}{2}-0\right) = e^{i\varphi_n^+}f\left(\frac{x_{2n}+x_{2n-1}}{2}+0\right)$$

$$\Rightarrow f\left(\frac{x_{2n}+x_{2n-1}}{2}-0\right) = f\left(\frac{x_{2n}+x_{2n-1}}{2}+0\right). \tag{4.3.7}$$

The first derivatives are continuous as well.

It follows that the operator $\mathbf{V}_a\mathbf{U}^{-1}L_q\mathbf{U}\mathbf{V}_a^{-1}$ is the magnetic Schrödinger operator on Γ defined on the functions satisfying vertex conditions with zero free phases.

4.4 Clarifying example

Consider the following quantum graph Γ_∞ obtained by joining two loops at a single vertex. The end points joined in the vertex V_1 are x_1, x_2, x_3, x_4.

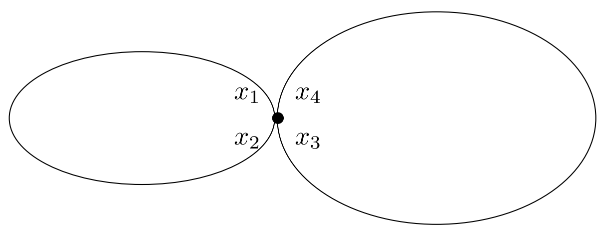

FIGURE 4.2: The Γ_∞ graph.

Define the Laplace operator on Γ_∞ by the differential expression

$$L\psi(x) = -\psi''(x)$$

on the functions from the Sobolev space $W_2^2([x_1,x_2]\cup[x_3,x_4])$ satisfying vertex conditions (4.1.2)

$$i(\hat{\mathbf{S}}_1 - I)\vec{\psi}_1 = (\hat{\mathbf{S}}_1 + \mathbf{I})\partial\vec{\psi}_1$$

where $\hat{\mathbf{S}}_1$ is the unitary matrix given by $\hat{\mathbf{S}}_1 = \mathbf{D}_1^*\mathbf{S}_1\mathbf{D}_1$ with

$$\mathbf{S}_1 = \frac{1}{\sqrt{3+\cos^2\beta}}\begin{pmatrix} \cos\beta & 1 & 1 & 1 \\ 1 & \cos\beta & -e^{i\beta} & -e^{-i\beta} \\ 1 & -e^{-i\beta} & -\cos\beta & e^{-i\beta} \\ 1 & -e^{i\beta} & e^{i\beta} & -\cos\beta \end{pmatrix}, \beta \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right) \tag{4.4.1}$$

and $\mathbf{D}_1 = \mathrm{diag}\left(1, e^{i\varphi_1}, e^{i\varphi_2}, e^{i\varphi_3}\right)$, $\varphi_j \in [-\pi, \pi)$. For $a = -e^{i\beta}$, $t = \frac{1}{\sqrt{3+\cos^2\beta}}$ and $r = \frac{\cos\beta}{\sqrt{3+\cos^2\beta}}$ we write the above matrix as

$$\mathbf{S}_1 = \begin{pmatrix} r & t & t & t \\ t & r & at & \overline{a}t \\ t & \overline{a}t & -r & -\overline{a}t \\ t & at & -at & -r \end{pmatrix}.$$

This is a zero-trace equi-transmitting unitary Hermitian matrix in the proof of Theorem 3.6.1. The transition probabilities are determined by the real parameter β or the unitary parameter a.

The defined operator L is determined by 4 real parameters: one in the matrix $\mathbf{S}_1$ and three in $\mathbf{D}_1$. The parameter included in $\mathbf{S}_1$ determine different transition probabilities through the central vertex, while not all phases included in $\mathbf{D}_1$ are important leading to unitary equivalent operators. Let us calculate the spectrum explicitly in order to see this phenomena.

The solution to the Laplace equation $L\psi = k^2\psi$ is given by

$$\psi(x) = \begin{cases} a_1 e^{ik|x-x_1|} + a_2 e^{ik|x-x_2|}, & x \in [x_1, x_2], \\ a_3 e^{ik|x-x_3|} + a_4 e^{ik|x-x_4|}, & x \in [x_3, x_4]. \end{cases}$$

Let $l_1 = x_2 - x_1$ and $l_2 = x_4 - x_3$. Since the unitary matrix $\hat{S}_1$ is also Hermitian, it plays the role of the vertex scattering matrix connecting the amplitudes of the incoming and outgoing waves at the vertex. In other words, vertex conditions (4.1.2) imposed on ψ imply that

$$\hat{\mathbf{S}}_1 \begin{pmatrix} e^{ikl_1} a_2 \\ e^{ikl_1} a_1 \\ e^{ikl_2} a_4 \\ e^{ikl_2} a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}. \tag{4.4.2}$$

This equation can be written as

$$(\mathbf{S}_1 \mathbf{S}_E - \mathbf{I}) \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = 0, \tag{4.4.3}$$

where

$$\mathbf{S}_1 = \begin{pmatrix} 0 & e^{ikl_1} & 0 & 0 \\ e^{ikl_1} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{ikl_2} \\ 0 & 0 & e^{ikl_2} & 0 \end{pmatrix}.$$

Hence the spectrum of L is determined by the secular equation $\det(\mathbf{S}_1\mathbf{S}_E - I) = 0$ which shows that the spectrum depends on β, the phase φ_1 and the difference $\varphi_3 - \varphi_2$, i.e. one of the phase parameters can be eliminated as far as the spectrum is concerned. The original equations is

$$
\begin{aligned}
&1+\left\{7t^4+2r^2t^2+rt^3\left(4e^{-i\beta}+e^{i\beta}\right)+\cos\left(2\beta\right)+rt^3e^{i(\beta-\varphi_1)}\right\}e^{2ik(l_1+l_2)}\\
&+2t\left\{\left(r^2-3t^2\right)e^{ik(2l_1+l_2)}+2te^{ik(l_1+l_2)}-e^{ikl_2}\right\}\cos\left(\beta-\varphi_3+\varphi_2\right)\\
&-2te^{ikl_1}\left(t^2e^{2ikl_2}+1\right)\cos\varphi_1-2t\left(2t^2-r^2+rt\cos\beta\right)e^{ik(l_1+2l_2)}\cos\varphi_1\\
&-2rt^2e^{ik(2l_1+l_2)}\left(\cos\varphi_1+\cos\left(2\beta-\varphi_3+\varphi_2\right)\right)=0.
\end{aligned}
$$

Introducing $\phi_1=\varphi_1,\phi_2=\varphi_3-\varphi_2$ we rewrite the secular equation as follows

$$
\begin{aligned}
&1+\left\{7t^4+2r^2t^2+rt^3\left(4e^{-i\beta}+e^{i\beta}\right)+\cos\left(2\beta\right)+rt^3e^{i(\beta-\phi_1)}\right\}e^{2ik(l_1+l_2)}\\
&+2t\left\{\left(r^2-3t^2\right)e^{ik(2l_1+l_2)}+2te^{ik(l_1+l_2)}-e^{ikl_2}\right\}\cos\left(\beta-\phi_2\right)\\
&-2te^{ikl_1}\left(t^2e^{2ikl_2}+1\right)\cos\phi_1-2t\left(2t^2-r^2+rt\cos\beta\right)e^{ik(l_1+2l_2)}\cos\phi_1\\
&-2rt^2e^{ik(2l_1+l_2)}\left(\cos\phi_1+\cos\left(2\beta-\phi_2\right)\right)=0.
\end{aligned}
$$

Thus the spectrum depends only on three of the parameters; β, $\phi_1=\varphi_1$, $\phi_2=\varphi_3-\varphi_2$. This can be explained using the following transformation $\mathbf{U}$ on $\psi\in L_2\left(\Gamma_\infty\right)$;

$$
\mathbf{U}\psi\left(x\right)=\begin{cases}\psi\left(x\right), & x\in E_1=\left[x_1,x_2\right]\\ e^{-i\varphi_2}\psi\left(x\right), & x\in E_2=\left[x_3,x_4\right].\end{cases}
$$

This unitary transformation does not change the differential operator, but amends the vertex scattering matrix as follows

$$
\tilde{\mathbf{S}}_1=\mathbf{U}_1^{-1}\hat{\mathbf{S}}_1\mathbf{U}_1=\mathrm{diag}\left(1,e^{-i\phi_1},1,e^{-i\phi_2}\right)S_1\,\mathrm{diag}\left(1,e^{i\phi_1},1,e^{i\phi_2}\right) \tag{4.4.4}
$$

where $\mathbf{U}_1=\mathrm{diag}\left(1,1,e^{-i\varphi_2},e^{-i\varphi_2}\right)$. Since $\mathbf{U}_1\mathbf{S}_E=\mathbf{S}_E\mathbf{U}_1$ we have

$$
\det\left(\tilde{\mathbf{S}}_1\mathbf{S}_E-\mathbf{I}\right)=\det\left(\mathbf{U}_1^{-1}\hat{\mathbf{S}}_1\mathbf{U}_1\mathbf{S}_E-\mathbf{U}_1^{-1}\mathbf{U}_1\right)=\cdots=\det\left(\hat{\mathbf{S}}_1\mathbf{S}_E-\mathbf{I}\right).
$$

Thus the secular equation remains unchanged despite one of the parameters having been eliminated.

The parameters $\phi_{1,2}$ are associated with the the two loops forming Γ_∞ and can be interpreted as fluxes of the magnetic filed through the loops, since these phases disappear if the magnetic potential on the edges is chosen appropriately as described in the previous section.

CONCLUSION

We have studied scattering matrices used for vertex conditions in quantum graphs where there is uniform transition probabilities as well as uniform reflection probabilities. We have shown that RET-matrices exist only in even orders. We have determined all such matrices up to order six. Matrices of order two comprises one-parameter family of matrices. RET-matrices of order four comprises two three-parameter family of matrices.

In order six we obtained 30 six-parameter families of matrices. Five of these parameters are called phase parameters and do not play a central role. Getting rid of these five parameters we arrived at one-parameter families of matrices $\mathbf{C}$. The families intersect at 12 very special real-valued matrices. Indeed each of the twelve is an intersection of five of the 60 parameter free matrices. It turned out that these twelve matrices are also conference matrices of order six. They determine the vertices of a bipartite $5-$regular combinatorial graph (see Figure 2.2) where the edges correspond to the 30 six-parameter families of matrices. A complete description of RET-matrices of orders greater than six remains an open problem.

We have shown that the SMC-matrix determines ET-matrices for all $n \geq 3$ and these are the only ET-matrices when the order of the matrix in question is odd and $n \leq 5$. We have determined all ET-matrices of even order up to order five. We observed that when the order is even then there exist ET-matrices not equivalent to SMC-matrix but all such matrices have zero trace. The cases of nonzero trace matrices which are not equivalent to SMC-matrices remains open for investigations.

The number of parameter dependent ET-matrices when n is even grows with the order of the matrix. When $n = 2$ there is only one one-parameter family of ET-matrices $\hat{\mathbf{C}}$. When $n = 4$ then the family of ET-matrices $\hat{\mathbf{C}}$ have at most one parameter. When $n = 6$ the ET-matrices $\hat{\mathbf{C}}$ have at most two parameters. As in the case of RET-matrices complete determination of ET-matrices of orders greater six still remains an open problem. Also the existence of ET-matrices in the cases $(2, 0)$, $(2, 1)$, $(3, 4)$ and $(3, 5)$ when $n = 6$ is yet to be determined.

We have shown that there are no ET-matrices for the cases (n^+, ν^+) and $(n - n^+, n - \nu^+)$ when $\nu^+ \in \{0, 1\}$ for all n. We conjecture that ET-matrices exist only in the following two cases

1. When the transition probabilities are the same as those of the SMC-matrix and this is true for all $n \geq 3$.

2. When n is even and the trace of the matrix is zero.

It remains to verify our conjecture and construct a proof. It will also be of interest to determine any relationship among the ET-matrices of order 6.

We have shown that the phase parameters in vertex conditions play a secondary role. The spectrum of a quantum graph does not depend on all such parameters but just a certain $g = N - M + 1$ of them. We have also shown that for any Schrödinger operator on a graph Γ with electric potential q and defined on functions satisfying (4.1.2) with $d_m - 1$ arbitrary vertex phases at each vertex V_m there exists a unitary equivalent magnetic Schrödinger operator on Γ with the same electric potential and zero phases in vertex conditions.

Computations for non-zero trace matrices when $n = 5$

Case $(2,1)$. In this case only one diagonal entry is positive while two eigenvalues are positive. The values r and t are $\frac{1}{3}$ and $\frac{\sqrt{2}}{3}$ respectively. The corresponding matrix C is represented as follows

$$C = \begin{pmatrix} r & t & t & t & t \\ t & -r & at & bt & ct \\ t & \overline{a}t & -r & dt & et \\ t & \overline{b}t & \overline{d}t & -r & ft \\ t & \overline{c}t & \overline{e}t & \overline{f}t & -r \end{pmatrix},$$

where $a, \ldots, f \in \{z \in \mathbf{C} : |z| = 1\}$. Since the rows of C are orthogonal, their inner products yield the following system of equations

$$\begin{cases} a + b + c = 0 & (1) \\ \overline{a} + d + e = 0 & (2) \\ \overline{b} + \overline{d} + f = 0 & (3) \\ \overline{c} + \overline{e} + \overline{f} = 0 & (4) \end{cases} \qquad \begin{cases} -2\overline{a}r + t\left(1 + \overline{b}d + \overline{c}e\right) = 0 & (5) \\ -2\overline{b}r + t\left(1 + \overline{a}\overline{d} + \overline{c}f\right) = 0 & (6) \\ -2\overline{c}r + t\left(1 + \overline{ae} + \overline{bf}\right) = 0 & (7) \end{cases} \tag{.0.5}$$

$$\begin{cases} -2\overline{d}r + t\left(1 + a\overline{b} + \overline{e}f\right) = 0 & (8) \\ -2\overline{e}r + t\left(1 + a\overline{c} + \overline{df}\right) = 0 & (9) \end{cases} \qquad \begin{cases} -2\overline{f}r + t\,(1 + b\overline{c} + d\overline{e}) = 0 & (10). \end{cases}$$

In what follows we determine the characteristic polynomial of matrix C from its spectrum and by direct computation from the entries of C. Now $\sigma(C) = \{1, 1, -1, -1, -1\}$ so that

$$\Delta_C(\lambda) = -(\lambda - 1)^2 (\lambda + 1)^3 = -\left(\lambda^5 + \lambda^4 - 2\lambda^3 - 2\lambda^2 + \lambda + 1\right). \tag{.0.6}$$

On the other hand by direct computation

$$\Delta_C(\lambda) = -\lambda^5 - 3r\lambda^4 + \left(10t^2 - 2r^2\right)\lambda^3 + \Big\{18rt^2 + 2r^3$$

$$+ t^3 \left[\underbrace{a + a\bar{b}d + a\bar{c}e}_{eq\,5=\alpha} + \underbrace{b + \bar{a}b\bar{d} + b\bar{c}f}_{eq\,6=\alpha} + \underbrace{c + \bar{a}c\bar{e} + \bar{b}c\bar{f}}_{eq\,7=\alpha}\right. \tag{.0.7}$$

$$\left. + \underbrace{\bar{a} + d + e}_{eq\,2=0} + \underbrace{\bar{b} + \bar{d} + f}_{eq\,3=0} + \underbrace{\bar{c} + \bar{e} + \bar{f}}_{eq\,4=0} + \underbrace{d\bar{e}f}_{eq\,8=\alpha-d-a\bar{b}d} + \underbrace{\bar{d}e\bar{f}}_{eq\,9=\alpha-d-a\bar{c}e}\right]\Big\}\lambda^2 + \cdots$$

Thus we rewrite the polynomial as

$$\Delta_C(\lambda) = -\lambda^5 - 3r\lambda^4 + \left(10t^2 - 2r^2\right)\lambda^3 + \left(18rt^2 + 2r^3 + t^3\left[5\alpha + a + \bar{a}\right]\right)\lambda^2 + \cdots \tag{.0.8}$$

Substituting the values of r and t and comparing the corresponding coefficients in (.0.6) and (.0.8) we readily see that the coefficients of λ^5 and λ^4 are equal. Simplifying the coefficient of λ^3 in (.0.8) we obtain that

$$10 \cdot \frac{2}{9} - 2 \cdot \frac{1}{9} = 2$$

in agreement with the value in (.0.6). Equating the coefficients of λ^2 we obtain

$$18rt^2 + 2r^3 + t^3\left(5\alpha + a + \bar{a}\right) = 2$$

which when simplified we obtain

$$\Re(a) = \frac{\alpha}{2}.$$

By making appropriate combinations in the coefficient of t^3 in (.0.7) we have

$$\Re(a) = \Re(b) = \Re(c) = \frac{\alpha}{2}.$$

The imaginary parts of a, b and c may coincide or differ by a sign. Hence it is impossible that (eq(1))

$$a + b + c = 0.$$

This contradiction implies that no ET-matrix can be obtained in this case.

Case $(3, 4)$. In this case only one diagonal entry is negative while three eigenvalues are positive. The values r and t are $\frac{1}{3}$ and $\frac{\sqrt{2}}{3}$ respectively. The corresponding matrix C is represented as follows

$$C = \begin{pmatrix} r & t & t & t & t \\ t & r & at & bt & ct \\ t & \overline{a}t & r & dt & et \\ t & \overline{b}t & \overline{d}t & r & ft \\ t & \overline{c}t & \overline{e}t & \overline{f}t & -r \end{pmatrix},$$

where $a, \ldots, f \in \{z \in \mathbf{C} : |z| = 1\}$. Since the rows of C are orthogonal, their inner products yield the following system of equations

$$\begin{cases} 2r + t\,(a + b + c) = 0 & (1) \\ 2r + t\,(\overline{a} + d + e) = 0 & (2) \\ 2r + t\left(\overline{b} + \overline{d} + f\right) = 0 & (3) \\ \overline{c} + \overline{e} + \overline{f} = 0 & (4) \end{cases} \qquad \begin{cases} 2\overline{a}r + t\left(1 + \overline{b}d + \overline{c}e\right) = 0 & (5) \\ 2\overline{b}r + t\left(1 + \overline{a}\overline{d} + \overline{c}f\right) = 0 & (6) \\ 1 + \overline{ae} + \overline{bf} = 0 & (7) \end{cases} \tag{.0.9}$$

$$\begin{cases} 2\overline{d}r + t\left(1 + a\overline{b} + \overline{e}f\right) = 0 & (8) \\ 1 + a\overline{c} + \overline{df} = 0 & (9) \end{cases} \qquad \begin{cases} 1 + b\overline{c} + d\overline{e} = 0 \quad (10). \end{cases}$$

In what follows we determine the characteristic polynomial of matrix C from its spectrum and by direct computation from the entries of C. Now $\sigma\,(C) = \{1, 1, 1, -1, -1\}$ so that

$$\Delta_C\,(\lambda) = -\,(\lambda - 1)^3\,(\lambda + 1)^2 = -\left(\lambda^5 - \lambda^4 - 2\lambda^3 + 2\lambda^2 + \lambda - 1\right). \tag{.0.10}$$

On the other hand by direct computation

$$\begin{aligned} \Delta_C\,(\lambda) = {} & -\lambda^5 + 3r\lambda^4 + \left(10t^2 - 2r^2\right)\lambda^3 + \left\{-24rt^2 - 2r^3\right. \\ & + t^3 \left[\underbrace{a + a\overline{b}d + a\overline{c}e}_{eq\,5 = -\alpha} + \underbrace{b + \overline{a}b\overline{d} + b\overline{c}f}_{eq\,6 = -\alpha} + \underbrace{c + \overline{a}c\overline{e} + \overline{b}c\overline{f}}_{eq\,7 = 0}\right. \\ & \left.\left. + \underbrace{\overline{a} + d + e}_{eq\,2 = -\alpha} + \underbrace{\overline{b} + \overline{d} + f}_{eq\,3 = -\alpha} + \underbrace{\overline{c} + \overline{e} + \overline{f}}_{eq\,4 = 0} + \underbrace{d\overline{e}f}_{eq\,8 = -\alpha - d - a\overline{b}d} + \underbrace{\overline{d}e\overline{f}}_{eq\,9 = -d - a\overline{c}e}\right]\right\}\lambda^2 + \cdots \end{aligned} \tag{.0.11}$$

Thus we rewrite the polynomial as

$$\Delta_C\,(\lambda) = -\lambda^5 + 3r\lambda^4 + \left(10t^2 - 2r^2\right)\lambda^3 + \left(-24rt^2 - 2r^3 + t^3\left[-2\alpha + a + \overline{a}\right]\right)\lambda^2 + \cdots \tag{.0.12}$$

Substituting the values of r and t and comparing the corresponding coefficients in (.0.10) and

(.0.12) we readily see that the coefficients of λ^5 and λ^4 are equal. Simplifying the coefficient of λ^3 in (.0.12) we obtain that

$$10 \cdot \frac{2}{9} - 2 \cdot \frac{1}{9} = 2$$

in agreement with the value in (.0.10). Equating the coefficients of λ^2 we obtain

$$-24rt^2 - 2r^3 + t^3\left(-2\alpha + a + \overline{a}\right) = -2$$

which when simplified we obtain

$$\Re\left(a\right) = \frac{\alpha}{2}.$$

By making appropriate combinations in the coefficient of t^3 in (.0.11) we have

$$\Re\left(a\right) = \Re\left(b\right) = \Re\left(c\right) = \frac{\alpha}{2}.$$

The imaginary parts of a, b and c may coincide or differ by a sign. Hence it is impossible that (eq(1))

$$a + b + c = -\alpha.$$

This contradiction implies that no ET-matrix can be obtained in this case.

Case $(3, 5)$. In this case all diagonal entries are positive while two eigenvalues are negative. The values r and t are $\frac{1}{5}$ and $\frac{\sqrt{6}}{5}$ respectively. The corresponding matrix C is represented as follows

$$C = \begin{pmatrix} r & t & t & t & t \\ t & r & at & bt & ct \\ t & \overline{a}t & r & dt & et \\ t & \overline{b}t & \overline{d}t & r & ft \\ t & \overline{c}t & \overline{e}t & \overline{f}t & r \end{pmatrix},$$

where $a, \ldots, f \in \{z \in \mathbf{C} : |z| = 1\}$. Since the rows of C are orthogonal, their inner products yield the following system of equations

$$\begin{cases} 2r + t\,(a+b+c) = 0 & (1) \\ 2r + t\,(\overline{a}+d+e) = 0 & (2) \\ 2r + t\left(\overline{b}+\overline{d}+f\right) = 0 & (3) \\ 2r + t\left(\overline{c}+\overline{e}+\overline{f}\right) = 0 & (4) \end{cases} \qquad \begin{cases} 2\overline{a}r + t\left(1+\overline{b}d+\overline{c}e\right) = 0 & (5) \\ 2\overline{b}r + t\left(1+\overline{a}\overline{d}+\overline{c}f\right) = 0 & (6) \\ 2\overline{c}r + t\left(1+\overline{a}\overline{e}+\overline{b}\overline{f}\right) = 0 & (7) \end{cases} \tag{.0.13}$$

$$\begin{cases} 2\overline{d}r + t\left(1+a\overline{b}+\overline{e}f\right) = 0 & (8) \\ 2\overline{e}r + t\left(1+a\overline{c}+\overline{d}\overline{f}\right) = 0 & (9) \end{cases} \qquad \begin{cases} 2\overline{f}r + t\,(1+b\overline{c}+d\overline{e}) = 0 & (10). \end{cases}$$

In what follows we determine the characteristic polynomial of matrix C from its spectrum and by direct computation from the entries of C. Now $\sigma(C) = \{1,1,1,-1,-1\}$ so that

$$\Delta_C(\lambda) = -(\lambda-1)^3(\lambda+1)^2 = -\left(\lambda^5 - \lambda^4 - 2\lambda^3 + 2\lambda^2 + \lambda - 1\right). \tag{.0.14}$$

On the other hand by direct computation

$$\begin{aligned} \Delta_C(\lambda) = {} & -\lambda^5 + 5r\lambda^4 + 10\left(t^2 - r^2\right)\lambda^3 + \Big\{10r^3 - 30rt^2 \\ & + t^3 \Bigg[\underbrace{a + a\overline{b}d + a\overline{c}e}_{eq\,5 = -\alpha} + \underbrace{b + \overline{a}b\overline{d} + b\overline{c}f}_{eq\,6 = -\alpha} + \underbrace{c + \overline{a}c\overline{e} + \overline{b}c\overline{f}}_{eq\,7 = -\alpha} \\ & + \underbrace{\overline{a} + d + e}_{eq\,2 = -\alpha} + \underbrace{\overline{b} + \overline{d} + f}_{eq\,3 = -\alpha} + \underbrace{\overline{c} + \overline{e} + \overline{f}}_{eq\,4 = -\alpha} + \underbrace{d\overline{e}f}_{eq\,8 = -\alpha - d - a\overline{b}d} + \underbrace{\overline{d}e\overline{f}}_{eq\,9 = -\alpha - d - a\overline{c}e} \Bigg] \Big\} \lambda^2 + \cdots \end{aligned} \tag{.0.15}$$

Thus we rewrite the polynomial as

$$\Delta_C(\lambda) = -\lambda^5 + 5r\lambda^4 + 10\left(t^2 - r^2\right)\lambda^3 + \left(10r^3 - 30rt^2 - t^3\left[-6\alpha + a + \overline{a}\right]\right)\lambda^2 + \cdots \tag{.0.16}$$

Substituting the values of r and t and comparing the corresponding coefficients in (.0.14) and (.0.16) we readily see that the coefficients of λ^5 and λ^4 are equal. Simplifying the coefficient of λ^3 in (.0.16) we obtain that

$$10\left(\frac{6}{25} - \frac{1}{25}\right) = 2$$

in agreement with the value in (.0.14). Equating the coefficients of λ^2 we obtain

$$10r^3 - 30rt^2 - t^3\left(-6\alpha + a + \overline{a}\right) = -2$$

which when simplified we obtain

$$\Re\left(a\right) = -\frac{\alpha}{3}.$$

By making appropriate combinations in the coefficient of t^3 in (.0.15) we have

$$\Re\left(a\right) = \Re\left(b\right) = \Re\left(c\right) = -\frac{\alpha}{3}.$$

The imaginary parts of a, b and c may coincide or differ by a sign. Hence it is impossible that (eq(1))

$$a + b + c = -\alpha.$$

This contradiction implies that no ET-matrix can be obtained in this case.

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