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THE LAPLACIAN ON DISCRETE AND QUANTUM GRAPHS, AN APPROACH FOR MATHEMATICAL BIOLOGY.

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Introducción

En este trabajo proporcionamos una introducción accesible y autónoma a las gráficas cuánticas y gráficas discretas, más aún, damos algunas posibles direcciones de investigación en el contexto de Biología Matemática. Revisamos artículos recientes sobre las aplicaciones de gráficas a Biología, éstas están basadas en gráficas discretas regularmente. Nuestra intención principal en esta tesis es una comparación entre gráficas cuánticas y gráficas discretas, enfocándonos en cómo las gráficas cuánticas pueden entrar en el dominio de la Biología. Nosotros creemos que las gráficas cuánticas pueden proveer una contribución importante a la Biología por las siguientes tres razones:

- El espectro de una gráfica cuántica finita es infinito, en contraste con el espectro de una gráfica discreta finita que es finito. Por lo que, la información que una gráfica cuántica puede proporcionar para el modelado de un fenómeno puede ser superior.
- Existe una cantidad muy grande de trabajos en la comunidad de Física Matemática sobre gráficas cuánticas. Nosotros creemos que los biólogos matemáticos deberían tomar ventaja de este trabajo.
- Además de la teoría espectral (que es una de las herramientas principales para los modelos que analizamos sobre las gráficas discretas), en gráficas cuánticas la teoría de dispersión juega un papel central (el cual da herramientas matemáticas adicionales e información).

En la sección 1.1, para el caso de gráficas discretas, consideramos el espacio de funciones definidas en los vértices de una gráfica finita y conexa y con valores en los reales o en los números complejos, y dentro de éste, un producto interno designado con pesos. El Laplaciano de una gráfica es definido en este espacio en términos de estos pesos y notamos que resulta ser autoadjunto.

Las gráficas métricas son definidas en la sección 1.2 con una gráfica discreta y dirigida subyacente, pero sus aristas son consideradas como intervalos reales con una coordenada en cada uno de éstas. Las funciones definidas sobre estas gráficas toman valores en todos los puntos de las aristas (incluyendo los vértices). En este caso, el operador Laplaciano es $\Delta = -\frac{d^2}{dx^2}$ (i.e. menos la segunda derivada distribucional tomada sobre cada arista). El espacio que consideramos para el dominio de Δ es $H^2(\Gamma)$, el espacio de Sobolev de funciones definidas sobre Γ con derivadas distribucionales, hasta de orden dos, cuadrado integrables. Con el propósito de garantizar que este operador es autoadjunto, necesitamos imponer algunas condiciones de frontera locales a la funciones en el dominio de Δ.

En la sección 1.3, demostramos que, si el Laplaciano Δ es definido en un dominio que contiene al espacio C_0^∞ (con condiciones de frontera locales mixtas de Dirichlet o Neumann), entonces el dominio del operador adjunto Δ^* es un subconjunto del espacio de Sobolev $H^2(\Gamma)$. Para la demostración de este hecho usamos la regularidad del Laplaciano de Dirichlet en intervalos finitos y semi infinitos. Incluimos la prueba de ésto en el escrito presente por dos razones: la primera es mantener el trabajo tan autónomo como sea posible y la segunda (y más importante) es que el estudio de operadores elípticos en gráficas no requiere la (sofisticada) maquinaria completa desarrollada en la teoría general de operadores elípticos en conjuntos abiertos en $\mathbb{R}^n$ (o variedades de Riemann), pero tiene la ventaja de que (en gráficas) la prueba puede ser presentada de una manera corta, intuitiva, autónoma y accesible. Esta presentación incluye todas las ideas clave que pueden ser generalizadas para variedades, por lo tanto, ésto es valioso para estudiantes de maestría que desean comprender las ideas principales de regularidad elíptica de una manera económica. Adicionalmente, recalcamos que el entendimiento de las gráficas cuánticas no requiere la teoría plena de ecuaciones diferenciales parciales elípticas, y este texto suministra el conocimiento básico para los estudiantes que quieren empezar una investigación en gráficas cuánticas sin entrar en la ecuaciones diferenciales parciales.

En la sección 1.4, siguiendo las ideas de [9] y considerando Γ una gráfica métrica finita y conexa, para funciones f en el dominio del Laplaciano damos algunas *condiciones de frontera* locales que son suficientes y necesarias para asegurar que este operador es autoadjunto. Estas condiciones son establecidas en el teorema 1.4.8, el cual es demostrado considerando sólo una parte pequeña de la gráfica (una vecindad de un vértice que parece una gráfica estrella) ya que las condiciones son locales.

Las gráficas son aplicadas en muchos modelos matemáticos en Biología. Los ejemplos van desde redes neuronales, modelos de proteínas o genes, hasta cadenas tróficas y árboles filogenéticos. En el último capítulo, escribimos una reseña de algunas aplicaciones matemáticas a redes biológicas, con particular énfasis sobre el espectro del Laplaciano de una gráfica discreta e indagando cómo las gráficas cuánticas pueden incluirse en estos modelos.

Introduction

In this work we provide an accessible and self-contained introduction to quantum graphs and discrete graphs and we give possible research directions in the context of Mathematical Biology. We revise recent research papers on applications of graphs to Biology. These applications are regularly based on discrete graphs. Our main intention in this thesis is a comparison between quantum and discrete graphs focusing on how quantum graphs could entry into the domain of Biology. We believe that quantum graphs could provide an important input in Biology for the following three reasons:

(1) The spectrum of a finite quantum graph is infinite, in contrast with the spectrum of a finite discrete graph that is finite. Therefore, the information that a quantum graph might provide to the modeling of a phenomenon might be superior.
(2) There is a huge amount of work in the Mathematical Physics community on quantum graphs. We believe that the mathematical biologists should take advantage of this work.
(3) Apart from spectral theory (which is one of the main tools for the models we analyze on discrete graphs), in quantum graphs the scattering theory plays a central role (which gives additional mathematical tools and information).

In Section 1.1, for the case of discrete graphs, we will consider the space of real or complex valued functions defined on the vertices of a finite connected graph and, defined therein, an inner product designated with weights. The graph Laplacian is defined on this space in terms of these weights and we will see that it turns out to be self-adjoint.

Metric graphs are defined in Section 1.2 with an underlying directed discrete graph, but its edges will be considered as real intervals with a coordinate on each one. The functions defined on these graphs take values in all the points of the edges (including the vertices). In this case, the Laplace operator is going to be $\Delta = -\frac{d^2}{dx^2}$ (i.e. the negative second distributional derivate taken on each edge). The space consider for the domain of Δ is $H^2(\Gamma)$, the Sobolev Space of functions defined on Γ with square integrable distributional derivates up to order two. In order to guarantee self-adjointness, we need to impose some local *boundary conditions* to the functions in the domain of Δ.

In Section 1.3, we demonstrate that, if the Laplacian Δ is defined with domain containing $C_0^\infty(\Gamma)$ (with mixed Dirichlet or Neumann local boundary conditions), then the domain of the adjoint operator Δ^* is a subset of the Sobolev space $H^2(\Gamma)$. The proof of this fact uses regularity of the Dirichlet Laplacian in finite and semi-infinite intervals. We include the demonstration of this in the present manuscript for two reasons: The first is to keep this work as self-contained as possible and the second (and the most relevant one) is that studying elliptic operators in graphs does not require the full (sophisticated) machinery developed in the general theory of elliptic operators in open sets in $\mathbb{R}^n$ (or Riemannian manifolds), but it has the advantage that the proof can be presented (in graphs) in a short, intuitive, self-contained and accessible way. This presentation already includes all key ideas that can be generalized to manifolds, and it is, therefore, valuable to master students that may want to grasp the main ideas of elliptic regularity in an economic way. Additionally, we stress that understanding quantum graphs does not require the full theory of elliptic PDE's, and this text provides the basic knowledge to scholars who might want to start doing research on quantum graphs without going into PDE's.

In Section 1.4, following ideas from [9] and considering Γ a finite connected metric graph, for functions f in the domain of the Laplacian we give some local *boundary conditions* which are sufficient and necessary to assure the self-adjointness of this operator. These conditions are settled on Theorem 1.4.8, which is proved just considering a small part of the graph (a vicinity of a vertex which looks like a star graph) being that the conditions are local.

Graphs are applied in many biological mathematical models. The examples go from neuronal networks, protein or genetic models, to trophic chains and phylogenetic trees. In the last Chapter, we write a review of some mathematical applications to biological networks, with particular emphasis on the spectrum of the discrete graph Laplacian, and enquiring how quantum graphs could make an entry in these models.

CHAPTER 1

The Graph Laplacian

A **discrete graph** or **combinatorial** Γ consists of a numerable set $\mathcal{V} = \{v_i\}$ of vertices and a set $\mathcal{E} = \{e_j\}$ of edges between vertices. If no confusion arises, we just say *graph* instead of discrete graph. Two vertices u and v are **adjacent** if there exists an edge between them and we will detone by $u \sim v$.

We will use the notation $v \in e$ to indicate that v is a vertex of e. The **degree** d_v of a vertex v is the number of edges which proceed from it, i.e.,

$$d_v = \big|\{e \in \mathcal{E} \colon v \in e\}\big|.$$

We will assume that all the degrees are finite.

A **path** in Γ is a finite sequence of distinct vertices $\{v_0, v_1, \dots, v_k\} \subset \mathcal{V}$ and edges $\{e_1, e_2, \dots, e_k\} \subset \mathcal{E}$, such that $v_{i-1} \in e_i$ and $v_i \in e_i$ for all $i = 1, 2, \dots, k$. We say that a graph is **connected** if there is a path between any two vertices.

We will say that a graph is a **directed**, or a **digraph**, if each of its edges has an assigned direction, i.e. there are functions $o \colon \mathcal{E} \to \mathcal{V}$ and $t \colon \mathcal{E} \to \mathcal{V}$ such that, for every $e \in \mathcal{E}$, $o(e)$ represents the **origin vertex** of e and $t(e)$ the **terminal vertex**.

1.1. The Laplacian on Discrete Graphs

Consider Γ a finite and connected discrete graph. A real or complex valued **function** f **on** Γ is defined on the vertices of Γ. We will denote by $L^2(\Gamma)$ the set of functions from Γ to $\mathbb{C}$.

Introducing an L^2-product:

$$(f, g) := \sum_{v \in \mathcal{V}} b_v f(v) \overline{g(v)},$$

where the *weights* b_i are positive reals, the **Discrete Graph Laplacian** is defined as follows:

$$\Delta \colon L^2(\Gamma) \to L^2(\Gamma)$$

$$\Delta f(v) := \frac{1}{b_v}\Big(d_v f(v) - \sum_{u \sim v} f(u)\Big) \qquad \forall f \in L^2(\Gamma). \tag{1}$$

An important property of Δ is that it is a **self-adjoint** operator. This follows from the symmetry of the adjacency relation. Indeed, from the definition of the product with weights we have

$$\begin{aligned}
(f, \Delta g) &= \sum_{v\in\mathcal{V}} b_v f(v) \overline{\frac{1}{b_v}\Big(d_v g(v) - \sum_{u\sim v} g(u)\Big)} \\
&= \sum_{v\in\mathcal{V}} f(v)\Big(d_v \overline{g(v)} - \sum_{u\sim v} \overline{g(u)}\Big) \\
&= \sum_{v\in\mathcal{V}} \Big(d_v f(v)\overline{g(v)} - \sum_{u\sim v} f(v)\overline{g(u)}\Big) \\
&= \sum_{v\in\mathcal{V}} \Big(d_v f(v) - \sum_{u\sim v} f(u)\Big)\overline{g(v)} \\
&= \sum_{v\in\mathcal{V}} b_v \frac{1}{b_v}\Big(d_v f(v) - \sum_{u\sim v} f(u)\Big)\overline{g(v)} \\
&= (\Delta f, g)
\end{aligned}$$

for any $f, g \in L^2(\Gamma)$.

1.2. Metric Graphs

Now we will consider edges not only as relations between vertices, but also as intervals, providing a metric to the graph.

Definition 1.2.1. *Let Γ be graph with set of vertices $\mathcal{V}$ and set of edges $\mathcal{E}$. We will say that Γ is a **metric graph** if it satisfies the following conditions:*

(1) Γ is directed and for every edge $e \in \mathcal{E}$ there is a length $L_e \in (0, \infty]$.

(2) To each edge there is a coordinate $x_e \in [0, L_e]$ increasing in the direction of the edge.

Henceforth, we identify the edges e with the intervals $[0, L_e]$ if $L_e < \infty$ and with the intervals $[0, \infty)$ if $L_e = \infty$. Furthermore, we denote by $\mathring{e}$ the interior of the edge e, defined by means of the identifications above, that is to say,

$$\mathring{e} \equiv (0, L_e)$$

In order to define a metric naturally, we will assume that a metric graph is *connected*. If $\{e_j\}_{j=1}^M$ is a sequence of edges which form a path, its length is defined as $\sum L_{e_j}$. For every two vertices v and w, the distance $\rho(v, w)$ is the minimal element of the lengths of the paths which join them. The distance $\rho(x, y)$ between two points x and y of two edges can be defined in an analogous way. For example, if $\{e_j\}_{j=1}^M$ is a sequence of edges such that they form a "path" between $x \in e_1$ and $y \in e_M$, and $t(e_1) \in e_2$ and

$o(e_M) \in e_{M-1}$, then its length will be $(L_{e_1} - x) + \sum_{j=2}^{M-1} L_{e_j} + y$. The other cases are similar.

We consider a function $f(x)$ on Γ defined along the edges. Before the next definitions, let us introduce the notation f_e and $f_{\mathring{e}}$ to refer the restriction of a function f defined on Γ to the edge e and to $\mathring{e}$, respectively. Also remark that the norm on the function space $L^2(e)$ is given by

$$\|f_e\|^2_{L^2(e)} = \int_e |f_e(x)|^2 dx,$$

and that if $D^k f_{\mathring{e}} \equiv \frac{d^k f}{dx^k} \equiv \frac{d^k f}{dx_e^k}$ is the k-th distributional derivate of $f_{\mathring{e}}$, then

$$H^k(\mathring{e}) = \{f_{\mathring{e}} \in L^2(\mathring{e}) \mid D^\alpha f_{\mathring{e}} \in L^2(\mathring{e}), \alpha = 0, \dots, k\}$$

is the Sobolev space with norm

$$\|f_{\mathring{e}}\|^2_{H^k(\mathring{e})} = \sum_{\alpha=0}^{k} \|D^\alpha f_{\mathring{e}}\|^2_{L^2(\mathring{e})}.$$

Definition 1.2.2. *Let Γ be a metric graph. The* ***space*** *$L^2(\Gamma)$ consists of functions f on Γ such that $f_e \in L^2(e)$ for every edge e of Γ and such that*

$$\|f\|^2_{L^2(\Gamma)} := \sum_{e \in \mathcal{E}} \|f_e\|^2_{L^2(e)} < \infty. \tag{2}$$

The ***Sobolev space*** *$H^k(\Gamma)$ consists of functions f on Γ such that $f_{\mathring{e}} \in H^k(\mathring{e})$ for every edge e of Γ and such that*

$$\|f\|^2_{H^k(\Gamma)} := \sum_{e \in \mathcal{E}} \|f_{\mathring{e}}\|^2_{H^k(\mathring{e})} < \infty. \tag{3}$$

Note 1.2.3. *Due to the Sobolev inequalities (see [12],Theorem 5, page 269), for a function $f_e \in H^1((0, L_e))$, there exists a function $f_e^* \in C^{0,1/2}([0, L_e])$ that is equal to f_e (except on a null set) and such that*

$$\|f_e^*\|_{C^{0,1/2}([0,L_e])} \le C \|f_e\|_{H^1((0,L_e))}$$

for some constant C. So henceforth, we will identify a function $f_e \in H^1(e)$ with its continuous version f_e^*.

1.3. Regularity

We study the Laplace operator in various domains. We define

$$C_0^\infty(\Gamma) := \bigoplus_{e \in \mathcal{E}} C_0^\infty(\mathring{e}).$$

We use the notation $\mathsf{Dom}(\Delta)$ to specify a possible domain. We assume that

$$C_0^\infty(\Gamma) \le \mathsf{Dom}(\Delta) \le H^2(\Gamma).$$

For every $\mathsf{Dom}(\Delta)$, we denote by $(\Delta;\mathsf{Dom}(\Delta))$ the Laplace operator with domain $\mathsf{Dom}(\Delta)$ that is given by minus the second distributional derivative operator, i.e.

$$\Delta(f) = -\frac{d^2f}{dx} \qquad \forall f \in \mathsf{Dom}(\Delta),$$

and by $(\Delta;\mathsf{Dom}(\Delta))^* := (\Delta^*;\mathsf{Dom}(\Delta^*))$, we denote the adjoint operator of $(\Delta;\mathsf{Dom}(\Delta))$.

The purpose of this section is to prove that, if $C_0^\infty(\Gamma) \leq \mathsf{Dom}(\Delta)$, then the domain of $(\Delta;\mathsf{Dom}(\Delta))^*$ is contained in $H^2(\Gamma)$. Recall that, for every $e \in \mathcal{E}$, $f_{\mathring{e}}$ is the restriction of f to the open ser $\mathring{e}$, and that each edge has a coordinate $x_e \in [0, L_e]$ (if its length is finite) or $x_e \in [0,\infty)$.

So, to our purpose, we have to prove two things about $f \in \mathsf{Dom}(\Delta^*)$:

- that $f_{\mathring{e}} \in H^2((0, L_e))$ if e has finite length and
- that $f_{\mathring{e}} \in H^2((0,\infty))$ if e has infinite length.

To simplify the notation, we will avoid the subindex in f_e and just write f. Let us begin with the case when e has infinite length. Consider the operator $(\Delta; C_0^\infty((0,\infty))$. Consider the following property of the elements of the domain of $(\Delta; C_0^\infty((0,\infty)))^*$:

$$f \in \mathsf{Dom}(\Delta^*) \iff \exists g \in L^2((0,\infty))\colon \langle f, \Delta h\rangle = \langle g, h\rangle \quad \forall h \in \mathsf{Dom}(\Delta)$$

$$\iff \int_{(0,\infty)} f \cdot \Delta h = \int_{(0,\infty)} g \cdot h \quad \forall h \in C_0^\infty((0,\infty)) \iff T_g = \Delta T_f, \tag{4}$$

where T_g and ΔT_f are the distributions which satisfy

$$T_g(h) = \int_{(0,\infty)} g(x)h(x)dx \qquad \forall h \in C_0^\infty((0,\infty))$$

and

$$\Delta T_f(h) = \int_{(0,\infty)} f(x)\Delta h(x)dx \qquad \forall h \in C_0^\infty((0,\infty)),$$

respectively.

Proposition 1.3.1. *(*Translations are continuous in L^P*). Let $t \in \mathbb{R}$ and define $\tau_t(f) := f_t$, where $f_t(x) := f(x+t)$. If $1 \leq p < \infty$, then for every $f \in L^p(\mathbb{R})$*

$$\|f_t - f\|_p \to 0 \qquad as \quad t \to 0.$$

Proof. As the set of finite linear combinations of characteristic functions of intervals is dense in $L^P(\mathbb{R})$, take ϕ a finite linear combination of characteristic functions of intervals such that $\|f-\phi\|_p$ is enough small. Without loss of generality, consider the characteristic function of an open interval (a,b), then

$$\|\tau_t(\chi_{(a,b)}) - \chi_{(a,b)}\|_p \leq (2|t|)^{1/p} \underset{t\to 0}{\longrightarrow} 0.$$

Thus we have

$$\|\tau_t(\phi) - \phi\|_p \underset{t\to 0}{\longrightarrow} 0.$$

But then,

$$\begin{aligned}\|f_t - f\|_p &\leq \|f_t - \phi_t\|_p + \|\phi_t - \phi\|_p + \|\phi - f\|_p \\ &= 2\|f - \phi\|_p + \|\phi_t - \phi\|_p \underset{t\to 0}{\longrightarrow} 0.\end{aligned}$$

□

Consider an even function $\eta \in C_0^\infty(\mathbb{R})$ such that $supp(\eta) \subset \overline{B(0,1)}$, $\eta \geq 0$ and η is not identically zero. For example, the function

$$\eta(x) = \begin{cases} Ce^{1/(|x|^2-1)} & \text{if} \quad |x| < 1 \\ 0 & \text{if} \quad |x| \geq 1 \end{cases}$$

whith $C > 0$ a constant such that $\int \eta(x)dx = 1$. We obtain then a sequence of *mollifiers* by letting $\eta_\epsilon(x) = \frac{1}{\epsilon}\eta(\frac{x}{\epsilon})$, i.e. a sequence $(\eta_\epsilon)_{\epsilon>0}$ of functions satisfying

(i) $\eta_\epsilon \in C_0^\infty(\mathbb{R})$,
(ii) $supp(\eta_\epsilon) \subset \overline{B(0,\epsilon)}$,
(iii) $\int \eta_\epsilon = 1$,
(iv) $\eta_\epsilon \geq 0$ in $\mathbb{R}$ and
(v) $\eta_\epsilon(x) = \eta_\epsilon(-x)$ for every $x \in \mathbb{R}$.

Lemma 1.3.2. *Let us consider a function $f \in L^2\big(\mathbb{R}\big)$ and a sequence of mollifiers $(\eta_\epsilon)_{\epsilon>0}$. Define*

$$f_\epsilon(x) := f * \eta_\epsilon(x) := \int_{-\infty}^{\infty} f(y)\eta_\epsilon(x-y)dy \qquad \forall x \in \mathbb{R}.$$

Then, the following statements hold:

(1) $f_\epsilon \in \mathcal{C}^\infty(\mathbb{R})$
(2) $\frac{d^n}{dx^n} f_\epsilon = f * \frac{d^n}{dx^n}\eta_\epsilon$ *for every* $n \in \mathbb{N}$,
(3) $f_\epsilon \in L^2(\mathbb{R})$ *for every* $\epsilon > 0$ *and* $f_\epsilon \underset{\epsilon\to 0}{\longrightarrow} f$ *in* $L^2\big(\mathbb{R}\big)$.

Proof. By the definition of f_ϵ, for every $x \in \mathbb{R}$ we have that

$$\frac{f_\epsilon(x+h) - f_\epsilon(x)}{h} = \int_{-\infty}^{\infty} \Big(\frac{\eta_\epsilon(x-y+h) - \eta_\epsilon(x-y)}{h}\Big) f(y)dy.$$

Then, by the Dominated Convergence Theorem follows

$$\lim_{h\to 0}\frac{f_\epsilon(x+h)-f_\epsilon(x)}{h}=\int_{-\infty}^{\infty}\frac{d\eta_\epsilon}{dx}(x-y)f(y)dy=\Big(f*\frac{d\eta_\epsilon}{dx}\Big)(x).$$

Hence, $\frac{df_\epsilon}{dx}(x)$ exists and

$$\frac{df_\epsilon}{dx}(x)=\Big(f*\frac{d\eta_\epsilon}{dx}\Big)(x).$$

A similar argument shows that $\frac{d^n}{dx^n}f_\epsilon$ exists and

$$\frac{d^n}{dx^n}f_\epsilon(x)=\int_{-\infty}^{\infty}\frac{d^n}{dx^n}\eta_\epsilon(x-y)f(y)dy=\Big(f*\frac{d^n}{dx^n}\eta_\epsilon\Big)(x)\qquad\forall x\in\mathbb{R},$$

for each $n=0,1,2,...$ Hence, points (1) and (2) are satisfied.

To demonstrate (3), we make reference to Theorem 4.22 in [10] to verify $f_\epsilon\in L^2(\mathbb{R})$ and

$$f*\eta_\epsilon\xrightarrow[\epsilon\to 0]{} f$$

in $L^2(\mathbb{R})$.

□

Lemma 1.3.3. *Let $f,g\in L^2((0,\infty))$. Suposse $\Delta T_f=T_g$. Then, for any $\epsilon>0$, there is a function $\phi\in C^\infty([0,\infty))$ such that*

$$\|f-\phi\|_{L^2((0,\infty))}<\epsilon\qquad \textit{and}\qquad \|g-\Delta\phi\|_{L^2((0,\infty))}<\epsilon.$$

Proof. For every $\delta>0$, define the functions $\tau_\delta(f),\tau_\delta(g):(-\delta,\infty)\to\mathbb{R}$ as follows:

$$\tau_\delta(f)(x)=f(x+\delta),\qquad\qquad \tau_\delta(g)(x)=g(x+\delta).\tag{5}$$

It is easy to see that $\tau_\delta(f),\tau_\delta(g)\in L^2((-\delta,\infty))$. By Propositon (1.3.1) there exists $\delta_0>0$ such that

$$\|\tau_{\delta_0}(f)-f\|_{L^2((0,\infty))}<\epsilon/2,\qquad \|\tau_{\delta_0}(g)-g\|_{L^2((0,\infty))}<\epsilon/2.\tag{6}$$

We extend the functions $\tau_{\delta_0}(f),\tau_{\delta_0}(g)$ to $\mathbb{R}$, without changing notation, defining them as 0 in $(-\infty,-\delta]$. Using Lemma 1.3.2 we obtain that there is $\epsilon_0\in(0,\delta_0)$ which satisfies

$$\|\tau_{\delta_0}(f)*\eta_{\epsilon_0}-\tau_{\delta_0}(f)\|_{L^2(\mathbb{R})}<\epsilon/2,\qquad \|\tau_{\delta_0}(g)*\eta_{\epsilon_0}-\tau_{\delta_0}(g)\|_{L^2(\mathbb{R})}<\epsilon/2.\tag{7}$$

Now we can define the function which satisfies the claims of this Lemma as follows:

$$\phi:=\tau_{\delta_0}(f)*\eta_{\epsilon_0}.$$

It follows from Lemma 1.3.2 that $\phi \in C^\infty([0,\infty))$. Moreover, by Equations (6) y (7) we have

$$\|f-\phi\|_{L^2((0,\infty))} \leq \|f-\tau_{\delta_0}(f)\|_{L^2((0,\infty))} + \|\tau_{\delta_0}(f)-\phi\|_{L^2((0,\infty))} < \epsilon.$$

Now we will prove that

$$\Delta(\tau_{\delta_0}(f) * \eta_{\epsilon_0}) = \Delta\tau_{\delta_0}(f) * \eta_{\epsilon_0} = \tau_{\delta_0}(g) * \eta_{\epsilon_0},$$

on $[0,\infty)$. From Lemma 1.3.2,

$$\Delta(\tau_{\delta_0}(f) * \eta_{\epsilon_0}) = \tau_{\delta_0}(f) * \Delta\eta_{\epsilon_0}.$$

Let $T_{\tau_{\delta_0}(f)}$ the distribution on $(-\delta_0,\infty)$ associated to $\tau_{\delta_0}(f)$. In the same way define $T_{\tau_{\delta_0}(g)}$. We will show that $\Delta T_{\tau_{\delta_0}(f)} = T_{\tau_{\delta_0}(g)}$. If $u \in C_0^\infty\big((-\delta_0,\infty)\big)$, then

$$\begin{aligned}\Delta T_{\tau_{\delta_0}(f)}(u) &= \int_{(-\delta_0,\infty)} \tau_{\delta_0}(f)\Delta u = \int_{(0,\infty)} f\tau_{-\delta_0}(\Delta u)\\ &=\Delta T_f(\tau_{-\delta_0}(u)) = T_g(\tau_{-\delta_0}(u)) = T_{\tau_{\delta_0}(g)}(u),\end{aligned}$$

since $\tau_{-\delta_0}(u) \in C_0^\infty\big((0,\infty)\big)$. The next step is to prove that $\tau_{\delta_0}(f) * \Delta\eta_{\epsilon_0} = \tau_{\delta_0}(g) * \eta_{\epsilon_0}$ as functions on $[0,\infty)$. Take $x \in [0,\infty)$,

$$\begin{aligned}\tau_{\delta_0}(f) * \Delta\eta_{\epsilon_0}(x) &= \int_{\mathbb{R}} \tau_{\delta_0}(f)(y)\Delta\eta_{\epsilon_0}(x-y)dy = \int_{\mathbb{R}} \tau_{\delta_0}(f)(y)\Delta\eta_{\epsilon_0}(y-x)dy\\ &= \int_{\mathbb{R}} \tau_{\delta_0}(f)(y)\Delta\tau_{-x}(\eta_{\epsilon_0}(y))dy = \Delta T_{\tau_{\delta_0}(f)}(\tau_{-x}(\eta_{\epsilon_0}))\\ &=T_{\tau_{\delta_0}(g)}(\tau_{-x}(\eta_{\epsilon_0})) = \tau_{\delta_0}(g) * \eta_{\epsilon_0}(x),\end{aligned}$$

where we used that $\tau_{-x}(\eta_{\epsilon_0}) \in C_0^\infty(-\delta_0,\infty)$, since $\epsilon_0 < \delta_0$ and $x \geq 0$. Finally, we obtain

$$\begin{aligned}\|g-\Delta\phi\|_{L^2((0,\infty))} &\leq \|g-\tau_{\delta_0}(g)\|_{L^2((0,\infty))} + \|\tau_{\delta_0}(g)-\Delta\phi\|_{L^2((0,\infty))}\\ &= \|g-\tau_{\delta_0}(g)\|_{L^2((0,\infty))} + \|\tau_{\delta_0}(g)-\tau_{\delta_0}(g) * \eta_{\epsilon_0}\|_{L^2((0,\infty))} < \epsilon.\end{aligned}$$

□

Lemma 1.3.4. *Let $\phi \in C^\infty([0,\infty))$. There exists $\widetilde{C} > 0$ such that*

$$\|\phi\|_{H^2((0,\infty))} \leq \widetilde{C}(\|\phi\|_{L^2((0,\infty))} + \|\Delta\phi\|_{L^2((0,\infty))}).$$

Proof. If $x \in [0,\infty)$, note that

$$\phi(x+y) - \phi(x) = \int_x^{x+y} \phi' \qquad \forall y \in (-x,\infty),$$

thereby, using Cauchy-Schwarz inequality,

$$|\phi(x)| \leq |\phi(x+y)| + \Big(\int_x^{x+y} |\phi'|^2\Big)^{1/2} |y|^{1/2} \qquad \forall y \in (-x, \infty).$$

Let $\epsilon > 0$. By integrating we obtain

$$\begin{aligned}\epsilon|\phi(x)| \leq &\int_0^{\epsilon} |\phi(x+y)|dy + \frac{2}{3}\|\phi'\|_{L^2((0,\infty))}\epsilon^{3/2}\\ \leq &\|\phi\|_{L^2((0,\infty))}\epsilon^{1/2} + \frac{2}{3}\|\phi'\|_{L^2((0,\infty))}\epsilon^{3/2}.\end{aligned}$$

Thus,

$$|\phi(x)| \leq \|\phi\|_{L^2((0,\infty))}\epsilon^{-1/2} + \frac{2}{3}\|\phi'\|_{L^2((0,\infty))}\epsilon^{1/2}.$$

Similarly, when $\epsilon = 1$, we have

$$|\phi'(x)| \leq \|\phi'\|_{L^2((0,\infty))} + \frac{2}{3}\|\phi''\|_{L^2((0,\infty))}.$$

Recall that

$$ab \leq \frac{1}{2}(a^2+b^2) \leq a^2 + b^2 \qquad \forall a, b > 0$$

and

$$ab = \Big(\frac{1}{\epsilon}a\Big)(\epsilon b) \leq \Big(\frac{a}{\epsilon}\Big)^2 + (\epsilon b)^2 \qquad \forall a, b > 0.$$

Then, we have for any $x \in [0, \infty)$ and $\epsilon > 0$,

$$\begin{aligned}|\phi(x)||\phi'(x)| \leq &\Big(\|\phi\|_{L^2((0,\infty))}\epsilon^{-1/2} + \frac{2}{3}\|\phi'\|_{L^2((0,\infty))}\epsilon^{1/2}\Big)\Big(\|\phi'\|_{L^2((0,\infty))} + \frac{2}{3}\|\phi''\|_{L^2((0,\infty))}\Big)\\ = &\epsilon^{-1/2}\|\phi\|_{L^2((0,\infty))}\|\phi'\|_{L^2((0,\infty))} + \frac{2}{3}\epsilon^{-1/2}\|\phi\|_{L^2((0,\infty))}\|\phi''\|_{L^2((0,\infty))}\\ &+ \frac{2}{3}\epsilon^{1/2}\|\phi'\|^2_{L^2((0,\infty))} + \frac{4}{9}\epsilon^{1/2}\|\phi'\|_{L^2((0,\infty))}\|\phi''\|_{L^2((0,\infty))}\\ \leq &\big(\epsilon^{-1}\|\phi\|_{L^2((0,\infty))}\big)^2 + \big(\epsilon^{1/2}\|\phi'\|_{L^2((0,\infty))}\big)^2 + \frac{2}{3}\epsilon^{-1/2}\big(\|\phi\|^2_{L^2((0,\infty))} + \|\phi''\|^2_{L^2((0,\infty))}\big)\\ &+ \frac{2}{3}\epsilon^{1/2}\|\phi'\|^2_{L^2((0,\infty))} + \frac{4}{9}\epsilon^{1/2}\big(\|\phi'\|^2_{L^2((0,\infty))} + \|\phi''\|^2_{L^2((0,\infty))}\big)\\ = &\|\phi\|^2_{L^2((0,\infty))}\Big(\epsilon^{-2} + \frac{2}{3}\epsilon^{-1/2}\Big) + \|\phi'\|^2_{L^2((0,\infty))}\Big(\epsilon + \frac{10}{9}\epsilon^{1/2}\Big)\\ &+ \|\phi''\|^2_{L^2((0,\infty))}\Big(\frac{2}{3}\epsilon^{-1/2} + \frac{4}{9}\epsilon^{1/2}\Big)\\ = &\alpha\|\phi\|^2_{L^2((0,\infty))} + \beta\|\phi'\|^2_{L^2((0,\infty))} + \gamma\|\phi''\|^2_{L^2((0,\infty))},\end{aligned}$$

that is to say,

$$|\phi(x)||\phi'(x)| \leq \alpha\|\phi\|^2_{L^2((0,\infty))} + \beta\|\phi'\|^2_{L^2((0,\infty))} + \gamma\|\phi''\|^2_{L^2((0,\infty))} \tag{8}$$

where $\alpha := \epsilon^{-2} + \frac{2}{3}\epsilon^{-1/2}, \beta := \epsilon + \frac{10}{9}\epsilon^{1/2}$ and $\gamma = \frac{2}{3}\epsilon^{-1/2} + \frac{4}{9}\epsilon^{1/2}$. Consider $\epsilon > 0$ such that $2\beta < 1$.

Take $N \in \mathbb{N}$ and compute the next inequality using (8):

$$\begin{aligned}
\int_0^N |\phi'|^2 =& \phi'\overline{\phi}\Big|_0^N - \int_0^N \phi''\overline{\phi} \\
\leq& |\phi'(N)||\phi(N)| + |\phi'(0)||\phi(0)| + \|\phi''\|_{L^2((0,\infty))}\|\phi\|_{L^2((0,\infty))} \\
\leq& |\phi'(N)||\phi(N)| + |\phi'(0)||\phi(0)| + \frac{1}{2}\big(\|\phi''\|^2_{L^2((0,\infty))} + \|\phi\|^2_{L^2((0,\infty))}\big) \\
\leq& 2\big(\alpha\|\phi\|^2_{L^2((0,\infty))} + \beta\|\phi'\|^2_{L^2((0,\infty))} + \gamma\|\phi''\|^2_{L^2((0,\infty))}\big) + \|\phi''\|^2_{L^2((0,\infty))} + \|\phi\|^2_{L^2((0,\infty))}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\|\phi'\|^2_{L^2((0,\infty))} =& \lim_{N\to\infty}\int_0^N |\phi'|^2 \\
\leq& 2\big(\alpha\|\phi\|^2_{L^2((0,\infty))} + \beta\|\phi'\|^2_{L^2((0,\infty))} + \gamma\|\phi''\|^2_{L^2((0,\infty))}\big) + \|\phi''\|^2_{L^2((0,\infty))} + \|\phi\|^2_{L^2((0,\infty))},
\end{aligned}$$

which implies

$$\begin{aligned}
\|\phi'\|^2_{L^2((0,\infty))} \leq& \frac{1}{1-2\beta}\big((2\alpha+1)\|\phi\|^2_{L^2((0,\infty))} + (2\gamma+1)\|\phi''\|^2_{L^2((0,\infty))}\big) \\
\leq& \bar{C}\big(\|\phi\|^2_{L^2((0,\infty))} + \|\phi''\|^2_{L^2((0,\infty))}\big),
\end{aligned}$$

where $\bar{C} = \max\{\frac{2\alpha+1}{1-2\beta}, \frac{2\gamma+1}{1-2\beta}\}$. Finally, from the fact that

$$a^2 + b^2 \leq (a+b)^2 \qquad \forall a, b \geq 0,$$

follows

$$\|\phi'\|_{L^2((0,\infty))} \leq \bar{C}^{1/2}\big(\|\phi\|_{L^2((0,\infty))} + \|\phi''\|_{L^2((0,\infty))}\big).$$

By letting $\widetilde{C} := 1 + \bar{C}^{1/2}$ we obtain the desired result. □

Theorem 1.3.5. *Suppose that $f \in L^2\big((0,\infty)\big)$ is such that $\Delta T_f = T_g$, for some $g \in L^2\big((0,\infty)\big)$. Then $f \in H^2\big((0,\infty)\big)$.*

PROOF. By Lemma 1.3.3, there is a sequence of functions $(\phi_n)_{n\in\mathbb{N}}$ on $C^\infty\big((0,\infty)\big)$ satisfying

$$\lim_{n\to\infty} \|\phi_n - f\|_{L^2((0,\infty))} + \|\Delta\phi_n - g\|_{L^2((0,\infty))} = 0,$$

which implies that

$$\lim_{m,n\to\infty} \|\phi_n - \phi_m\|_{L^2((0,\infty))} + \|\Delta\phi_n - \Delta\phi_m\|_{L^2((0,\infty))} = 0.$$

From Lemma 1.3.4 we have

$$\|\phi_n - \phi_m\|_{H^2((0,\infty))} \leq C\Big[\|\phi_n - \phi_m\|_{L^2((0,\infty))} + \|\Delta\phi_n - \Delta\phi_m\|_{L^2((0,\infty))}\Big],$$

which implies that

$$\lim_{m,n\to\infty} \|\phi_n - \phi_m\|_{H^2((0,\infty))} = 0.$$

Thus, $(\phi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in $H^2\big((0,\infty)\big)$. Since $H^2((0,\infty))$ is complete, there exists $h \in H^2\big((0,\infty)\big)$ such that

$$h = \lim_{n\to\infty} \phi_n.$$

But $f = \lim_{n\to\infty} \phi_n$ in L^2, then we have $f = h$ (maybe except on a null set). We conclude $f \in H^2\big((0,\infty)\big)$.

□

Corollary 1.3.6. *The domain of $\big(\Delta; C_0^\infty((0,\infty))\big)^*$ is a subset of $H^2\big((0,\infty)\big)$.*

PROOF. It follows from Equation (4) and Theorem 1.3.5.

□

Corollary 1.3.7. *If $C_0^\infty((0,\infty)) \leq \mathsf{Dom}(\Delta)$, then the domain of $(\Delta, \mathsf{Dom}(\Delta))^*$ is a subset of $H^2((0,\infty))$.*

PROOF. Recall that if A and B are two operators such that $\mathsf{Dom}(A) \subset \mathsf{Dom}(B)$, then $\mathsf{Dom}(B^*) \subset \mathsf{Dom}(A^*)$. Then the result follows from the containment

$$C_0^\infty((0,\infty)) \subset \mathsf{Dom}(\Delta),$$

and the Corollary 1.3.6. □

To prove the second case (i.e. when e has finite length), let us obtain analogous results for functions in $L^2((0,b))$, where $b < \infty$. Similarly, we have the property of the elements of the domain of $(\Delta; C_0^\infty((0,b)))^*$:

$$f \in \mathsf{Dom}(\Delta^*) \iff \exists g \in L^2((0,b))\colon \langle f, \Delta h\rangle = \langle g, h\rangle \quad \forall h \in \mathsf{Dom}(\Delta)$$

$$\iff \int_{(0,b)} f \cdot \Delta h = \int_{(0,b)} g \cdot h \quad \forall h \in C_0^\infty((0,b)) \iff T_g = \Delta T_f, \tag{9}$$

where T_g and ΔT_f are the distributions which satisfy

$$T_g(h) = \int_{(0,b)} g(x)h(x)dx \qquad \forall h \in C_0^\infty((0,b))$$

and

$$\Delta T_f(h) = \int_{(0,b)} f(x)\Delta h(x)dx \qquad \forall h \in C_0^\infty((0,b)),$$

respectively.

Proposition 1.3.8. *Let $\epsilon \in (-1/2, \infty)$ and define $E_\epsilon(f)(x) := f\big(\frac{x}{1+2\epsilon}\big)$. Then for every $f \in L^p(\mathbb{R})$*

$$\|E_\epsilon(f) - f\|_p \to 0 \qquad as \quad \epsilon \to 0.$$

Proof. As the set of finite linear combinations of characteristic functions of intervals is dense in L^p, take ϕ a finite linear combination of characteristics functions of intervals, such that $\|f - \phi\|_p$ is enough small. Without loss of generality, we only consider characteristic functions of open intervals. For each interval (a, b), we have two different cases for the homothety $E_\epsilon(\chi_{(a,b))})$ depending on $(1+2\epsilon)$. First consider that $0 < (1+2\epsilon) < 1$, then $a(1+2\epsilon) < a \le b(1+2\epsilon) < b$. This implies that

$$\|E_\epsilon(\chi_{(a,b)}) - \chi_{(a,b)}\|_p \le (|a2\epsilon| + |b2\epsilon|)^{1/p} \underset{\epsilon\to 0}{\longrightarrow} 0, \tag{10}$$

since the function $E_\epsilon(\chi_{(a,b)}) - \chi_{(a,b)}$ is different from zero only in the intervals $(a(1+2\epsilon), a]$ and $[b(1+2\epsilon), b)$.

On the other hand, if $(1+2\epsilon) \ge 1$, then $a \le a(1+2\epsilon) \le b \le b(1+2\epsilon)$. Similarly, we obtain (10).

Thus, as ϕ is a finite linear combination of characteristics functions of intervals, we have

$$\|E_\epsilon(\phi) - \phi\|_p \underset{\epsilon\to 0}{\longrightarrow} 0.$$

But then,

$$\begin{aligned}\|E_\epsilon(f) - f\|_p &\le \|E_\epsilon(f) - E_\epsilon(\phi)\|_p + \|E_\epsilon(\phi) - \phi\|_p + \|\phi - f\|_p \\ &= (1 + (1+2\epsilon)^{1/p})\|f - \phi\|_p + \|E_\epsilon(\phi) - \phi\|_p \underset{\epsilon\to 0}{\longrightarrow} 0.\end{aligned}$$

∎

The proof of the following Lemma is similar to that in Lemma 1.3.3.

Lemma 1.3.9. *Let $f, g \in L^2((0,b))$ such that $\Delta T_f = T_g$. Then, for all $\epsilon > 0$, there is a function $\phi \in C^\infty([0,b])$ satisfying $\|f - \phi\|_{L^2((0,b))} < \epsilon$ and $\|g - \Delta\phi\|_{L^2((0,b))} < \epsilon$.*

Proof. For any $\delta, \epsilon > 0$, we define functions $\tau_\epsilon E_\delta(f), \tau_\epsilon E_\delta(g) : [-\epsilon, b(1+2\delta) - \epsilon] \to \mathbb{R}$ as follows:

$$\tau_\epsilon E_\delta(f)(x) = f\Big(\frac{x+\epsilon}{1+2\delta}\Big), \qquad \tau_\epsilon E_\delta(g)(x) = g\Big(\frac{x+\epsilon}{1+2\delta}\Big). \tag{11}$$

It is easy to see that $\tau_\epsilon E_\delta(f), \tau_\epsilon E_\delta(g) \in L^2([-\epsilon, b(1+2\delta)-\epsilon])$. We extend these functions to $\mathbb{R}$, whitout changing notation, defining them as 0 in $(-\infty, -\epsilon) \cup (b(1+2\delta) - \epsilon, \infty)$. By propositions (1.3.1) and (1.3.8), there are $\epsilon_1 > 0$ and $\delta_0 > 0$ such that $\epsilon_1 < 2b\delta_0$ and

$$\|\tau_{\epsilon_1} E_{\delta_0}(f) - f\|_{L^2(\mathbb{R})} < \epsilon/2, \qquad \|\tau_{\epsilon_1} E_{\delta_0}(g) - g\|_{L^2(\mathbb{R})} < \epsilon/2. \tag{12}$$

It follows from Lemma 1.3.2 that there is $\epsilon_0 \in (0, \epsilon_1)$ such that $\epsilon_0 + \epsilon_1 < 2b\delta_0$ and

$$\|\tau_{\epsilon_1} E_{\delta_0}(f) * \eta_{\epsilon_0} - \tau_{\epsilon_1} E_{\delta_0}(f)\|_{L^2(\mathbb{R})} < \epsilon/2, \qquad \|\tau_{\epsilon_1} E_{\delta_0}(g) * \eta_{\epsilon_0} - \tau_{\epsilon_1} E_{\delta_0}(g)\|_{L^2(\mathbb{R})} < \epsilon/2. \tag{13}$$

Thus, if we define

$$\phi := \tau_{\epsilon_1} E_{\delta_0}(f) * \eta_{\epsilon_0},$$

by Equations (12) and (13) we have

$$\|f - \phi\|_{L^2((0,b))} \le \|f - \tau_{\epsilon_1} E_{\delta_0}(f)\|_{L^2((0,b))} + \|\tau_{\epsilon_1} E_{\delta_0}(f) - \phi\|_{L^2((0,b))} < \epsilon.$$

Now let us see that

$$\Delta(\tau_{\epsilon_1} E_{\delta_0}(f) * \eta_{\epsilon_0}) = \Delta\tau_{\epsilon_1} E_{\delta_0}(f) * \eta_{\epsilon_0} = \tau_{\epsilon_1} E_{\delta_0}(g) * \eta_{\epsilon_0},$$

on $[\epsilon_0 - \epsilon_1, b(1+2\delta) - \epsilon_0 - \epsilon_1]$. From Lemma 1.3.2,

$$\Delta(\tau_{\epsilon_1} E_{\delta_0}(f) * \eta_{\epsilon_0}) = \tau_{\epsilon_1} E_{\delta_0}(f) * \Delta\eta_{\epsilon_0}.$$

Let $T_{E_{\delta_0}(f)}$ the distribution on $(0, b(1+2\delta_0))$ corresponding to $E_{\delta_0}(f)$. In the same way we definine $T_{E_{\delta_0}(g)}$. We will show that $\Delta T_{E_{\delta_0}(f)} = T_{E_{\delta_0}(g)}$. Let $u \in C_0^\infty\big[(0, b(1+2\delta_0))\big]$, then

$$\begin{aligned}\Delta T_{E_{\delta_0}(f)}(u) &= \int_{(0,b(1+2\delta_0))} E_{\delta_0}(f)\Delta u = (1+2\delta)\int_{(0,b)} f(x)\Delta u(x(1+2\delta))dx \\ &= (1+2\delta)\Delta T_f[u(x(1+2\delta))] = (1+2\delta)T_g[u(x(1+2\delta))] \\ &= \int_{(0,b(1+2\delta))} g\Big(\frac{x}{1+2\delta}\Big)u(x)dx = T_{E_{\delta_0}(g)}(u).\end{aligned}$$

since $u(x(1+2\delta)) \in C_0^\infty\big[(0,b)\big]$. Our next goal is to prove $\tau_{\epsilon_1}E_{\delta_0}(f) * \Delta\eta_{\epsilon_0} = \tau_{\epsilon_1}E_{\delta_0}(g) * \eta_{\epsilon_0}$ as functions on $[\epsilon_0 - \epsilon_1, b(1+2\delta) - \epsilon_0 - \epsilon_1]$. Take $x \in [\epsilon_0 - \epsilon_1, b(1+2\delta) - \epsilon_0 - \epsilon_1]$, then

$$
\begin{aligned}
\tau_{\epsilon_1}E_{\delta_0}(f) * \Delta\eta_{\epsilon_0}(x) = &\int_{\mathbb{R}} \tau_{\epsilon_1}E_{\delta_0}(f)(y)\Delta\eta_{\epsilon_0}(x-y)dy = \int_{\mathbb{R}} \tau_{\epsilon_1}E_{\delta_0}(f)(y)\Delta\eta_{\epsilon_0}(y-x)dy \\
= &\int_{\mathbb{R}} E_{\delta_0}(f)(y)\Delta\tau_{-\epsilon_1-x}\eta_{\epsilon_0}(y)dy = T_{E_{\delta_0}(g)}(\tau_{-\epsilon_1-x}(\eta_{\epsilon_0})) \\
=&T_{\tau_{\epsilon_1}E_{\delta_0}(g)}(\tau_{-x}(\eta_{\epsilon_0})) = \tau_{\epsilon_1}E_{\delta_0}(g) * \eta_{\epsilon_0}(x),
\end{aligned}
$$

where we used that $\tau_{-\epsilon_1-x}(\eta_{\epsilon_0}) \in C_0^\infty((0, b(1+2\delta_0)))$.

Due to $[0,b] \subset [\epsilon_0 - \epsilon_1, b(1+2\delta_0) - \epsilon_0 - \epsilon_1]$, by Equations (12) y (13) we obtain

$$
\begin{aligned}
\|g - \Delta\phi\|_{L^2((0,b))} \leq &\|g - \tau_{\epsilon_1}E_{\delta_0}(g)\|_{L^2((0,b))} + \|\tau_{\epsilon_1}E_{\delta_0}(g) - \Delta\phi\|_{L^2((0,b))} \\
= &\|g - \tau_{\epsilon_1}E_{\delta_0}(g)\|_{L^2((0,b))} + \|\tau_{\epsilon_1}E_{\delta_0}(g) - \tau_{\epsilon_1}E_{\delta_0}(g) * \eta_{\epsilon_0}\|_{L^2((0,b))} < \epsilon.
\end{aligned}
$$

$\square$

Lemma 1.3.10. *Let $\phi \in C^\infty([0,b])$. Then there is $\widetilde{C} > 0$ such that*

$$\|\phi\|_{H^2((0,b))} \leq \widetilde{C}(\|\phi\|_{L^2((0,b))} + \|\Delta\phi\|_{L^2((0,b))}).$$

Proof. Let $x \in [0,b]$. Notice that

$$\phi(x+y) - \phi(x) = \int_x^{x+y} \phi' \qquad \forall y \in (-x, b-x).$$

Thus, using Cauchy-Schwarz inequality,

$$|\phi(x)| \leq |\phi(x+y)| + \Big(\int_x^{x+y} |\phi'|^2\Big)^{1/2} |y|^{1/2} \qquad \forall y \in (-x, b-x).$$

Let $|\epsilon| < b/2$. By integrating we obtain,

$$
\begin{aligned}
|\epsilon| \cdot |\phi(x)| \leq &\int_0^\epsilon |\phi(x+y)|dy + \frac{2}{3}\|\phi'\|_{L^2((0,b))}|\epsilon|^{3/2} \\
\leq &\int_x^{x+\epsilon} |\phi(y)|dy + \frac{2}{3}\|\phi'\|_{L^2((0,b))}|\epsilon|^{3/2} \\
\leq &\|\phi\|_{L^2((0,b))}|\epsilon|^{1/2} + \frac{2}{3}\|\phi'\|_{L^2((0,b))}|\epsilon|^{3/2}.
\end{aligned}
$$

where we choose $\epsilon \in (0, b/2)$ if $x \leq b/2$ and $\epsilon \in (-b/2, 0)$ if $x > b/2$. Then we have,

$$|\phi(x)| \leq \|\phi\|_{L^2((0,b))}|\epsilon|^{-1/2} + \frac{2}{3}\|\phi'\|_{L^2((0,b))}|\epsilon|^{1/2}.$$

Let us recall that

$$ab \le \frac{1}{2}(a^2 + b^2) \le a^2 + b^2 \qquad \forall a, b > 0$$

and

$$ab = \Big(\frac{1}{|\epsilon|}a\Big)(|\epsilon|b) \le \Big(\frac{a}{|\epsilon|}\Big)^2 + (|\epsilon|b)^2 \qquad \forall a, b > 0.$$

Using these last inequalities and considering real numbers κ with $|\kappa| = b/4$, we obtain

$$\begin{aligned}
|\phi(x)||\phi'(x)| \le& (\|\phi\|_{L^2((0,b))}|\epsilon|^{-1/2} + \frac{2}{3}\|\phi'\|_{L^2((0,b))}|\epsilon|^{1/2})(\|\phi'\|_{L^2((0,b))}|\kappa|^{-1/2} + \frac{2}{3}\|\phi''\|_{L^2((0,b))}|\kappa|^{1/2}) \\
=& |\epsilon|^{-1/2}|\kappa|^{-1/2}\|\phi\|_{L^2((0,b))}\|\phi'\|_{L^2((0,b))} + \frac{2}{3}|\epsilon|^{-1/2}|\kappa|^{1/2}\|\phi\|_{L^2((0,b))}\|\phi''\|_{L^2((0,b))} \\
&+ \frac{2}{3}|\epsilon|^{1/2}|\kappa|^{-1/2}\|\phi'\|^2_{L^2((0,b))} + \frac{4}{9}|\epsilon|^{1/2}|\kappa|^{1/2}\|\phi'\|_{L^2((0,b))}\|\phi''\|_{L^2((0,b))} \\
\le& (|\epsilon|^{-1}|\kappa|^{-1/2}\|\phi\|_{L^2((0,b))})^2 + (|\epsilon|^{1/2}\|\phi'\|_{L^2((0,b))})^2 + \frac{2}{3}(|\epsilon|^{-1}\|\phi\|^2_{L^2((0,b))} + |\kappa|\|\phi''\|^2_{L^2((0,b))}) \\
&+ \frac{2}{3}|\epsilon|^{1/2}|\kappa|^{-1/2}\|\phi'\|^2_{L^2((0,b))} + \frac{4}{9}(|\epsilon|\|\phi'\|^2_{L^2((0,b))} + |\kappa|\|\phi''\|^2_{L^2((0,b))}) \\
=& \Big(|\epsilon|^{-2}|\kappa|^{-1} + \frac{2}{3}|\epsilon|^{-1}\Big)\|\phi\|^2_{L^2((0,b))} + \Big(\frac{13}{9}|\epsilon| + \frac{2}{3}|\epsilon|^{1/2}|\kappa|^{-1/2}\Big)\|\phi'\|^2_{L^2((0,b))} \\
&+ \|\phi''\|^2_{L^2((0,b))}\Big(\frac{10}{9}|\kappa|\Big) \\
=& \alpha\|\phi\|^2_{L^2((0,b))} + \beta\|\phi'\|^2_{L^2((0,b))} + \gamma\|\phi''\|^2_{L^2((0,b))},
\end{aligned}$$

where $\alpha := |\epsilon|^{-2}|\kappa|^{-1} + \frac{2}{3}|\epsilon|^{-1}, \beta := \frac{13}{9}|\epsilon| + \frac{2}{3}|\epsilon|^{1/2}|\kappa|^{-1/2}$ and $\gamma = \frac{10}{9}|\kappa|$. Choose $\epsilon > 0$ such that $2\beta < 1$.

Now we calculate,

$$\begin{aligned}
\int_0^b |\phi'|^2 =& \phi'\overline{\phi}\Big|_0^b - \int_0^b \phi''\overline{\phi} \\
\le& |\phi'(b)||\overline{\phi}(b)| + |\phi'(0)||\overline{\phi}(0)| + \|\phi''\|_{L^2((0,b))}\|\phi\|_{L^2((0,b))} \\
\le& |\phi'(b)||\overline{\phi}(b)| + |\phi'(0)||\overline{\phi}(0)| + \frac{1}{2}\big(\|\phi''\|^2_{L^2((0,b))} + \|\phi\|^2_{L^2((0,b))}\big) \\
\le& 2\big(\alpha\|\phi\|^2_{L^2((0,b))} + \beta\|\phi'\|^2_{L^2((0,b))} + \gamma\|\phi''\|^2_{L^2((0,b))}\big) + \|\phi''\|^2_{L^2((0,b))} + \|\phi\|^2_{L^2((0,b))}.
\end{aligned}$$

Thereby,

$$\|\phi'\|^2_{L^2((0,b))} = \int_0^b |\phi'|^2 \leq 2\big(\alpha\|\phi\|^2_{L^2((0,b))} + \beta\|\phi'\|^2_{L^2((0,b))} + \gamma\|\phi''\|^2_{L^2((0,b))}\big) + \|\phi''\|^2_{L^2((0,b))} + \|\phi\|^2_{L^2((0,b))}.$$

This last inequality implies

$$\begin{aligned}\|\phi'\|^2_{L^2((0,b))} \leq & \frac{1}{1-2\beta}\big((2\alpha+1)\|\phi\|^2_{L^2((0,b))} + (2\gamma+1)\|\phi''\|^2_{L^2((0,b))}\big)\\ \leq & \bar{C}\big(\|\phi\|^2_{L^2((0,b))} + \|\phi''\|^2_{L^2((0,b))}\big),\end{aligned}$$

where $\bar{C} = \max\{\frac{2\alpha+1}{1-2\beta}, \frac{2\gamma+1}{1-2\beta}\}$. Finally, using the fact that

$$a^2 + b^2 \leq (a+b)^2 \qquad \forall a, b \geq 0,$$

we have

$$\|\phi'\|_{L^2((0,b))} \leq \bar{C}^{1/2}\big(\|\phi\|_{L^2((0,b))} + \|\phi''\|_{L^2((0,b))}\big).$$

Letting $\widetilde{C} := 1 + \bar{C}^{1/2}$ we obtain the desired result. □

Theorem 1.3.11. *Suppose that $f \in L^2\big((0,b)\big)$ is such that $\Delta T_f = T_g$ for some $g \in L^2\big((0,b)\big)$. Then $f \in H^2\big((0,b)\big)$.*

Proof. By Lemma 1.3.9 there exists a sequence of functions $(\phi_n)_{n\in\mathbb{N}}$ in $C^\infty\big((0,b)\big)$ such that

$$\lim_{n\to\infty} \|\phi_n - f\|_{L^2((0,b))} + \|\Delta\phi_n - g\|_{L^2((0,b))} = 0,$$

implying that

$$\lim_{m,n\to\infty} \|\phi_n - \phi_m\|_{L^2((0,b))} + \|\Delta\phi_n - \Delta\phi_m\|_{L^2((0,b))} = 0.$$

According to Lemma 1.3.10, there is $C > 0$ such that

$$\|\phi_n - \phi_m\|_{H^2\left((0,b)\right)} \leq C\Big[\|\phi_n - \phi_m\|_{L^2((0,b))} + \|\Delta\phi_n - \Delta\phi_m\|_{L^2((0,b))}\Big],$$

thus

$$\lim_{m,n\to\infty} \|\phi_n - \phi_m\|_{H^2((0,b))} = 0.$$

Then $(\phi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in $H^2\big((0,b)\big)$. Since $H^2((0,b))$ is complete, there exists $h \in H^2\big((0,b)\big)$ such that

$$h = \lim_{n\to\infty} \phi_n.$$

But $f = \lim_{n\to\infty} \phi_n$ in L^2, then $f = h$ (maybe except on a null set). Hence $f \in H^2\big((0,b)\big)$.

□

Corollary 1.3.12. *The domain of* $\big(\Delta; C_0^\infty((0,b))\big)^*$ *is a subset of* $H^2\big((0,b)\big)$.

Proof. It follows from Equation (9) and Theorem 1.3.11. □

Corollary 1.3.13. *If* $C_0^\infty((0,b)) \leq \mathsf{Dom}(\Delta)$*, then domain of* $(\Delta, \mathsf{Dom}(\Delta))^*$ *is a subset of* $H^2((0,b))$.

Proof. The result follows from the containment

$$C_0^\infty((0,b)) \subset \mathsf{Dom}(\Delta),$$

and the Corollary 1.3.12.

□

1.4. Quantum Graphs and the Laplacian on Metric Graphs

Definition 1.4.1. *A* ***quantum graph*** *is a metric graph* Γ *with a self-adjoint differential operator* $\mathcal{H}$ *(called Hamiltonian) in a space of functions defined on* Γ.

In this work, we will consider the Hamiltonian to be the Laplacian operator Δ, i.e. the negative second order distributional derivate of functions which take values at each edge of the graph. But for the self-adjointness of Δ, we will need to impose some **vertex conditions** to these functions.

Notice that for the Laplacian

$$f(x) \mapsto -\frac{d^2 f}{dx^2}$$

the direction of the coordinate is irrelevant since $\Delta f(x) = \Delta f(-x)$ for all $x \in \mathbb{R}$, so the direction on which the derivate is taken in each edge is not relevant.

As the operator involves a second distributional derivate, we will assume that the functions of the domain of Δ belong to the Sobolev space $H^2(\Gamma)$. We will give some **local vertex conditions** for the self-adjointness of the Laplacian, so henceforth we only consider parts of the graph which are star graphs (see Figure 1).

Consider $f \in H^2(\Gamma)$ and any vertex v of Γ. As we suppose that the degree of each vertex is finite, we can enumerate all the neighbours of v and all the edges between v and its neighbours, i.e., there exist a subset of vertices $\{u_1, u_2, \ldots, u_{d_v}\} \subset \mathcal{V}$ and some edges $\{e_1, e_2, \ldots, e_{d_v}\} \subset \mathcal{E}$ such that $v \in e_i$ and $u_i \in e_i$ for every $i = 1, 2, \ldots, d_v$. Also, we establish that f_i refers to the restriction f_{e_i} for $i = 1, 2, \ldots, d_v$. Then, we can denote by $F(v)$ the vector

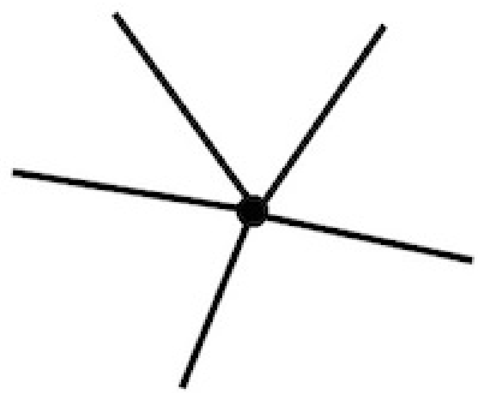

FIGURE 1. Star graph.

column

$$F(v) := (f_1(v), \dots, f_{d_v}(v))^t = \begin{pmatrix} f_1(v) \\ \cdots \\ \cdots \\ f_{d_v}(v) \end{pmatrix}. \tag{14}$$

and, similarly,

$$F'(v) := (f'_1(v), \dots, f'_{d_v}(v))^t = \begin{pmatrix} f'_1(v) \\ \cdots \\ \cdots \\ f'_{d_v}(v) \end{pmatrix}. \tag{15}$$

Note 1.4.2. *As $f \in H^1(\Gamma)$, by the Trace Theorem for Sobolev spaces (see [12], p. 258), F and F' are well defined on v. Thus, the boundary conditions will be given just considering the values which take the function f and its distributional derivate df/dx on the vertices v.*

Lemma 1.4.3. *Let A and B matrices of $d \times d$ satisfying the following conditions:*

$$\text{the matrix} \quad (A|B) \in Mat_{d\times 2d} \quad \text{has maximal rank,} \tag{16}$$

$$\text{the matrix} \quad AB^* \quad \text{is self-adjoint.} \tag{17}$$

Then, for any real $k \neq 0$, the matrix $A + ikB$ is invertible and $\sigma(k) = -(A + ikB)^{-1}(A - ikB)$ is a unitary matrix.

PROOF. Condition (17) implies that $AB^* = (AB^*)^* = BA^*$, then

$$
\begin{aligned}
(A+ikB)(A^*-ikB^*) &= AA^* - ikAB^* + ikBA^* + k^2BB^* \qquad (18)\\
&= AA^* + k^2BB^* \qquad (19)\\
&= (A-ikB)(A^*+ikB^*)\\
&= (A|kB)\begin{pmatrix} A^* \\ kB^* \end{pmatrix},
\end{aligned}
$$

where $(A|kB)$ denotes the matrix $d_v \times 2d_v$ composed by A and kB. Now note that $(A+ikB)^* = (A^*-ikB^*)$ and, due to the fact that $\mathsf{rank}(TT^*) = \mathsf{rank}(T)$ for any finite matrix T (see [13], section 6.4, exercise 18), we can demonstrate that $A+ikB$ has maximal rank:

$$
\begin{aligned}
\mathsf{rank}(A+ikB) &= \mathsf{rank}((A+ikB)(A^*-ikB^*))\\
&= \mathsf{rank}\Big((A|kB)\begin{pmatrix} A^* \\ kB^* \end{pmatrix}\Big)\\
&= \mathsf{rank}((A|kB)(A|kB)^*)\\
&= \mathsf{rank}((A|kB)) = d_v.
\end{aligned}
$$

Therefore, $A+ikB$ is invertible and the matrix $\sigma(k)$ is well defined.

Following the same reasoning we get that the matrix $(A-ikB)$ is invertible, then, also its adjoint (A^*+ikB^*) is invertible. Using Equation (18) we have

$$
\begin{aligned}
\sigma(k) &= -(A+ikB)^{-1}(A-ikB)\\
&= -(A+ikB)^{-1}(A-ikB)(A^*+ikB^*)(A^*+ikB^*)^{-1}\\
&= -(A+ikB)^{-1}(A+ikB)(A^*-ikB^*)(A^*+ikB^*)^{-1}\\
&= -(A^*-ikB^*)(A^*+ikB^*)^{-1}.
\end{aligned}
$$

Thus, we can verify that $\sigma(k)$ is unitary :

$$
\begin{aligned}
\sigma(k)\sigma(k)^* &= -(A^*-ikB^*)(A^*+ikB^*)^{-1}[-(A+ikB)^{-1}(A-ikB)]^*\\
&= (A^*-ikB^*)(A^*+ikB^*)^{-1}(A-ikB)^*[(A+ikB)^{-1}]^*\\
&= (A^*-ikB^*)(A^*+ikB^*)^{-1}(A^*+ikB^*)[(A+ikB)^*]^{-1}\\
&= (A^*-ikB^*)(A^*-ikB^*)^{-1} = \mathbb{I},
\end{aligned}
$$

and similarly,

$$\begin{aligned}\sigma(k)^*\sigma(k) &= [-(A+ikB)^{-1}(A-ikB)]^*[-(A^*-ikB^*)(A^*+ikB^*)^{-1}]\\ &= (A-ikB)^*[(A+ikB)^{-1}]^*(A^*-ikB^*)(A^*+ikB^*)^{-1}\\ &= (A^*+ikB^*)[(A+ikB)^*]^{-1}(A^*-ikB^*)(A^*+ikB^*)^{-1}\\ &= (A^*+ikB^*)(A^*-ikB^*)^{-1}(A^*-ikB^*)(A^*+ikB^*)^{-1}\\ &= (A^*+ikB^*)(A^*+ikB^*)^{-1} = \mathbb{I}.\end{aligned}$$

□

Note 1.4.4. *We do not consider the point at infinity as a vertex, so edges with infinite length do not have more than one vertex.*

In the following lemmas, we will give some equivalent descriptions of the domain of Δ in terms of *vertex conditions*, which are necessary and sufficient to guarantee the self-adjointness of the Laplacian operator.

Besides, as all the conditions are local, we will consider only one vertex v and a vicinity of it where the graph is like a star graph. Thus, in the demonstrations, we avoid de notation $A_v, B_v, d_v, F(v), F'(v), \ldots$ and instead we use $A, B, d, F, F', \ldots$, respectively.

Lemma 1.4.5. *Let Γ be a metric graph with finite number of edges. For every vertex $v \in \mathcal{V}$, take A_v and B_v matrices $d_v \times d_v$ such that*

$$(A_v|B_v) \in \mathsf{Mat}_{d_v\times 2d_v} \quad \text{has maximal rank and}$$

$$A_vB_v^* \quad \text{is self-adjoint.}$$

Furthermore, define for every vertex $v \in \mathcal{V}$

$$U_v = -(A-ikB)^{-1}(A+ikB) \in \mathsf{Mat}_{d_v\times d_v}.$$

Then, U_v is a unitary matrix for every v and

$$\{f \in H^2(\Gamma)\colon A_vF(v) + B_vF'(v) = 0 \quad \forall v \in \mathcal{V}\} =$$

$$\{f \in H^2(\Gamma)\colon i(U_v - \mathbb{I})F(v) + (U_v + \mathbb{I})F'(v) = 0 \quad \forall v \in \mathcal{V}\},$$

where $\mathbb{I} \in \mathsf{Mat}_{d_v\times d_v}$ is the identity matrix.

Proof. Using Lemma 1.4.3, notice that

$$\begin{aligned}-2i(A+ikB)^{-1}A &= -2i(A+ikB)^{-1}\frac{1}{2}((A-ikB)+(A+ikB))\\ &= i(\sigma(k)-\mathbb{I}),\end{aligned}$$

where the matrix $\sigma(k) = -(A + ikB)^{-1}(A - ikB)$ is unitary for every real $k \neq 0$ according to Lemma 1.4.3. Similarly,

$$\begin{aligned}-2i(A+ikB)^{-1}B &= -2i(A+ikB)^{-1}\frac{1}{2ik}((A+ikB)-(A-ikB)) \\ &= -\frac{1}{k}(\mathbb{I}+\sigma(k)).\end{aligned}$$

From these equalities follows that

$$\begin{aligned}&AF + BF' = 0 \\ \iff& -2i(A+ikB)^{-1}(AF+BF') = 0 \\ \iff& i(\sigma(k)-\mathbb{I})F - \frac{1}{k}(\mathbb{I}+\sigma(k))F' = 0.\end{aligned}$$

Taking $k = -1$ we obtain

$$\begin{aligned}&AF + BF' = 0 \\ \iff& i(U-\mathbb{I})F + (U+\mathbb{I})F' = 0,\end{aligned}$$

where $U = \sigma(-1)$ is unitary. □

Lemma 1.4.6. *Let Γ be a metric graph with finite number of edges. For every vertex v of Γ consider a unitary matrix $U_v \in \mathsf{Mat}_{d_v\times d_v}$. Let $P_{D,v}$ and $P_{N,v}$ be the orthogonal projectors onto the eigenspaces of the matrix U_v with eigenvalues -1 and $+1$, respectively, and $P_{R,v} := \mathbb{I} - P_{D,v} - P_{N,v}$. Furthermore, we define $\Lambda_v : P_{R,v}[\mathbb{C}^{d_v}] \to P_{R,v}[\mathbb{C}^{d_v}]$ by*

$$\Lambda_v := -i\Big(P_{R,v}(U_v+\mathbb{I})P_{R,v}\Big)^{-1}P_{R,v}(U_v-\mathbb{I})P_{R,v}.$$

Then Λ_v is invertible and self-adjoint and

$$\begin{aligned}&\{f \in H^2(\Gamma) \colon i(U_v-\mathbb{I})F(v) + (U_v+\mathbb{I})F'(v) = 0 \quad \forall v \in \mathcal{V}\} = \\ &\{f \in H^2(\Gamma) \colon (P_{D,v} - \Lambda_v P_{R,v})F(v) + (P_{N,v}+P_{R,v})F'(v) = 0 \quad \forall v \in \mathcal{V}\}.\end{aligned}$$

Notice that $(P_{D,v} - \Lambda_v P_{R,v})F(v) + (P_{N,v}+P_{R,v})F'(v) = 0$ if and only if

$$P_{D,v}F(v) = 0, \qquad P_{N,v}F'(v) = 0$$

and

$$P_{R,v}F'(v) = \Lambda_v P_{R,v}F(v).$$

Proof. As P_D and P_N are the orthogonal projectors onto the eigenspaces of the matrix U with eigenvalue -1 and $+1$, respectively, then $P_R = \mathbb{I} - P_D - P_N$ is the projection onto the eigenspaces of all the eigenvalues different from -1 and $+1$. These three projectors conmute with U and thus with $U - \mathbb{I}$ and

$U + \mathbb{I}$, by the spectral theorem.
We first suppose that

$$i(U - \mathbb{I})F(v) + (U + \mathbb{I})F'(v) = 0 \tag{20}$$

and prove that

$$(P_{D,v} - \Lambda_v P_{R,v})F(v) + (P_{N,v} + P_{R,v})F'(v) = 0.$$

Multiplying (20) by P_D and commuting, we have

$$\begin{aligned} & i(U - \mathbb{I})F(v) + (U + \mathbb{I})F'(v) = 0 \\ \Longrightarrow\ & iP_D(U - \mathbb{I})F(v) + P_D(U + \mathbb{I})F'(v) = 0 \\ \Longleftrightarrow\ & i(U - \mathbb{I})P_D F(v) + (U + \mathbb{I})P_D F'(v) = 0. \end{aligned} \tag{21}$$

It follows from the definition of P_D that $(U+\mathbb{I})P_D = 0$ and $(U-\mathbb{I})P_D = -2P_D$, reducing equation (21) to

$$-2iP_D F(v) = 0.$$

Hence, $P_D F(v) = 0$.
In the same way, multiplying (20) by P_N and commuting,

$$\begin{aligned} & i(U - \mathbb{I})F(v) + (U + \mathbb{I})F'(v) = 0 \\ \Longrightarrow\ & iP_N(U - \mathbb{I})F(v) + P_N(U + \mathbb{I})F'(v) = 0 \\ \Longleftrightarrow\ & i(U - \mathbb{I})P_N F(v) + (U + \mathbb{I})P_N F'(v) = 0. \end{aligned} \tag{22}$$

From the definition of P_N we have $(U + \mathbb{I})P_N = 2P_N$ and $(U - \mathbb{I})P_N = 0$, reducing the equation (22) to

$$2P_N F'(v) = 0.$$

Therefore, $P_N F'(v) = 0$.

Now let $(U+\mathbb{I})_R$ and $(U-\mathbb{I})_R$ the restrictions of $(U+\mathbb{I})$ and $(U-\mathbb{I})$ to the space $P_R\mathbb{C}^d$, respectively; due to $\ker(U + \mathbb{I})_R = \{0\}$ and $\ker(U - \mathbb{I})_R = \{0\}$, there exist $(U + \mathbb{I})_R^{-1}$ and $(U - \mathbb{I})_R^{-1}$. Newly, multiplying (20) by P_R and commuting,

$$\begin{aligned} & i(U - \mathbb{I})F(v) + (U + \mathbb{I})F'(v) = 0 \\ \Longrightarrow & iP_R(U - \mathbb{I})F(v) + P_R(U + \mathbb{I})F'(v) = 0 \\ \Longleftrightarrow\ & i(U - \mathbb{I})P_R F(v) + (U + \mathbb{I})P_R F'(v) = 0 \\ \Longleftrightarrow\ & -(U + \mathbb{I})_R^{-1}[i(U - \mathbb{I})_R P_R F(v) + (U + \mathbb{I})_R P_R F'(v)] = 0 \\ \Longleftrightarrow\ & -i(U + \mathbb{I})_R^{-1}(U - \mathbb{I})_R P_R F(v) - P_R F'(v) = 0. \end{aligned}$$

As $\Lambda = -i(U + \mathbb{I})_R^{-1}(U - \mathbb{I})_R$, we deduce

$$\Lambda P_R F(v) = P_R F'(v).$$

Further, Λ is invertible, as it is the composition of invertible operators, and it is self-adjoint since

$$\begin{aligned}
&\Lambda = \Lambda^* \\
\iff & -i(U+\mathbb{I})_R^{-1}(U-\mathbb{I})_R = i(U-\mathbb{I})_R^*[(U+\mathbb{I})_R^{-1}]^* \\
\iff & -(U-\mathbb{I})_R(U+\mathbb{I})_R^* = (U+\mathbb{I})_R(U-\mathbb{I})_R^* \\
\iff & -(U-\mathbb{I})_R(U^*+\mathbb{I})_R = (U+\mathbb{I})_R(U^*-\mathbb{I})_R \\
\iff & -(U-U^*)_R = (-U+U^*)_R.
\end{aligned}$$

We now suppose that

$$(P_{D,v} - \Lambda_v P_{R,v})F(v) + (P_{N,v} + P_{R,v})F'(v) = 0.$$

and prove that

$$i(U-\mathbb{I})F(v) + (U+\mathbb{I})F'(v) = 0.$$

Since $P_D F(v) = 0$, $P_N F(v) = 0$ and $\Lambda P_R F(v) = P_R F'(v)$, then

$$\begin{gathered}
iP_D(U-\mathbb{I})F(v) + P_D(U+\mathbb{I})F'(v) = 0, \\
iP_N(U-\mathbb{I})F(v) + P_N(U+\mathbb{I})F'(v) = 0 \qquad \text{and} \\
iP_R(U-\mathbb{I})F(v) + P_R(U+\mathbb{I})F'(v) = 0,
\end{gathered}$$

which implies that

$$i(U-\mathbb{I})F(v) + (U+\mathbb{I})F'(v) = 0.$$

□

Lemma 1.4.7. *Let Γ be a metric graph with finite number of edges. Suppose that for each vertex v there are complementary orthogonal projections $P_{D,v}$, $P_{N,v}$ and $P_{R,v}$ (i.e. $P_{D,v} + P_{N,v} + P_{R,v} = \mathbb{I}$ and their images are orthogonal to each other), and an invertible self-adjoint map $\Lambda_v : P_{R,v}[\mathbb{C}^{d_v}] \to P_{R,v}[\mathbb{C}^{d_v}]$.*

For every vertex $v \in \mathcal{V}$ define the operators

$$A_v := P_{D,v} - \Lambda P_{R,v} \qquad \textit{and} \qquad B_v := P_{N,v} + P_{R,v},$$

and, without loss of generality, the matrix representations of these operators are denoted by A_v and B_v,respectively. Then

$$\begin{gathered}
(A_v|B_v) \in \mathsf{Mat}_{d_v \times 2d_v} \quad \textit{has maximal rank and} \\
A_v B_v^* \quad \textit{is self-adjoint.}
\end{gathered}$$

Further,

$$\begin{aligned}
&\{f \in H^2(\Gamma) \colon (P_{D,v} - \Lambda_v P_{R,v})F(v) + (P_{N,v} + P_{R,v})F'(v) = 0 \quad \forall v \in \mathcal{V}\} \\
&\quad = \{f \in H^2(\Gamma) \colon A_v F(v) + B_v F'(v) = 0 \quad \forall v \in \mathcal{V}\}.
\end{aligned}$$

Proof. Notice that, if $P_D F = 0$, $P_N F' = 0$ and $P_R F' = \Lambda P_R F$ (i.e. $(P_{D,v} - \Lambda_v P_{R,v})F(v) + (P_{N,v} + P_{R,v})F'(v) = 0$), then

$$\begin{aligned} AF + BF' =& (P_D - \Lambda P_R)F + (P_N + P_R)F' \\ =& -\Lambda P_R F + P_R F' = 0. \end{aligned}$$

Conversely, if $AF + BF' = 0$, then

$$P_D F + P_N F' + (P_R F' - \Lambda P_R F) = 0.$$

Therefore, as P_D and P_N are orthogonal and $P_R = \mathbb{I} - P_D - P_N$, we obtain

$$P_D F = 0, \quad P_N F' = 0 \quad \text{and} \quad P_R F' = \Lambda P_R F.$$

Now let us see that AB^* is self adjoint. On the one hand,

$$\begin{aligned} AB^* =& (P_D - \Lambda P_R)(P_N + P_R)^* \\ =& (P_D - \Lambda P_R)(P_N + P_R) \\ =& -\Lambda P_R, \end{aligned}$$

and on the other hand,

$$\begin{aligned} A^*B =& (P_D - \Lambda P_R)^*(P_N + P_R) \\ =& (P_D - P_R \Lambda P_R)^*(P_N + P_R) \\ =& (P_D - P_R^* \Lambda^* P_R^*)(P_N + P_R) \\ =& (P_D - \Lambda P_R)(P_N + P_R) \\ =& -\Lambda P_R, \end{aligned}$$

where we have use the fact that Λ is self-adjoint. Hence, $AB^* = A^*B$. Finally, to show that $(A|B) = (P_D - \Lambda P_R | P_N + P_R)$ has maximal rank, observe that for any $u \in \mathbb{C}^d$,

$$\begin{aligned} (P_D - \Lambda P_R)(P_D u) + (P_N + P_R)(\bar{0}) =& P_D u, \\ (P_D - \Lambda P_R)(\bar{0}) + (P_N + P_R)(P_N u) =& P_N u \qquad \text{and} \\ (P_D - \Lambda P_R)(\bar{0}) + (P_N + P_R)(P_R u) =& P_R u, \end{aligned}$$

where $\bar{0}$ denotes de zero vector in $\mathbb{C}^d$. These equalities imply that

$$\dim((A|B)\mathbb{C}^{2d}) \geq \dim(P_D \mathbb{C}^d) + \dim(P_N \mathbb{C}^d) + \dim(P_R \mathbb{C}^d) = d.$$

We conclude that $(A|B)$ has maximal rank. $\square$

Theorem 1.4.8. *Let Γ be a metric graph with finite number of edges. Consider the operator $\Delta = -\frac{d^2}{dx^2}$ (i.e. minus the second distributional derivate) with domain*

$$\mathsf{Dom}(\Delta) = \{f \in H^2(\Gamma)\colon A_v F(v) + B_v F'(v) = 0 \quad \forall v \in \mathcal{V}\},$$

where A_v and B_v are matrices $d_v \times d_v$. Then, Δ is self-adjoint if, and only if,

$$(A_v|B_v) \in Mat_{d_v \times 2d_v} \quad \textit{has maximal rank,} \tag{23}$$

$$\textit{and} \quad A_v B_v^* \quad \textit{is self-adjoint.}^{[9]} \tag{24}$$

Proof. We recall that, as all the conditions are local, we consider only one vertex v and a vicinity of it where the graph is like a star graph. Therefore, we avoid using notations $A_v, B_v, d_v, F(v), F'(v), ...$ and instead we use $A, B, d, F, F', ...$, respectively. We furthermore assume, without loss of generality, that for each edge e, the coordinate x_e is such that $o(e) = v$, recall that $o(e)$ is the initial point of the edge e.

We will demonstrate that if Δ is self-adjoint, then the conditions (23) and (24) are satisfied. Conversely, by Lemmas 1.4.5 and 1.4.6, we have that if conditions (23) and (24) hold, then there exist complementary orthogonal projectors P_D, P_N and P_R, and Λ an invertible self-adjoint operator on $P_R\mathbb{C}^d$ such that

$$P_D F = 0$$

$$P_N F' = 0 \qquad \text{and}$$

$$\Lambda P_R F = P_R F'.$$

Moreover, for every vertex v of Γ,

$$\{f \in H^2(\Gamma)\colon A_v F(v) + B_v F'(v) = 0\} =$$

$$\{f \in H^2(\Gamma)\colon (P_{D,v} - \Lambda_v P_{R,v})F(v) + (P_{N,v} + P_{R,v})F'(v) = 0\}$$

Under these conditions, we will prove that if

$$\mathsf{Dom}(\Delta) = \{f \in H^2(\Gamma)\colon (P_D - \Lambda P_R)F + (P_N + P_R)F' = 0\},$$

then Δ is self-adjoint.

We begin supposing that Δ is self-adjoint. Let $f \in \mathsf{Dom}(\Delta)$ and $g \in \oplus_{e\in\mathcal{E}} C^\infty(e)$ such that becomes zero outside of a neigbourhood of the vertex v. Since Δ is self-adjoint, we have

$$\sum_{e\in\mathcal{E}} \int_e \frac{d^2 f_e(x)}{dx^2}\overline{g_e(x)}dx = \sum_{e\in\mathcal{E}} \int_e f_e(x)\frac{d^2\overline{g_e(x)}}{dx^2}dx. \tag{25}$$

As g is zero on all vertices different from v, integrating by parts we obtain

$$\begin{aligned}\sum_{e\in\mathcal{E}}\int_e \frac{d^2 f_e(x)}{dx^2}\overline{g_e(x)}dx &= \sum_{e\in\mathcal{E}}\left(-f_e'(v)\overline{g_e(v)} - \int_e \frac{df_e(x)}{dx}\frac{d\overline{g_e(x)}}{dx}dx\right)\\ &= \sum_{e\in\mathcal{E}}\left(-f_e'(v)\overline{g_e(v)} + f_e(v)\overline{g_e'(v)} + \int_e f_e(x)\frac{d^2\overline{g_e(x)}}{dx^2}dx\right).\end{aligned}$$

Then, by (25),

$$\sum_{e\in\mathcal{E}} f_e'(v)\overline{g_e(v)} - \sum_{e\in\mathcal{E}} f_e(v)\overline{g_e'(v)} = \langle F', G\rangle - \langle F, G'\rangle = 0, \tag{26}$$

where $\langle,\rangle$ denotes the standar hermitian product on $\mathbb{C}^{d_v}$. Thus, $g \in \mathsf{Dom}(\Delta^*)$ is equivalent to satisfy (26) for any $f \in \mathsf{Dom}(\Delta)$. But $g \in \mathsf{Dom}(\Delta^*) = \mathsf{Dom}(\Delta)$ is equivalent to

$$AG + BG' = 0.$$

Thus, we have that for $g \in \mathsf{Dom}(\Delta^*)$ the following conditions are equivalent:

(i) $AG + BG' = 0$ and
(ii) $\langle F', G\rangle - \langle F, G'\rangle = 0$ for all $f \in \mathsf{Dom}(\Delta)$.

By the rank-nullity Theorem for linear functions we have

$$\dim(\mathsf{Ran}(A|B)) = \dim(\mathbb{C}^{2d}) - \dim(\mathsf{Ker}(A|B)) = 2d - \dim(\mathsf{Ker}(A|B)). \tag{27}$$

But, from the equivalence between the points (i) and (ii) follows that

$$\begin{aligned}\mathsf{Ker}(A|B) =& \left\{ \begin{pmatrix} G \\ G' \end{pmatrix} : AG + BG' = 0 \right\}\\ =& \left\{ \begin{pmatrix} G \\ G' \end{pmatrix} : \langle F, G'\rangle - \langle F', G\rangle = 0 \quad \forall f \in \mathsf{Dom}(\Delta) \right\}\end{aligned} \tag{28}$$

Consider the following inner product in $\mathbb{C}^d \times \mathbb{C}^d \equiv \mathbb{C}^{2d}$,

$$\left\langle \begin{pmatrix} X \\ Y \end{pmatrix}, \begin{pmatrix} Z \\ W \end{pmatrix} \right\rangle = < X, Z > + < Y, W > \qquad \forall \begin{pmatrix} X \\ Y \end{pmatrix}, \begin{pmatrix} Z \\ W \end{pmatrix} \in \mathbb{C}^{2d},$$

and define the operator $V : \mathbb{C}^{2d} \to \mathbb{C}^{2d}$ by

$$V\begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} Y \\ -X \end{pmatrix} \qquad \forall \begin{pmatrix} X \\ Y \end{pmatrix} \in \mathbb{C}^{2d}.$$

It is easy to see that V is unitary, i.e.

$$VV^* = V^*V = \mathbb{I}.$$

Using Equation (28), we can write $\mathsf{Ker}(A|B)$ in terms of V and obtain

$$\begin{aligned}\mathsf{Ker}(A|B) &= \left\{ \begin{pmatrix} G \\ G' \end{pmatrix} : \left\langle \begin{pmatrix} F \\ F' \end{pmatrix}, V \begin{pmatrix} G \\ G' \end{pmatrix} \right\rangle = 0 \quad \forall f \in \mathsf{Dom}(\Delta) \right\} \\ &= \left\{ \begin{pmatrix} G \\ G' \end{pmatrix} : \left\langle V^* \begin{pmatrix} F \\ F' \end{pmatrix}, \begin{pmatrix} G \\ G' \end{pmatrix} \right\rangle = 0 \quad \forall f \in \mathsf{Dom}(\Delta) \right\} \\ &= [V^*(\mathsf{Dom}(\Delta))]^{\perp} \\ &= [V^*(\mathsf{Ker}(A|B))]^{\perp}.\end{aligned}$$

This implies that

$$\begin{aligned} dim(\mathsf{Ker}(A|B)) =& 2d - dim(V^*(\mathsf{Ker}(A|B))) \\ =& 2d - dim(\mathsf{Ker}(A|B)),\end{aligned}$$

where the last equality occurs since V^* is bijective. Thus, $dim(\mathsf{Ker}(A|B)) = d$. Therefore, by the Equation (27), the rank of $(A|B)$ is d, i.e, $(A|B)$ has maximal rank.

Moreover, for any $a, b \in \mathbb{R}$ we can produce a function $g_e \in C^{\infty}([0, L_e])$ (vanishing outside a small vicinity of v) such that $g(0) = a$ and $g'(0) = b$. Then, if we take any vector $h \in \mathbb{C}^d$, we can produce a function $g \in \oplus_{e \in \mathcal{E}} C^{\infty}(e)$ such that $G = -B^*h$ y $G' = A^*h$. Thereby, for every $f \in \mathsf{Dom}(\Delta)$

$$\begin{aligned}\langle F', G\rangle - \langle F, G'\rangle &= \langle F', -B^*h\rangle - \langle F, A^*h\rangle \\ &= -\langle BF', h\rangle - \langle AF, h\rangle \\ &= -\langle BF' + AF, h\rangle = 0.\end{aligned}$$

Then $(G|G') = (-B^*h|A^*h)$ satisfy (ii). Equivalently, $(-AB^* + BA^*)h = 0$ for any h. Hence, $AB^* = A^*B$, which means that condition (24) is satisfied.

Now we suppose that

$$\mathsf{Dom}(\Delta) = \{f \in H^2(\Gamma)\colon (P_{D,v} - \Lambda_v P_{R,v})F(v) + (P_{N,v} + P_{R,v})F'(v) = 0 \quad \forall v \in \mathcal{V}\},$$

where $P_{D,v}$, $P_{N,v}$ and $\Lambda P_{R,v} := \mathbb{I} - P_{D,v} - P_{N,v}$ are orthogonal projectors acting on $\mathbb{C}^{d_v}$ and Λ_v is an invertible self-adjoint operator on $P_{R,v}\mathbb{C}^{d_v}$. It follows that

$$\begin{gathered} P_{D,v}F(v) = 0, \quad P_{N,v}F'(v) = 0 \quad \text{and} \\ P_{R,v}F'(v) = \Lambda_v P_{R,v} F(v). \end{gathered} \tag{29}$$

We will show that this implies the self-adjointness for Δ.

First we demonstrate that Δ is a symmetric operator, i.e. $\mathsf{Dom}(\Delta) \subset \mathsf{Dom}(\Delta^*)$ and $\Delta(f) = \Delta^*(f)$ for all $f \in \mathsf{Dom}(\Delta)$. Let $f, g \in \mathsf{Dom}(\Delta)$. We will use $\mathbb{I} = P_D + P_N + P_R$ and that the projectors are self-adjoint operators in order to compute

$$\begin{aligned}\langle F', G\rangle &= \langle F', (P_D + P_N + P_R)G\rangle \\ &= \langle F', P_D G\rangle + \langle P_N F', G\rangle + \langle P_R F', G\rangle \\ &= \langle P_R F', G\rangle \\ &= \langle P_R F', P_R G\rangle \\ &= \langle \Lambda P_R F, P_R G\rangle\end{aligned}$$

and

$$\begin{aligned}\langle F, G'\rangle &= \langle F, (P_D + P_N + P_R)G'\rangle \\ &= \langle P_D F, G'\rangle + \langle F, P_N G'\rangle + \langle F, P_R G'\rangle \\ &= \langle F, P_R G'\rangle \\ &= \langle P_R F, P_R G'\rangle \\ &= \langle P_R F, \Lambda P_R G\rangle\end{aligned}$$

Since Λ is self-adjoint we conclude

$$\begin{aligned}\langle F', G\rangle - \langle F, G'\rangle &= \langle \Lambda P_R F, P_R G\rangle - \langle P_R F, \Lambda P_R G\rangle \\ &= \langle \Lambda P_R F, P_R G\rangle - \langle \Lambda P_R F, P_R G\rangle = 0.\end{aligned}$$

Thereby, integrating by parts twice we obtain

$$\sum_{e\in\mathcal{E}} \int_e \frac{d^2 f_e(x)}{dx^2} \overline{g_e(x)} dx = \sum_{e\in\mathcal{E}} \int_e f_e(x) \frac{d^2 \overline{g_e(x)}}{dx^2} dx.$$

We conclude that $f \in \mathsf{Dom}(\Delta^*)$ and $\Delta^* f = \Delta f$. Thus Δ is a symmetric operator (i.e. $\Delta \subset \Delta^*$).

Also, we have to prove that $\mathsf{Dom}(\Delta^*) \subset \mathsf{Dom}(\Delta)$. Let $g \in \mathsf{Dom}(\Delta^*)$, then

$$\langle \Delta f, g\rangle = \langle f, \Delta^* g\rangle \qquad \forall f \in \mathsf{Dom}(\Delta).$$

Notice that $C_0^\infty(\Gamma) \subset \mathsf{Dom}(\Delta)$ since $f(v) = 0$ for all $f \in C_0^\infty(\Gamma)$. Thus, from Corollaries 1.3.7 and 1.3.13, we have

$$\mathsf{Dom}(\Delta^*) \subset H^2(\Gamma).$$

Subsequently we can integrate by parts and obtain

$$\langle f, \Delta^* g\rangle = \langle \Delta f, g\rangle = -\langle F', G\rangle + \langle F, G'\rangle + \langle f, \Delta g\rangle \tag{30}$$

for every $f \in \mathsf{Dom}(\Delta)$. Particularly,

$$\langle f, \Delta^* g\rangle = \langle f, \Delta g\rangle \qquad \forall f \in C_0^\infty(\Gamma).$$

Since $C_0^\infty(\Gamma)$ is dense in $L^2(\Gamma)$, we conclude that $\Delta g = \Delta^* g$ for every $g \in \mathsf{Dom}(\Delta^*)$.

Moreover, from Equation (30) it follows

$$\langle F', G\rangle - \langle F, G'\rangle = 0 \qquad \forall f \in \mathsf{Dom}(\Delta). \tag{31}$$

Now define $A = P_D - \Lambda P_R$ and $B = P_N + P_R$. For every $h \in \mathbb{C}^d$ we can construct a function $\tilde{f} \in H^2(\Gamma)$ such that $\tilde{F} = -B^*h$ and $\tilde{F}' = A^*h$. Notice that $\tilde{f}$ satisfies (29) as the projectors P_D, P_N and P_R are orthogonal. Indeed,

$$P_D\tilde{F} = P_D(-B^*h) = P_D((-P_N - P_R)h) = 0,$$

$$P_N\tilde{F}' = P_N(A^*h) = P_N((P_D - \Lambda P_R)h) = 0 \qquad \text{and}$$

$$\begin{aligned}\Lambda P_R\tilde{F} =& \Lambda P_R(-B^*h) = \Lambda P_R((-P_N - P_R)h) = -\Lambda P_R h\\ =& P_R((P_D - \Lambda P_R)h) = P_R(A^*h) = P_R\tilde{F}'.\end{aligned}$$

Thus, $\tilde{f} \in \mathsf{Dom}(\Delta)$ and it follows from equation (31) that

$$\begin{aligned}0 = \langle \tilde{F}', G\rangle - \langle \tilde{F}, G'\rangle &= \langle A^*h, G\rangle - \langle -B^*h, G'\rangle\\ \langle h, AG\rangle - \langle h, -BG'\rangle &= \langle h, AG + BG'\rangle.\end{aligned}$$

This implies that $AG + BG' = 0$ and then

$$0 = (P_D - \Lambda P_R)G + (P_N + P_R)G' = P_D G + P_N G' + P_R(-\Lambda P_R G + P_R G').$$

As the projectors are orthogonal, we conclude that

$$P_D G = 0, \quad P_N G' = 0 \quad \text{and} \quad -\Lambda P_R G + P_R G' = 0.$$

This last statement implicates that $g \in \mathsf{Dom}(\Delta)$. Hence, we infer that Δ is self-adjoint.

□

Note 1.4.9. *Theorem 1.4.8 together with Lemmas 1.4.5, 1.4.6 and 1.4.7 give different characterizations of the domains of Laplace operators giving rise to self-adjoint operators, when boundary conditions are local. The first demonstrations are allocated to Kostrykin and Schrader in [19] and to Harmer in [14]. A deeper study of the matrices A and B (using arguments of diagonalization) leads to self-adjointness conditions that can be reduced to Neumann or Dirichlet conditions on each edge. This is achieved in [3], [4] and [5], where low and high energy limits of scattering operators are studied, in the case that electric potentials are added to the Laplacian in the context of quantum mechanics and Schroedinger operators in star graphs (or matrix Schroedinger operators in the half-line).*

CHAPTER 2

The spectrum of the Laplacian

Consider Γ a finite connected discrete graph. We have already defined the Discrete Graph Laplacian as

$$\Delta\colon L^2(\Gamma) \to L^2(\Gamma)$$
$$\Delta f(v) := \frac{1}{b_v}\Big(\sum_{u\sim v} f(u) - d_v f(v)\Big) \qquad \forall f \in L^2(\Gamma). \tag{32}$$

We have proven that this operator is **self-adjoint**, besides it is **nonpositive**, i.e.,

$$(\Delta u, u) \leq 0, \tag{33}$$

and $\Delta u = 0$ when u is constant.

Notice that if u is an eigenfunction of Δ w.r.t. the eigenvalue λ, then $\lambda \in \mathbb{R}$ since Δ is self-adjoint and

$$(\Delta u, u) = (\lambda u, u) = \lambda(u, u) \leq 0.$$

Thus, the eigenvalues of Δ are nonpositive.

It is known that there exists an **orthonormal basis** of $L^2(\Gamma)$ consisting of eigenvalues of Δ.[15] Moreover, if $\{u_1, u_2, \dots, u_k\}$ is an orthonormal basis of $L^2(\Gamma)$ such that u_i is an eigenfunction of Δ w.r.t. the eigenvalue λ_i for every $i = 1, 2, \dots, k$, then any $f \in L^2(\Gamma)$ admits a decomposition

$$f(v) = \sum_{i=1}^{k} (f, u_i) u_i(v) \tag{34}$$

for every vertex v of Γ.

Based in the description above (following [15]) and seeking to establish a result for the quantum graphs analogous to (34), in this chapter we add some propositions and theorems taken from [9] provided with the necessary definitions. Also, we give a theorem which offers a relation between the spectra of the discrete graph Laplacian and the Laplacian on a quantum graph for the specific case of having a compact *equilateral* quantum graph. (Theorem 2.5.1).

2.1. The spectrum of a self-adjoint linear operator

Consider H a Hilbert space and A a self-adjoint linear operator in H. We define the **resolvent** set of A as

$$\rho(A) := \{\lambda \in \mathbb{C}\colon (A - \lambda\mathbb{I})^{-1} \text{ exists and it is bounded}\}.$$

And we define the **spectrum** of A as the complement of its resolvent set, i.e.

$$\sigma(A) := \mathbb{C} \setminus \rho(A).$$

We say that $\lambda \in \mathbb{C}$ is an **eigenvalue** of A if $\mathsf{Ker}(A - \lambda\mathbb{I}) \neq \{0\}$, where $0 \in H$ is the identity element. Furthermore, the elements of this kernel which are different from 0 are called **eigenfunctions** with respect to λ. The set of all eigenvalues of A is designated the **point spectrum** and it is denoted by $\sigma_p(A)$.

The elements of $\sigma(A)$ can be classified according to some properties. The set of all eigenvalues of finite multiplicity which are not accumulation points is the **discrete spectrum** $\sigma_d(A)$, and its complement is the **essential spectrum**

$$\sigma_{ess}(A) := \sigma(A) \setminus \sigma_d(A).$$

Definition 2.1.1. *Let $\mathcal{H}$ a Hamiltonian related to a quantum graph Γ with set of edges $\mathcal{E}$. Referring to the Dirichlet conditions, we define the set $\sigma_D(\mathcal{H})$ by the next relation:*

a complex number λ is an element of $\sigma_D(\mathcal{H})$ if, and only if, there exists a function $f \in Dom(\mathcal{H})$ such that $\mathcal{H}f_e = \lambda f_e$ for some edge $e \in \mathcal{E}$ and f_e vanishes on the vertices of e.

Notice that, as $sin\left(\frac{\pi n x}{L_e}\right)$ is an eigenfunction of $-\frac{d^2}{dx}$ in the interval $[0, L_e]$, when $\mathcal{H} = -\frac{d^2}{dx}$,

$$\sigma_D(\mathcal{H}) = \bigcup_{e \in \mathcal{E}} \left\{ \left(\frac{\pi n}{L_e}\right)^2 \middle| n \in \mathbb{N} \right\}.$$

2.2. The Spectral Theorem and Spectral Measure

For the next theorem we recall that $L(H)$ is the Banach space of bounded linear operators from H to H with norm

$$\|T\| = \sup_{x \neq 0} \frac{\|Tx\|}{\|x\|} \qquad \forall T \in L(H).$$

Theorem 2.2.1. ***Spectral Theorem.*** *Let A be a self-adjoint operator in H. There exists a unique map*

$$\phi_A \colon C_0(\sigma(A)) \to L(H)$$

such that

(1) *ϕ_A is an algebraic $*$-homomorphism of $*$-algebras,*
(2) *$\|\phi_A(f)\| \leq \|f\|_{L^\infty}$,*
(3) *if $\lambda \notin \mathbb{R}$ and $r_\lambda(z) := (\lambda - z)^{-1}$, then $\phi_A(r_\lambda) = (\lambda\mathbb{I} - A)^{-1}$ and*
(4) *$\phi_A(f) = 0$ if $\mathsf{supp} f \cap \sigma(A) = \emptyset$.*

Using the Theorem 2.2.1, we can define for every $w \in H$ a **spectral measure** μ_w on $\sigma(A)$ such that

$$\int_{\sigma(A)} f(z) d\mu_w(z) := (w, \phi_A(f)w).$$

Considering that a measure $\mu : \mathcal{B} \to \mathbb{R}$ is **pure point** if, for every measurable set $X \in \mathcal{B}$,

$$\mu(X) = \sum_{x \in X} \mu(x),$$

we define the invariant subspace of A

$$H_{pp} := \{w \in H \colon \mu_w \text{ is pure point}\}.$$

We define the **pure point spectrum** of A as the spectrum of the restriction $A\big|_{H_{pp}}$, and we donoted by $\sigma_{pp}(A)$.

Definition 2.2.2. *Let $(X, \mathcal{B})$ be a measurable space, H a Hilbert space and $\mathcal{P} = \mathcal{P}(H)$ the set of orthogonal projections on H. Suppose that $\mu : \mathcal{B} \to \mathcal{P}$ is a function such that*

- *it is* countable additive, *i.e., if $\{\delta_n\}$ is a countable set of disjoint sets of $\mathcal{B}$ and $\delta = \cup_n \delta_n$, then $\mu(\delta) =$s-$\sum_n \mu(\delta_n)$ (the strong limit of partial sums),*
- *and it is* complet, *i.e., $\mu(X) = \mathbb{I}$.*

Then, we say that μ is a ***spectral measure*** *on H and $(X, \mathcal{B}, H, \mu)$ is a* ***spectral measure space****.*

Theorem 2.2.3. ***Spectral Theorem (projection valued measure form)*** *Let A be a self-adjoint operator on H. Then there exists a unique spectral measure*

$$\mu_A : \mathcal{B}_{\mathbb{R}} \to \mathcal{P}(H),$$

where $\mathcal{B}_{\mathbb{R}}$ denote the Borel σ-algebra on $\mathbb{R}$, such that

$$A = \int_{\mathbb{R}} s d\mu_A(s).$$

2.3. Quadratic form

Consider $\mathcal{H}$ a self-adjoint operator acting as the negative second derivative on a space of functions defined in a quantum graph Γ. We choose the vertex conditions to be of the form

$$\begin{cases} P_{D,v}F(v) = 0 \\ P_{N,v}F'(v) = 0 \\ P_{R,v}F'(v) = \lambda_v P_{R,v}F(v), \end{cases}$$

where $P_{D,v}, P_{N,v}$ and $P_{R,v} = \mathbb{I} - P_{D,v} - P_{N,v}$ are orthogonal projectors acting on $\mathbb{C}^{d_v}$ and Λ_v is a self-adjoint operator in $P_{R,v}\mathbb{C}^{d_v}$ for every vertex $v \in \mathcal{V}$.

The next theorem is taken from [9].

Theorem 2.3.1. *The quadratic form of $\mathcal{H}$ is given by*

$$\langle \mathcal{H}f, f\rangle = \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{dx}\right|^2 dx + \sum_{v\in\mathcal{V}} \langle \Lambda_v P_{R,v}F, P_{R,v}F\rangle. \tag{35}$$

The domain of this form is

$$\{f \in H^1(\Gamma) \colon P_{D,v}F = 0 \quad \forall v \in \mathcal{V}\}.$$

The sesqui-linear form of $\mathcal{H}$ is

$$\langle \mathcal{H}f, g\rangle = \sum_{e\in\mathcal{E}} \int_e \frac{df}{dx}\overline{\frac{dg}{dx}} dx + \sum_{v\in\mathcal{V}} \langle \Lambda_v P_{R,v}F, P_{R,v}G\rangle. \tag{36}$$

2.4. Discreteness of the Laplacian Spectrum

A bounded operator $T \in \mathcal{B}(X, Y)$ is **compact** if the image $\{Tu_n\}$ of any bounded sequence $\{u_n\}$ of X contains a Cauchy subsequence.

Lemma 2.4.1. *Let $T \in \mathcal{B}(X, Y)$ be a compact operator. Then, its spectrum $\sigma(T)$ is a countable set with no accumulation points different from zero. Each nonzero eigenvalue $\lambda \in \sigma(T)$ has finite multiplicity, and $\overline{\lambda}$ is an eigenvalue of T^* with the same multiplicity.* [17]

Theorem 2.4.2. *Let Γ a compact quantum graph together with the Laplacian $\Delta = -d^2/dx^2$ (i.e. the negative second distributional derivate) with domain given as*

$$\{f \in H^2(\Gamma) \colon A_v F(v) + B_v F'(v) = 0 \quad \forall v \in \mathcal{V}\},$$

where A_v, B_v are $d_v \times d_v$-matrices such that $(A_v|B_v)$ has maximal rank and AB^* is self-adjoint. Then the resolvent $(\Delta - i\mathbb{I})^{-1}$ is a compact operator in $L^2(\Gamma)$. [9]

Proof. The self-adjointness of Δ implies that the resolvent $(\Delta - i\mathbb{I})^{-1}$ is well defined from $L_2(\Gamma)$ to $Dom(\Delta) \subset H^2(\Gamma)$. The natural embedding

$$H^2(\Gamma) \mapsto L_2(\Gamma),$$

given by the Sobolev embedding Theorem [2], is compact. Thus, the resolvent is compact. $\square$

Corollary 2.4.3. *The spectrum of the Laplacian $\sigma(\Delta)$ consist of isolated eigenvalues λ_j of finite multiplicity and such that $\lambda_j \underset{j\to\infty}{\to} \infty$. [9]*

Proof. Notice that, for $u \in \mathsf{Dom}((\Delta - i\mathbb{I})^{-1})$ different from zero and a complex number $\gamma \neq 0$, the following is satisfied

$$\begin{aligned} &(\Delta - i\mathbb{I})^{-1}u = \gamma u \qquad (37)\\ \iff &u = (\Delta - i\mathbb{I})\gamma u \\ \iff &u + i\gamma u = \Delta\gamma u \\ \iff &\Delta u = \Big(\frac{1}{\gamma} + i\Big)u. \end{aligned}$$

Then, by Lemma 2.4.1 and Theorem 2.4.2, the spectrum of the Laplacian $\sigma(\Delta)$ is a countable set with no accumulation points of eigenvalues with finite multiplicity. Also notice that

$$\Big|\frac{1}{\gamma_j} + i\Big| \underset{\gamma_j\to 0}{\to} \infty,$$

then the eigenvalues of Δ, denoted as

$$\lambda_j := \Big(\frac{1}{\gamma_j} + i\Big),$$

diverge to infinity. $\square$

2.5. Relation between Spectra of Laplacians

We say that a metric graph is **equilateral** when the length of all its edges are equal. Now consider an equilateral quantum graph Γ such that its sets of vertices $\mathcal{V}$ and edges $\mathcal{E}$ are **countable**, and assume that the common length of its edges is L. Also, considering the Laplacian Δ (minus the second distributional derivate) on Γ, suppose that any $f \in Dom(\Delta)$ satisfies the **Neumann-Kirchhoff** conditions:

- $f(x)$ is continuos on Γ, that is to say, every restriction f_e is continuos for every $e \in \mathcal{E}$ and, for any $v \in \mathcal{V}$,
$$f_e(v) = f_{e'}(v) \qquad \forall e, e' \in \mathcal{E}_v,$$
where $\mathcal{E}_v$ denotes the set of all the edges which contain v.
- For every vertex v,
$$\sum_{e \in \mathcal{E}_v} \frac{df_e}{dx_e}(v) = 0,$$
where the derivates are taken in the direction away from the vertex.

We look for a relation between the spectrum of Δ and the **normalized discrete graph Laplacian**. Henceforth, in order to distinguish between both Laplacians, we use the notation Δ_c for the Laplacian considered on a quantum graph (which is given by minus the second distributional derivate) and Δ_d for the normalized discrete graph Laplacian defined as
$$\Delta_d f(v) = f(v) - \frac{1}{d_v} \sum_{u \sim v} f(u).$$

Using the Definition 2.1.1, we give the following relation between the elements of $\sigma(\Delta_c)$ and $\sigma(\Delta_d)$ spectra.

Theorem 2.5.1. *Consider Γ an equilateral quantum graph and $L \in (0, \infty)$ the length of its edges. Also, suppose that $0 < d_v < \infty$ for every vertex $v \in \mathcal{V}$ and that every function $f \in \mathsf{Dom}(\Delta_c)$ satisfies the Neumann-Kirchhoff conditions. Let $\lambda \in \mathbb{C} \setminus \sigma_D(\Delta_c)$ and $k^2 = \lambda$. Then, the next equivalence holds:*
$$\lambda \in \sigma_p(\Delta_c) \iff (1 - \cos kL) \in \sigma_p(\Delta_d).$$
The same relation occurs when we consider the spectrum σ and the spectral components σ_d, σ_{ess} and σ_{pp}.[9]

Note 2.5.2. *We only demonstrate one implication of the relation between the point spectra. For the complete proof we refer to [9] that mention a proof based on the* ***formula of Krein*** *and a technique developed in [23].*

Proof. Consider the eigenvalue equation
$$-\frac{d^2u}{dx} = k^2 u, \tag{38}$$
with boundary conditions $u(0) = f(0)$ and $u(L) = f(L)$ for every $e \in \mathcal{E}$.

Notice that the function u defined in each edge as
$$u_e(x) = \frac{1}{\sin(kL)} \left[f(0) \sin(k(L - x)) + f(L) \sin(kx) \right],$$
is a solution of the Equation (38).

Indeed, after some computations we obtain the first and the second derivatives of u_e:

$$u_e'(x) = \frac{k}{\sin(kL)}\big[-f(0)\cos(k(L-x)) + f(L)\cos(kx)\big] \tag{39}$$

$$\begin{aligned} u_e''(x) =& \frac{-k^2}{\sin(kL)}\big[f(0)\sin(k(L-x)) + f(L)\sin(kx)\big] \\ =& -k^2 u_e(x). \end{aligned} \tag{40}$$

Thus, substituting $x = 0$ in Equation (39) we have

$$u_e'(0) = \frac{k}{\sin(kL)}\big[-f(0)\cos(kL) + f(L)\big]. \tag{41}$$

Considering that we take the derivatives with direction from a vertex v to its neighbours, we have that $u_e'(0) \equiv u_e'(v)$ for every edge $e \in \mathcal{E}_v$. Then, writing the Neumann condition for the derivatives u_e' using the Equation (41), it follows

$$\sum_{e\in\mathcal{E}_v} \frac{du_e}{dx}(v) = \sum_{e\in\mathcal{E}_v} \frac{k}{\sin(kL)}\big[-f(0)\cos(kL) + f(L)\big] = 0. \tag{42}$$

We deduce that u satisfies the Neumann condition if, and only if,

$$\sum_{e\in\mathcal{E}_v} \big[-f(0)\cos(kL) + f(L)\big] = 0.$$

The last expression is equivalent to next equalities:

$$\begin{aligned} & f(v)d_v\cos(kL) - \sum_{u\sim v} f(u) = 0 \\ \iff\ & f(v) - \frac{1}{d_v}\sum_{u\sim v} f(u) = \big(1-\cos(kL)\big)f(v) \\ \iff\ & \Delta_d f(v) = (1-\cos(kL))f(v). \end{aligned}$$

The previous equality of the normalized graph Laplacian holds for every vertex $v \in \mathcal{V}$. Hence, we conclude that the function u satisfies the Neumann condition if, and only if, f is an eigenfunction with respect to the eigenvalue $(1-\cos(kL))$ of the normalized graph Laplacian. □

A fine achievement to enhance the relation between discrete graphs and quantum graphs would be to extent Theorem 2.5.1 for graphs that are not equilateral. Thus, we can enunciate the following new problem:

Problem 2.5.3. *For the case of graphs that are not equilateral, can we give a relation as in Theorem 2.5.1 between the spectra of the discrete graph Laplacian and the Laplacian on a quantum graph?*

2.6. Spectral decomposition in eigenfunctions

We aim to find a sort of Fourier decomposition in terms of the eigenfunctions of the Laplacian for the elements of $\mathsf{Dom}(\Delta)$.

Let Γ be a quantum graph with set of edges $e \in \mathcal{E}$ and denote by E the cardinality of $\mathcal{E}$. Define the set

$$\mathcal{A} := \{(A_v|B_v) \colon v \in \mathcal{V}\}$$

and the vector $\xi = \{\xi_e\} \in (\mathbb{C} \setminus \{0\})^E$. Consider the Hamiltonian

$$\mathcal{H}_{\mathcal{A},\xi} := -\xi^{-2} \frac{d^2}{dx^2}$$

on a quantum graph, with domain

$$\mathsf{Dom}(\mathcal{H}) = \{f \in H^2(\Gamma) \colon A_v F(v) + B_v F'(v) = 0 \quad \forall v \in \mathcal{V}\},$$

where, for every $v \in \mathcal{V}$, $(A_v|B_v) \in \mathcal{A}$ has maximal rank and $A_v B_v^*$ is self-adjoint. That it is, $\mathcal{H}$ acts as re-scaled version of the negative second distributional derivate

$$-\xi_e^{-2} \frac{d^2}{dx_e^2}$$

on every edge e.

The operator $\mathcal{H}_{\mathcal{A},\xi}$ is self-adjoint and its spectrum is real and discrete.

Definition 2.6.1. *A subset X of an analytic manifold M is called* ***analytic*** *if it can be locally described as the set of common zeros of several analytic functions, and it is called* ***principal analytic*** *if it can be locally described as the set of zeros of an analytic function.*

Theorem 2.6.2. *Define the following subset of $\mathbb{C}^{2\sum d_v^2} \times (\mathbb{C} \setminus \{0\})^E \times \mathbb{C}$*

$$\mathcal{S} := \{(\mathcal{A}, \xi, \lambda) \colon (\mathcal{H}_{\mathcal{A},\xi} - \lambda \mathbb{I}) \text{ does not have bounded inverse in } L^2(\Gamma)\}.$$

Then, $\mathcal{S}$ is principal analytic.
Also, for every $k \geq 1$, define the subset of $\mathbb{C}^{2\sum d_v^2} \times (\mathbb{C} \setminus \{0\})^E \times \mathbb{C}$

$$\mathcal{S}_k := \{(\mathcal{A}, \xi, \lambda) \colon \dim \mathsf{Ker}(\mathcal{H}_{\mathcal{A},\xi} - \lambda \mathbb{I}) \geq k\}.$$

Then, $\mathcal{S}_k$ is analytic for every $k \geq 1$. [9]

Note that $\mathcal{S}_{k+1} \subset \mathcal{S}_k \subset \mathcal{S}$ for every $k \geq 1$. The set $\mathcal{S}$ is the graph of the multiplie-valued function

$$(\mathcal{A}, \xi) \mapsto \sigma(\mathcal{H}_{\mathcal{A},\xi}),$$

which can be considered as a "**dispersion relation**".

The following definitions are reproduced from [16].

Definition 2.6.3. *A k-dimensional* ***vector bundle*** *consists of a total space E, a base M and a projection $\pi\colon E \to M$, where E and M are differentiable manifolds, π is differentiable, for each $x \in M$ the* fiber *$E_x := \pi^{-1}(x)$ has the structure of a k-dimensional vector space and there exists a neighbourhood U_x and a diffeomorphism (i.e. an isomorphism of smooth manifolds)*

$$\varphi_x\colon \pi^{-1}(U_x) \to U_x \times \mathbb{R}^k,$$

called local trivialization*, such that for every $y \in U_x$*

$$\varphi_{xy} := \varphi_x\big|_{E_y}\colon E_y \to \{y\} \times \mathbb{R}^k$$

is a vector space isomorphism.

If (E, π, M) is a k-dimensional vector bundle, $(U_\alpha)_{\alpha\in A}$ a covering of M by open sets and $\phi_\alpha\colon \pi^{-1}(U_\alpha) \to U_\alpha \times \mathbb{R}^k$ the corresponding local trivializations, for nonempty $U_\alpha \cap U_\beta$, we obtain **transitions maps**

$$\varphi_{\beta\alpha}\colon U_\alpha \cap U_\beta \to \mathsf{Gl}(k, \mathbb{R})$$

by

$$\varphi_\beta \circ \varphi_\alpha^{-1}(x, v) = (x, \varphi_{\beta\alpha}(x)v) \qquad \forall x \in U_\alpha \cap U_\beta, v \in \mathbb{R}^k,$$

where $\mathsf{Gl}(k, \mathbb{R})$ is the general linear group. If M is a complex manifold and the transitions maps are holomorphic, then (E, π, M) is an **holomorphic vector bundle**.

Theorem 2.6.4. *With the specifications above, the set $\mathsf{Ker}(\mathcal{H}_{\mathcal{A},\xi})$ is an holomorphic k-dimensional vector bundle over $\mathcal{S}_k \setminus \mathcal{S}_{k+1}$. As a consequence, if there exists a local analytic eigenvalue branch $\lambda(\mathcal{A}, \xi)$ of constant multiplicity k, then there is an analytic local basis of k eigenfunctions. [9]*

Although the next theorem could be generalized to infinite quantum graphs, we consider Γ a finite quantum graph, with set of vertices $\mathcal{V}$, and Δ the Laplacian operator defined on

$$\mathsf{Dom}(\Delta) = \{f \in H^2(\Gamma)\colon (P_{D,v} - \Lambda P_{R,v})F(v) + (P_{N,v} + P_{R,v})F'(v) = 0 \quad \forall v \in \mathcal{V}\},$$

where $P_{D,v}, P_{N,v}$ and $P_{R,v}$ are complementary orthogonal projectors and Λ is an invertible self-adjoint operator defined on $P_{R,v}\mathbb{C}^{d_v}$. Also, we assume that

- the lengths of the edges are bounded from below, i.e. there exists a positive number L_{min} satisfying

$$L_e \geq L_{min} > 0,$$

- the bijections Λ_v are uniformly bounded, i.e.

$$\|\Lambda_v\| \leq C < \infty.$$

Definition 2.6.5. *A function $\phi(x) \in H^2_{loc}(\Gamma)$ which satisfies*

$$(P_{D,v} - \Lambda P_{R,v})\phi(v) + (P_{N,v} + P_{R,v})\phi'(v) = 0 \qquad \forall v \in \mathcal{V},$$

is said to be a ***generalized eigenfunction*** *with respect to λ of the Laplacian Δ if*

$$\Delta\phi(x) = \lambda\phi(x) \qquad a.e. \ on \ \Gamma.$$

Note 2.6.6. *When we say that $\phi(x) \in H^2_{loc}(\Gamma)$, we suppose it is possible that ϕ is not square integrable on Γ (i.e. $\phi \notin L^2(\Gamma)$).*

Theorem 2.6.7. *Under the assumptions above, let μ be the spectral measure of Δ (see Theorem 2.2.3). Consider a function $w\colon \Gamma \to [1, \infty)$ continuous which satisfies $1/w \in L^2(\Gamma)$. Then there exist a "spectral decomposition" into functions ϕ_λ such that, for μ-almost all $\lambda \in \sigma(\Delta)$, ϕ_λ is a generalized eigenfunction of Δ and $w^{-1}\phi_\lambda \in L^2(\Gamma)$ for μ-almost all $\lambda \in \sigma(\Delta)$. [9]*

CHAPTER 3

Applications to Biology

3.1. GRN models

The large amount of genetic data has prompted the analysis of complex systems, with various components and interactions between them, using mathematical and computational resources. For example, these methods have contributed to comprehend plant growth and to understand genetic foundations of the evolution of plants. For the very large number of genes, and the complexity of interactions between them which regulate cell differentiation and development, schematic and intuitive models are not enough for responding the open questions about it in Biology. But mathematical representations and computational simulations allow structural and dynamical studies of complex collections of interconnected genes, proteins and other molecules, which are called gene regulatory networks (GRN).[6]

The GRN models - in which genes, mRNA or proteins are represented by nodes (vertices) and their regulatory interactions by links (edges) - have been elaborated using functional genomics to reverse engineer the identity of the network (graph), or using thorough molecular genetic experiments to suggest models of GRN structures for small gene networks. These models have permited the analysis of temporal change of gene activities (network dynamics) and of the manner in which genes are connected to each other (network architecture). [6]

Discrete and Continuous GRN Models: As development models involve an extensive range of scales and mechanisms, depending on the scale involved and the essence of the available information, a fitting mathematical framework must be selected. GRN models might incorporate continuous or discrete functions. Continuous models can include more detail and produce quantitative predictions; they are very useful for investigating signal transduction pathways and the circadian clock, for example. On the other hand, experiments evidence that gene expression is digital at the individual cell level. Thus, qualitative GRN models with discrete kinetics of gene activation are the most suitable representation of complex gene regulatory logics.

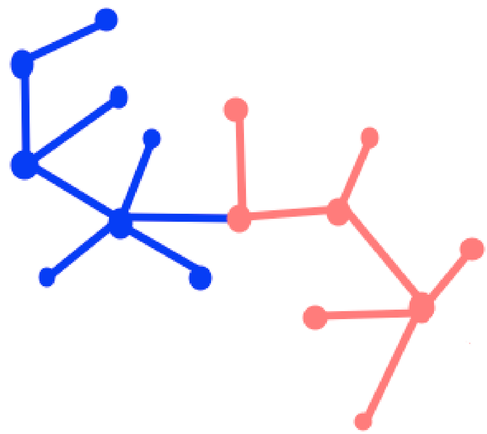

FIGURE 1. Motif joining.

However, different analyses of topologically equivalent continuous and discrete models reveal that both give analogous dynamic results. [6]

3.2. Eigenfunctions of the Graph Laplacian

From the analysis of the discrete graph Laplacian, qualitative properties of a graph can be deduced [15]. Laplacian graph spectra has been used for characterizing large networks and random graphs. Geometric properties of the eigenvectors are studied in several applications in Mathematical Biology and Combinatorial Optimization [24].

When a graph represents biological data as a structure that has evolved from simple precursors, there are characteristic traced by this process in the spectrum of the *normalized* graph Laplacian:

$$\Delta_\Gamma f(v) := f(v) - \frac{1}{d_v} \sum_{u \in \Gamma, u \sim v} f(u).$$

(Notice that this Laplacian is the same as the defined in Equation (1), but with weights $b_v = d_v$.) For example, when a graph Γ_0 is joined to an existing graph Γ in a vertex where an eigenfunction f of Γ_0 (i.e. $\Delta_{\Gamma_0} f - \lambda f = 0$ for some eigenvalue λ) vanishes, the new graph obtained preserve the eigenvalue λ with a *localized* eigenfunction, that is, and eigenfunction which agrees with f on Γ_0 and vanishes at other vertices [7].

Another example is when a small subgraph Γ_1 (*motif*) of Γ is doubling at Γ (i.e. an extension of Γ is constructed in the following way: A copy of

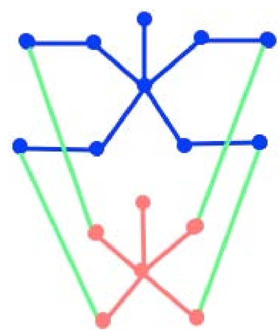

FIGURE 2. Motif duplication.

Γ_1 – denoted temporarily by Γ_1' – is added in such a way that each vertex of Γ_1' is connected to all closest neighbors, that do not belong to Γ_1, of the copied vertex – see Figure 2). Then the new graph possesses the eigenvalue λ of the graph Laplacian on Γ_1

$$\frac{1}{d_v}\sum_{u\in\Gamma_1, u\sim v} f(u) = (1-\lambda)f(v),$$

related to the eigenfunction f with a localized eigenfunction which is *double* (i.e. it agrees with $-f$ on the double of Γ_1) [7].
Constructions like the first (**motif joining**) or the second (**duplication**) could be functional to describe evolution hypothesis of a biological network starting from the data available [7].

An other application of the analysis of the graph Laplacian *eigenfunctions* is on *Landscape Theory*. A **landscape** is a triple $(X, \mathcal{X}, f)$ where X is a set of configurations, $\mathcal{X}$ is a topological structure on X and $f\colon X \to \mathbb{R}$ is a fitness function. The topological structure is often specified as a function $N : X \to 2^X$ constructed in a symmetric way, satisfying $x \in N(y) \iff y \in N(x)$. This relation yields an undirected graph related to $(X, \mathcal{X})$ [18].

The average cost of an arbitrary configuration is

$$\bar{f} = \frac{1}{|X|}\sum_{x\in X} f(x).$$

It has been noticed that in multiple cases the function $\tilde{f}$ defined as $\tilde{f}(x) = f(x) - \bar{f}$ turns out to be an eigenfunction of the Laplacian of the graph related to the configuration space $(X, \mathcal{X})$ [24].

Some of the properties in discrete graph have their analogous in metric graphs. For example, the eigenfunctions of the discrete graph Laplacian has parallel characteristic to the ones of the eigenfunctions of the continuous Laplacian given in the **Courant Nodal Domain Theorem for Elliptic Operators** which states the following: *Given a self-adjoint second order elliptic differential equation* $L[u] + \lambda\rho u = 0 \quad (\rho > 0)$ *in a domain* G *with arbitrary homogeneous boundary conditions; if its eigenfunctions are ordered according to increasing eigenvalues, then the nodes of the* n*-th eigenfunction* u_n *divide the domain into no more than* n *subdomains*. Here L could be the Laplacian and *nodes* are points where the eigenfunction u vanishes [24].

Associated with a graph $G(V, E)$, a symmetric matrix $\mathbf{M}$ is called a *generalized Laplacian* or *discrete Schrödinger operator* of G if $M_{xy} < 0$ whenever $x \sim y$ and $M_{xy} = 0$ when x and y are distinct and not adjacent. A *positive (negative) strong nodal domain* of a function f on $V(G)$ is a maximal connected induced subgraph of G with vertices $v \in V$ with $f(v) > 0 \quad (f(v) < 0)$. And a *positive (negative) weak nodal domain* of a function f on $V(G)$ is a maximal connected induced subgraph of G with vertices $v \in V$ with $f(v) \geq 0 \quad (f(v) \leq 0)$ that contains at least one nonzero vertex. The **Discrete Nodal Domain Theorem** establishes the following: *Let* $\mathbf{M}$ *be a generalized Laplacian of a connected graph with* n *vertices. Then any eigenfunction* f_k *corresponding to the* k*-th eigenvalue* λ_k *with multiplicity* r *has at most* k *weak nodal domains and* $k+r-1$ *strong nodal domains* [24].

3.3. Solitons, Quantum and Chaotic Graphs

There are also some investigations involving quantum graphs, solitons and Biology. For example, in [22] it is shown that models of proteins present pulses as solitons. Using the Schrödinger equation on a star quantum graph, it has been proved that a fast soliton splits in reflected and transmitted components after colliding with the central vertex of the graph [1]. And in [21] is analysed the stability of some solitons for pulse propagation in biomembranes and nerves.

In the discrete setting, soliton graphs are the fundamental graphs of soliton automata, which function as a mathematical model for molecular electronic switching [8].

The chaotic graphs are represented as many fuzzy fractal lines up to ∞ and are described as chaotic matrices. Some operations on the chaotic graphs such as the union and the intersection, the chaotic incidence matrices and the chaotic adjacency matrices has been studied. Chaotic systems are deterministic and sensible to their initial condition. Chaotic behaviour is common in systems as measles out break, heart rhythms, electrical brain activity, circadian rhythms, fluids and animal population. The generalization of discrete graphs are *fuzzy graphs*, whereas *chaotic graphs* are more general than fuzzy graphs. The biological properties of biological isomers represent a chain of ∞-chaotic graphs, which represent the biological properties like link, growth toxics and pharmaceuticals [11].

Quantum graphs attracted the interest of the quantum chaos community because they can be considered as typical and simple examples for the class of systems in which classically chaotic dynamics implies universal correlations in the semiclassical limit. Up to now there is only a limited understanding of the reasons for this universality, and quantum graph models provide a valuable opportunity for mathematically rigorous investigations of the phenomenon [20].

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