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On the inverse spectral problems for quantum graphs

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Abstract We review some aspects of inverse spectral problems for quantum graphs. Under hypothesis of rational independence of lengths of edges it is possible, thanks to trace formulas, to reconstruct informations on compact and not compact graphs from the knowledge, respectively, of the spectrum of Laplacian and of the scattering phase. In the case of Sturm-Liouville operators defined on compact graphs and in general for differential operators on compact star-graphs, unknown potentials can be recovered from the knowledge of the spectrum of operators obtained imposing different boundary conditions.

Introduction

Quantum graphs are metric graphs provided with a selfadjoint operator that describes the dynamics of waves on the graph. The most natural application of a quantum graph is in the study of nanoscopic networks and their quantum properties, and in the new important area of technological development in quantum wires. Quantum graphs are in general good models for wave dynamics in thin structures, for example in the case of photonic crystals, or in chemistry for the study of dynamics of π-electrons in naphtalene molecule (see [7]).

In the present work we deal with the spectral problems of quantum graphs. (Direct) spectral problem is usually referred at the problem of obtaining the

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spectrum of an operator from information about the graph; instead the inverse spectral problem is in general referred to acquiring information about the system from the knowledge of the spectrum of a selfadjoint operator defined on the graph.

We review some inverse problems under different sets of hypotheses. In the first section we introduce fundamental definitions concerning selfadjoint operators and quantum systems on graphs. In the second and third ones we study inverse problems on compact graphs and answering to the question of which information on the graph we can recover with or without the hypothesis of rational independence of lengths of edges. In the fourth section we consider non compact graphs and search for the relations between the scattering on graph, its spectrum and its topological structure. The final section is dedicated to recovering potentials of Sturm-Liouville operators defined on compact graphs from spectra of different problems that are obtained varying boundary conditions at vertices. We present the same problem for general differential operator on compact star-shaped graphs.

1 Fundamental definitions

A *graph* is a couple of at most countable sets: $\Gamma = (\mathcal{V}, \mathcal{E})$, with $\mathcal{V} = \{v_i\}_{i=1}^{V}$ set of *vertices* and $\mathcal{E} = \{e_i\}_{i=1}^{E}$ set of *edges*.

Every edge is a binary relation between two vertices: if $e \in \mathcal{E}$, then $e = \{v, w\} = \{w, v\}, v, w \in \mathcal{V}$; we say that the vertices v, w are *incident* to e and indicate it with $v, w \sim e$ (loops and multiple edges are also admitted, for example: $e = \{v, v\}$ is a loop).

With *oriented* graph we mean a graph in which an orientation has been defined on every edge. We will call *bonds* the oriented edges and indicate the set of bonds with $\mathcal{B}$, so if $b \in \mathcal{B}$, then $b = (v, w) \in \mathcal{V} \times \mathcal{V}$. The inverse bond of b is simply defined as $\bar{b} = (w, v)$. By definition, $\mathcal{B}$ contains the bonds and their inverse bonds (so $|\mathcal{B}| = 2E$), instead if we consider a precise orientation for every edge, we can indicate the set of such bonds always with $\mathcal{E}$, without considering the edges with inverse orientation. From now on we are going to consider only oriented graphs.

If we put an orientation on a graph it is possible to turn the graph into a metric system defining a length function. A *metric graph* is a graph with a length assigned to every bond: $L_b \in (0, +\infty]$ for every $b \in \mathcal{B}$ and the property that $L_b = L_{\bar{b}}$. So it is possible to define the length of every edge without contradiction: $L_e := L_b = L_{\bar{b}}$, if $b = (v, w)$ and $e = \{v, w\}$.

A *compact* graph is a graph with a finite number of edges with finite length, otherwise we will call it *non compact*.

On an edge e of a metric graph we can define a coordinate $x_e \in [0, L_e]$ and the respective Lebesgue measure dx_e (the coordinate increases following the orientation).

If we want a quantum system we need to identify a Hilbert space $\mathcal{H}$ as space of states. In our case, if not specified otherwise, we will always take the Hilbert space associated to one particle moving on the graph

$$\mathcal{H} = L^2(\Gamma) := \bigoplus_{e\in\mathcal{E}} L^2(e, dx_e)$$

that is, a square-integrable function on a metric graph can be thought as a collection of E L^2-functions defined on every edge:

$$\psi := (\psi_1(x_1), \psi_2(x_2), \dots \psi_E(x_E)), \quad x_1 \in [0, L_1], x_2 \in [0, L_2], \dots, x_E \in [0, L_E]$$

and so an operator on a graph acts on the set of these functions.

A *quantum graph* is a triple $(\Gamma, H, \mathcal{D}(H))$ with Γ metric graph and H a selfadjoint operator in its domain $\mathcal{D}(H) \subseteq \mathcal{H}$.

A concrete example is given by the *Laplacian* on a metric graph, defined as

$$H := -\frac{d^2}{dx^2} = \left(-\frac{d^2}{dx_e^2}\right)_{e\in\mathcal{E}}$$

that acts on every edge as a second derivative. A theorem from [1] guarantees conditions on its domain for selfadjointness. Let us denote the degree of a vertex v by d_v that is the number of edges incident to v, that we assume finite for every vertex:

$$d_v := |\{e \in \mathcal{E} : e = \{v, w\}, w \in \mathcal{V}\}|.$$

Theorem 1.1. *Let Γ be a metric graph and H the Laplacian with domain $\mathcal{D}(H) \subseteq \mathcal{H}$. The operator H is selfadjoint on $\mathcal{D}(H)$ if and only if $\mathcal{D}(H)$ is the set of ψ such that:*

(i) $\psi \in \bigoplus_{e\in\mathcal{E}} H^2(e, dx_e)$, *with $H^2(e, dx_e)$ Sobolev space on edge e:*

$$H^2(e, dx_e) := \{\phi_e \in L^2(e, dx_e) : \phi_e'' \in L^2(e, dx_e)\};$$

(ii) *(vertices condition) for every $v \in \mathcal{V}$ exist $A_v, B_v \in Mat(d_v)$ such that*

- $rk(A_v|B_v) = d_v$, *with $(A_v|B_v)$ matrix that has as columns the union of columns of A_v and B_v;*
- $A_v B_v^*$ *is selfadjoint;*
- $A_v\psi(v) + B_v\psi'(v) = 0$, *where $\psi(v)$ is the vector $(\psi_1(v), \dots, \psi_{d_v}(v))$ of the components of ψ on the edges incident to v valued in the coordinate corresponding to v on the edge.*

So with the previous conditions, $(\Gamma, H, \mathcal{D}(H))$ is a quantum graph.

We observe that the vertices conditions are implicitly determined also by assigning a *scattering matrix* σ^v at each vertex v, that we define

$$\sigma^v(k) := -(A_v + ikB_v)^{-1}(A_v - ikB_v), \quad k \in \mathbb{C}. \tag{1}$$

See [1] for the physical meaning of the scattering matrices and their relation with transmission through the vertices of waves moving along the graph.

Let us consider a particular case of conditions at vertices that assure self-adjointness thanks to the theorem 1.1. We take for every vertex v

$$A_v = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & 1 & -1 \\ 0 & 0 & \dots & \dots & 0 & 0 \end{pmatrix}, \quad B_v = \begin{pmatrix} 0 & 0 & \dots & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \dots & 0 & 0 \\ 1 & 1 & \dots & \dots & 1 & 1 \end{pmatrix}$$

and so we obtain *Kirchhoff-Neumann* (K-N) conditions: for every vertex v, ψ has to satisfy

$$\begin{cases} \psi \text{ continuous in } v \\ \sum_{e \sim v} \psi'_e(v) = 0. \end{cases} \tag{2}$$

where the derivatives are taken in the outgoing direction from the vertex v and the continuity condition is: $\psi_1(v) = \dots = \psi_{d_v}(v)$.

In this case the scattering matrices are k-indipendent (so energy indipendent, see [1]) and their elements have the explicit form ([9]):

$$\sigma^v_{i,j} = \frac{2}{d_v} - \delta_{i,j}, \tag{3}$$

where $\delta_{i,j}$ is the Kronecker delta.

2 Compact graphs: inverse problem with rational indipendence of edges lenghts

In this section we deal with the inverse spectral problem for compact quantum graphs. From now on Γ will be a metric compact graph, $(H, \mathcal{D}(H))$ the Laplacian with K-N conditions.

Under these hypotheses a *trace formula* exists that gives a relation between the spectrum of the Laplacian and the topological structure of the graph.

First of all let us remark that from [1] (theorem 3.1.1) we have that a compact quantum graph with K-N conditions has a discrete spectrum composed by positive eigenvalues with finite multiplicity and accumulation at infinity.

So we can express the spectrum in this way:

$$\sigma(H) = \{k_n^2\}_{n\in\mathbb{N}} \subseteq \mathbb{R}, \qquad 0 = k_0^2 < k_1^2 \leq k_2^2 \leq \dots$$

Now we can define a distribution, the *spectral density* u:

$$u(k) := 2\delta(k) + \sum_{n=1}^{\infty} (\delta(k-k_n) + \delta(k+k_n))$$

and its Fourier transform:

$$\sqrt{2\pi}\hat{u}(l) = 2 + \sum_{n=1}^{\infty} (e^{-ik_n l} + e^{ik_n l}).$$

The trace formula gives an alternative formula for the spectral density and its transform involving periodic orbits on the graph (see [11]).

Theorem 2.1. *Let Γ be a metric, compact, connected graph and $(H, \mathcal{D}(H))$ the K-N Laplacian. Then the following trace formulas establish the relation between the spectrum $\sigma(H) = \{k_n^2\}_{n\in\mathbb{N}}$ of H and the set of periodic orbits, the total length and the Euler characteristic of the graph:*

$$u(k) = \chi\delta(k) + \frac{L}{\pi} + \frac{1}{2\pi} \sum_{p\in\mathcal{P}} (\mathcal{A}_p e^{ikl_p} + \mathcal{A}_p^* e^{ikl_p}), \tag{4}$$

$$\sqrt{2\pi}\hat{u}(l) = \chi + 2L\delta(l) + \sum_{p\in\mathcal{P}} (\mathcal{A}_p \delta(l-l_p) + \mathcal{A}_p^* \delta(l+l_p)), \tag{5}$$

where

$$\mathcal{A}_p = l_{p'} \left(\prod_{\sigma_{ij}^v \in \mathcal{T}(p)} \sigma_{ij}^v \right), \quad \mathcal{A}_p^* = l_{p'} \left(\prod_{\sigma_{ij}^v \in \mathcal{T}(p)} \overline{\sigma_{ij}^v} \right),$$

- $\chi := V - E$ *is the Euler characteristic of the graph;*
- L *: sum of the lengths of the edges of Γ, called the total length;*
- $\mathcal{P}$ *set of periodic orbits on Γ. A periodic orbit is an equivalence class of oriented closed paths invariant under the action of a cyclic permutation of edges of the path;*
- p' *primitive orbit of p. If p has a length multiple of lengths of other orbits, p' is the orbit among these ones that has the minimal length;*
- l_p *length of the orbit p;*
- $\mathcal{T}(p)$ *set of all scattering matrices elements $\sigma_{i,j}^v$ associated to vertices v and edges i, j that belong to the periodic orbit p.*

Knowledge of the spectrum allows one to define the spectral density, and thanks to the trace formula we obtain that the support of (5) is the set of the lenghts of all periodic orbits of the graph. In [11], if we assume hypothesis of rational independence of edges lengths and cleaning of graph (absence of vertices with degree 2), an algorithmic procedure to recover information about the graph is presented. The most important steps are the definitions of three sets $\mathcal{L}'' \subseteq \mathcal{L}' \subseteq \mathcal{L}$ where:

- $\mathcal{L} := \{l_p \,:\, p \in \mathcal{P}\}$ is the set of the lengths of periodic orbits that can be obtained by the support of (5);
- $\mathcal{L}' := \left\{ l \in \mathcal{L} \,:\, \sum_{p\in\mathcal{P}: l = l_p} \mathcal{A}_p \neq 0 \right\}$ gives connectivity of the graph because it contains the lengths of the edges and combination of lengths of couples of edges that are connected;
- $\mathcal{L}'' := \{l \in \mathcal{L}' : l \leq 2L\}$, that is a finite set, and so one can find a basis of lengths whose a semi-integer combination can produce all the other elements of $\mathcal{L}''$. The basis with the minimal lengths is the set of the lengths of the edges of the graph or their double (depending if an edge forms a loop or not respectively).

And so it is possible to recover the edges lengths $\{L_e\}_{e\in\mathcal{E}}$ and how they are connected, i.e. it is possible to reconstruct the graph.

Theorem 2.2. *Let Γ be a compact, connected, quantum graph with $(H, \mathcal{D}(H))$ K-N Laplacian. If we suppose that*

(i) Γ is clean (no vertices of degree 2),
(ii) the lengths of the edges are rational independent,

then from the spectrum $\sigma(H)$ it is possible to reconstruct uniquely the graph Γ (that is, the lengths of edges and how they are connected).

In [4] a counterexample is produced that shows the failure of reconstruction of graphs without the hypothesis of rational independence. Let's take Γ_1 in Figure 1 and K-N Laplacian $(H, \mathcal{D}(H))$.

Its lengths are rational dependent. The spectrum of H is obtained solving the secular equation (see [4]), and consists of zeros of the function

$$f_1(k) = \tan(2(a+b)k) + \frac{2\tan(ak) + 2\tan(bk) + \tan((2a+b)k) + \tan((a+2b)k)}{1 - (2\tan(ak) + \tan(bk))(\tan(bk) + \tan((2a+b)k) + \tan((a+2b)k))}.$$

If we consider now $(H, \mathcal{D}(H))$ on graph Γ_2 in Figure 2, always with rational dependence lengths, this time the spectrum of H consists of zeros of the function

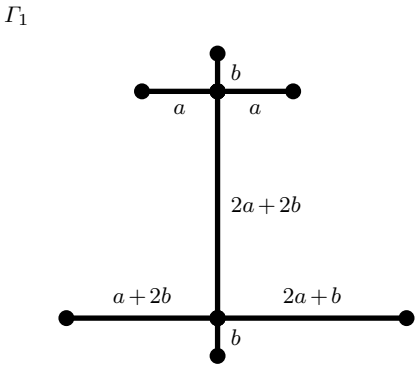

Fig. 1: graph Γ_1

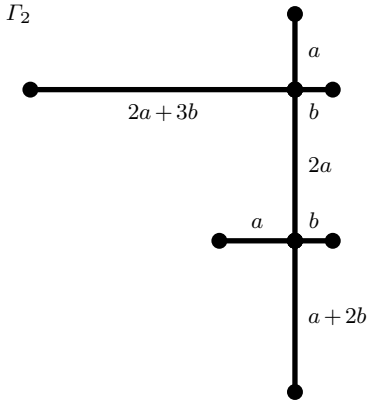

Fig. 2: graph Γ_2

$$f_2(k) = \tan(2ak)\cdot \frac{2\tan(ak)+2\tan(bk)+\tan((a+2b)k)+\tan((2a+3b)k)}{1-(\tan(ak)+\tan(bk)+\tan((a+2b)k)(\tan(ak)+\tan(bk)+\tan((2a+3b)k))}.$$

From [3] we have that zeros of f_1 and zeros of f_2 are the same, that is, Γ_1 and Γ_2 are isospectral graphs, so there's the failure of unique reconstruction of the graph from the spectrum of the Laplacian.

3 Compact graphs: inverse problem in general

Now we do not assume the rational independence of edges lenghts. Without this hypothesis only the Euler characteristic can be recovered (see [9]) and we have, thanks again to the trace formula, an explicit formula for χ.

Theorem 3.1. *Let Γ be a compact, connected, quantum graph with $(H, \mathcal{D}(H))$ the K-N Laplacian. Then from the spectrum $\sigma(H) = \{k_n^2\}_{n\in\mathbb{N}}$ it is possible to recover uniquely the Euler characteristic χ of the graph by the formula:*

$$\chi = 2 + 2 \lim_{t\to+\infty} \sum_{k_n\neq 0} \cos(k_n/t) \left(\frac{\sin(k_n/2t)}{k_n/2t}\right)^2 \tag{6}$$

$$= 2 - 2 \lim_{t\to+\infty} \sum_{k_n\neq 0} \frac{1 - 2\cos(k_n/t) + \cos(2k_n/t)}{(k_n/t)^2}. \tag{7}$$

It is possible to extend this result to bounded perturbation of the Laplacian (see [9]): let H_q be the operator

$$H_q = H + q, \quad \mathcal{D}(H_q) := \mathcal{D}(H).$$

where $q \in L^\infty(\Gamma)$ acts as a multiplication operator. H_q is selfadjoint in its domain and has a discrete spectrum: $\sigma(H_q) := \{(k'_n)^2\}_{n\in\mathbb{N}}$. Thanks to the asymptotical behaviour of the eigenvalues respect that of Laplacian eigenvalues ($|k_n - k'_n| = O\left(\frac{1}{n}\right)$) formula (6) holds the same replacing k_n with k'_n.

Theorem 3.2. *Let Γ be a compact, connected, quantum graph with $(H_q, \mathcal{D}(H_q))$ the operator defined above. Then from the spectrum $\sigma(H_q) = \{(k'_n)^2\}_{n\in\mathbb{N}}$ it is possible to recover uniquely the Euler characteristic χ of the graph by the formula:*

$$\chi = 2 + 2 \lim_{t\to+\infty} \sum_{n=0}^{\infty} \cos(k'_n/t) \left(\frac{\sin(k'_n/2t)}{k'_n/2t}\right)^2 \tag{8}$$

4 Non compact graphs: inverse problem with scattering

Now we are going to consider graphs with finite number of edges but also with infinite lengths. We deal with inverse problems for graphs that consist of a compact part and bonds of infinite length attached to some vertices and going to infinity. We call these bonds *leads*, their set $\mathcal{B}^{ext}$, and denote them with $(v, \infty) \in \mathcal{B}^{ext}$ (inverse bonds of leads are not admitted).

So the graph can be expressed in the form $\Gamma = (\mathcal{V}, \mathcal{B})$, $\mathcal{B} := \mathcal{B}^{int} \cup \mathcal{B}^{ext}$ where $\mathcal{B}^{int}$ are the bonds of the compact part.

Let us also make, for simplicity, the hypothesis of at most one lead attached to every vertex, so $|\mathcal{B}^{ext}| = N \leq V$. If we do not consider inverse bonds, we denote with $\mathcal{E} = \mathcal{E}^{int} \cup \mathcal{E}^{ext}$, $\mathcal{E}^{int}$ set of internal edges of compact part of the graph, and $\mathcal{E}^{ext}$ edges associated to leads (obviously $\mathcal{E}^{ext} = \mathcal{B}^{ext}$).

The eigenvalues problem for the Laplacian with general selfadjoint conditions at vertices

$$-\frac{d^2}{dx_b^2}\psi_b(x) = k^2\psi_b(x), \quad b \in \mathcal{B}$$

on the bonds in the compact part of the graph has the solutions:

$$\psi_b(x) = \alpha_b e^{ikx_b} + \alpha_{\bar{b}} e^{ikL_b} e^{-ikx_b}, \quad \text{if } b \in \mathcal{B}^{int} \tag{9}$$

while on leads we are interested in solution of the form:

$$\psi_b(x) = C_b^{in} e^{-ikx_b} + C_b^{out} e^{ikx_b}, \quad \text{if } b \in \mathcal{B}^{ext}. \tag{10}$$

In [1] it is explained how are related the $2E-$vector of coefficients of outgoing waves from vertices $\alpha := \{\alpha_b\}_{b\in\mathcal{B}^{int}}$, the $N-$vectors of coefficients of waves that leave the graph on leads $C^{out} := \{C_b^{out}\}_{b\in\mathcal{B}^{ext}}$ and the ones that reach the graph on the leads $C^{in} := \{C_b^{in}\}_{b\in\mathcal{B}^{ext}}$:

$$\begin{pmatrix} C^{out} \\ \alpha \end{pmatrix} = \begin{pmatrix} R(k) & T_o(k) \\ T_i(k) & S(k) \end{pmatrix} \begin{pmatrix} C^{in} \\ \alpha \end{pmatrix} \tag{11}$$

where the previous matrix is $(2E+N)\times(2E+N)$ and

- $S(k)$ describes the evolution of waves inside the compact part of the graph;
- $R(k)$ describes the immediate reflection of waves from the graph (from leads into leads);
- $T_o(k)$ and $T_i(k)$ describe transmission form the compact part out and from the leads into the compact part correspondingly.

Solving equation (11) (see [1] for explicit calculation) we find that

$$C^{out} = \Sigma(k) C^{in}$$

where $\Sigma(k) := R(k) + T_o(k)(\mathbb{1} - S(k))^{-1} T_i(k)$ is the *scattering matrix* [1] ($\mathbb{1}$ is the identity matrix). The knowledge of this matrix gives the opportunity

[1] the previous scattering matrix already defined can be thought as a restriction of this one for compact graphs. In fact in a proper base: $\Sigma = \mathrm{diag}(\sigma^1, \ldots, \sigma^V)$

to obtain again a method of reconstruction of a metric graph. If we define the *scattering phase* Φ by

$$\Phi(k) := -i \log \det(\Sigma(k))$$

and the *resonance density* u by

$$u(k) := \frac{1}{2\pi} \frac{d\Phi(k)}{dk}$$

we have in this case a trace formula for the resonance density (see [5] and [6]).

Theorem 4.1. *Let Γ be a non-compact, metric graph formed by a compact part with at most one lead attached to every vertex, $(H, \mathcal{D}(H))$ the K-N Laplacian and Σ the scattering matrix associated. The next formula holds for the resonance density:*

$$u(k) = \frac{\tilde{L}}{\pi} + \frac{1}{2\pi} \sum_{p \in \tilde{\mathcal{P}}} \left(\tilde{\mathcal{A}}_p e^{ikl_p} + \tilde{\mathcal{A}}_p^* e^{-ikl_p} \right)$$

where

$$\tilde{\mathcal{A}}_p = l_{p'} \left(\prod_{\sigma_{ij}^v \in \tilde{\mathcal{T}}(p)} \sigma_{ij}^v \right), \quad \tilde{\mathcal{A}}_p^* = l_{p'} \left(\prod_{\sigma_{ij}^v \in \tilde{\mathcal{T}}(p)} \overline{\sigma_{ij}^v} \right),$$

- $\tilde{L}$ *is the total length of the compact part of the graph:* $\tilde{L} := \frac{1}{2} \sum_{b \in \mathcal{B}^{int}} L_b$*;*
- $\tilde{\mathcal{P}}$ *is the set of periodic orbits in the compact part of the graph;*
- p' *primitive orbit of* p*;*
- l_p *the length of the orbit* p*;*
- $\tilde{\mathcal{T}}(p)$ *set of all scattering matrices* σ^v *associated to vertices that belong to the periodic orbit* p *in the compact part of the graph.*

As did in the compact case from the knowledge of spectrum, now from the knowledge of the scattering phase and under the same hypotheses of Kirchhoff-Neumann conditions, cleanliness and rational independence of lengths it is possible to reconstruct uniquely the graph with the same algorithm (find the support of the Fourier transform of u, and from it the lengths of edges and connectivity).

Theorem 4.2. *Let Γ be a non-compact, connected, quantum graph with $(H, \mathcal{D}(H))$ K-N Laplacian, formed by a compact part with at most one lead attached to every vertex. If we suppose that*

(*i*) *Γ is clean,*

(*ii*) *the lengths of the edges are rational independent,*

then from the scattering matrix Σ it is possible to reconstruct uniquely the compact part of the graph Γ.

It is possible to find, also in this case, some counterexamples. The impossibility of unique reconstruction holds also for more general operators respect to the Laplacian H: let Γ be a non-compact graph with a finite number of bonds and leads, and H_Q be the Schrödinger operator

$$H_Q := H + Q \tag{12}$$

$$H_Q\psi = \left\{ -\frac{d^2}{dx_e^2}\psi_e(x_e) + q_e(x_e)\psi_e(x_e) \right\}_{e\in\mathcal{E}}$$

where $Q = \{q_e\}_{e\in\mathcal{E}} \in L^1(\Gamma) := \bigoplus_{e\in\mathcal{E}} L^1(e)$, Q real-valued and on the leads b there is the further request

$$\int_b (1+|x_b|)|q_b(x_b)|dx_b < +\infty.$$

Previously, from the knowledge of the scattering matrix, one could find the scattering phase and, with the hypothesis of rational independence, reconstruct the graph.

The results given below show that if one knows the scattering matrix associated to operator (12) (defined in a similar way to the one of (10)) without further hypotheses on lengths of edges, reconstruction is no more possible. Also recovering other informations is not accessible, for example potential or information about Schrödinger operator.

We remark the fact that if two scattering matrices Σ and Σ' are similar (see [10]) then the respective Schrödinger operators are unitary equivalent. So the next results have to be intended up to unitary equivalence of operators and up to similarity for scattering matrices (for further details, see always [10]):

(*i*) (Bargmann) the knowledge of the graph, the selfadjoint boundary conditions at the vertices and the scattering matrix Σ for the Schrödinger operator H_Q is generally not enough to determine the real-valued potential Q (for a proof see [2]);

(*ii*) the knowledge of the scattering matrix Σ for the K-N Laplacian is generally not enough to determine the topological structure of the graph uniquely;

(*iii*) the knowledge of the topological structure of the graph and of the scattering matrix Σ for the K-N Laplacian is generally not enough to determine the graph uniquely;

(*iv*) the knowledge of the graph, the real-valued potential Q and the scattering matrix Σ for the Schrödinger operator H_Q is generally not enough to determine the Schrödinger operator uniquely.

Where not otherwise specified, the counterexamples are all shown in [10].

5 Inverse problem for Sturm-Liouville operators on graphs: recovering potential

We now consider the problem of reconstruction of potential from the knowledge of the spectrum of the operator associated to various vertices conditions on compact graphs in the case of Sturm-Liouville operators, and then more in general for differential operators of a variable order.

Let $\Gamma = (\mathcal{V}, \mathcal{E})$ be a compact graph. We call

$$\mathcal{V}_0 := \{v \in \mathcal{V} : d_v = 1\}$$

the set of *external vertices* the set of vertices of degree 1 ($|\mathcal{V}_0| = V_0$). The others are called *internal* and indicated with $\mathcal{V}_1$ ($|\mathcal{V}_1| = V_1$), so that

$$\mathcal{V} = \mathcal{V}_0 \cup \mathcal{V}_1, \quad V = V_0 + V_1.$$

Edges that are incident to external vertices are called *external edges* and indicated with $\mathcal{E}_0$ (the same for bonds).

A *cycle* is an ordered sequence of bonds $(b_1, b_2, \dots, b_n)$ such that they form a closed curve: $b_1 = b_n$. We indicate the set of edges whose bonds form a cycle with $\mathcal{E}_2$, instead the ones that do not form a cycle with $\mathcal{E}_1$. Obviously $\mathcal{E}_0 \subseteq \mathcal{E}_1$ because we are not considering inverse bonds.

We enumerate the edges as follows:

- $\mathcal{E}_0 := \{e_1, \dots, e_p\}$;
- $\mathcal{E}_1 := \{e_1, \dots, e_r\}$, $r \geq p$, $p = V_0$ (every external vertex is incident to only one external edge);
- $\mathcal{E}_2 := \{e_{r+1}, \dots, e_E\}$.

As always we assign lengths to edges and put an orientation on the graph so that coordinates on the edges are well defined. Let us take a function $\psi = (\psi_e)_{e \in \mathcal{E}}$ with every $\psi_e \in AC(e)$, where $AC(e)$ is the set of absolute continuous functions on e; we take $Q = (q_e)_{e \in \mathcal{E}} \in L^1(\Gamma)$ to play the role of potential.

We define the *Sturm-Liouville problem*:

$$-\frac{d^2}{dx_e^2}\psi_e(x) + q_e(x)\psi_e(x) = \lambda \psi_e(x), \quad e \in \mathcal{E} \tag{13}$$

with K-N conditions on every internal vertex, that here we rewrite for convenience: for every $v \in \mathcal{V}_1$

$$\begin{cases} \psi \text{ continuous in } v \\ \sum_{e\sim v} \psi'_e(v) = 0. \end{cases} \tag{14}$$

With the specification of conditions on external vertices, we can produce various associated problems:

- $L_0(\Gamma)$ *problem:* (13)-(14) problem with *Dirichlet* conditions on external vertices, that is: for every $v \in \mathcal{V}_0$

$$\psi_e(v) = 0, \quad \text{for every } \ e \sim v;$$

- $L_k(\Gamma)$ *problems,* $k = 1, \dots, p-1$: (13)-(14) problem with Dirichlet conditions on external vertices except for the vertex v_k, that has *Neumann* condition

$$\begin{aligned} &\psi'_e(v_k) = 0, \quad \text{for every } e \sim v_k, \\ &\psi_e(v) = 0, \quad \text{for every } v \in \mathcal{V}_0 - \{v_k\}, e \sim v; \end{aligned}$$

- $L^\xi_\nu(\Gamma)$ *problems,* $\xi = r+1, \dots, E$; $\nu = 0, 1$: ξ identifies an edge e_ξ part of a cycle. Denoting with v_ξ the vertex with coordinate zero on e_ξ, the $L^\xi_\nu(\Gamma)$ problem is (13) problem with K-N conditions on every internal vertex but not in v_ξ. Here we have K-N condition involving every incident edge except e_ξ[2], while along e_ξ, the problem with $\nu = 0$ corresponds to Dirichlet condition on v_ξ, instead the problem with $\nu = 1$ to Neumann condition on v_ξ. In the external vertices there are Dirichlet conditions:

$$\begin{cases} \psi_{e_\xi}(v_\xi) = 0, & \text{if } \nu = 0; \\ \psi'_{e_\xi}(v_\xi) = 0, & \text{if } \nu = 1; \end{cases}$$

$$\psi_e(v) = 0, \quad \text{for every } v \in \mathcal{V}_0, e \sim v_k.$$

Every problem defined above gives a different spectrum of the operator $H_Q := -\frac{d^2}{dx^2} + Q$ as solution. Let us associate every spectral set to problems in this way:

[2] So in the vertex v_ξ K-N conditions have to be rewritten as

$$\sum_{e_\xi \neq e \sim v_\xi} \psi'_e(v_\xi) = 0$$

Problems	**Eigenvalues sets**
$L_0(\Gamma)$	$\Lambda_0 := \{\lambda_{0n}\}_{n\geq 1}$
$L_k(\Gamma)$	$\Lambda_k := \{\lambda_{kn}\}_{n\geq 1}$
$L_\nu^\xi(\Gamma)$	$\Lambda_\nu^\xi := \{\lambda_{\nu n}^\xi\}_{n\geq 1}$

Knowledge of all this spectral sets allows one to recover an unknown potential of the H_Q operator, as stated in [13].

Theorem 5.1. *Let Γ be a metric, compact, graph, and $H_Q := -\frac{d^2}{dx^2} + Q$ a Schrödinger operator as previously defined. From the knowledge of*

- Λ_0 *;*
- Λ_k *for $k = 1, \dots, p-1$;*
- Λ_ν^ξ *for $\xi = r+1, \dots, E$ and $\nu = 0, 1$*

it is possible to recover uniquely the potential $Q = (q_e)_{e\in\mathcal{E}}$.

Let us now deal with the case of general differential operators of variable order. In this case, if we admit also the presence of cycles, we have a result for star-shaped graphs.

Let $\Gamma = (\mathcal{V}, \mathcal{E})$ be a metric, compact graph, more specifically a star-graph with a cycle, i.e. if $\mathcal{V} = \{v_0, \dots, v_{E-1}\}$ and $\mathcal{E} = \{e_0, \dots, e_{E-1}\}$ we suppose that $e_0 := (v_0, v_0)$ is a loop, and all the other edges are incident to v_0: $e_j := (v_j, v_0)$, with orientation in the direction entering in the vertex v_0 (so we can denote the edges simply with correspondent indices). Also in this case we take functions $\psi \in \bigoplus_{e\in\mathcal{E}} AC(e)$.

Fix numbers $2 = n_0 \leq n_1 \leq \ldots \leq n_{E-1}$, and consider differential equations

$$\psi_j^{(n_j)}(x) + \sum_{\mu=0}^{n_j-2} q_{\mu j}(x)\psi_j^{(\mu)}(x) = \lambda\psi_j(x). \quad j = 0, \dots, E-1 \tag{15}$$

where $q_{\mu j} \in L^1(e)$ for every j, and so we have a potential $Q := \{q_{\mu j}\}$ with $j = 0, \dots, E-1$ and $\mu = 0, \dots, n_j - 2$.

Let us define conditions on the vertex v_0. First of all we introduce the linear forms

$$U_{j\nu}(\psi_j) := \sum_{\mu=0}^{\nu} \gamma_{j\nu\mu}\psi_j^{(\mu)}(L_j)$$

with $j = 1, \dots, E-1$; $\nu = 0, \dots, n_j - 1$ and $0 \neq \gamma_{j\nu\mu} \in \mathbb{C}$ are fixed complex numbers. Consider also the form

$$U_{0\nu}(\psi_0) := \psi_0^{(\nu)}(L_0), \quad \nu = 0, 1.$$

We define continuity conditions $C(\nu), C(0,\alpha)$ and Kirchhoff conditions $K(\nu)$ of order ν as follows:

- $C(\nu)$:

$$U_{E-1,\nu}(\psi_{E-1}) = U_{j\nu}(\psi_j), \quad j = 0,\dots,E-2;\ \nu < n_j - 1;$$

- $C(0,\alpha) : C(0)$ conditions and $\alpha\psi_0(0) = \psi_0(L_0)$;
- $K(\nu)$:

$$\sum_{j:\nu<n_j} \psi_j^{(\nu)}(L_j) = \delta_{1\nu}\psi_0'(0)$$

where δ_{jk} is the Kronecker delta and $\alpha \in \mathbb{C} - \{0\}$.

We define now, for fixed s,k,μ, with $s \in \{1,\dots,E-1\}, k \in \{1,\dots,n_s - 1\}$ and $\mu \in \{k,\dots,n_s\}$, the $L_{sk\mu}$ problem for the variable order differential operators. It can be defined as the problem (15) with

(i) continuity conditions: $C(0,\alpha_s)$, $C(\nu)$, for $\nu = 1,\dots,k-1$, and $K(\nu)$, for $\nu = k,\dots,n_s - 1$ at the vertex v_0 (α_s being non-zero numbers at least two of which are different);
(ii) boundary conditions:

$$\psi_k^{(\nu-1)}(0) = 0, \quad \nu = 1,\dots,k-1,\mu;$$

$$\psi_j^{(\nu-1)}(0) = 0, \quad \nu = 1,\dots,n_j - k;\ j = 1,\dots,E-1;\ j \neq s : n_j < k;$$

$$\psi_j(0) = 0, \quad j = 1,\dots,E-1 : n_j \leq k$$

Solutions to these problems give discrete spectra $\Lambda_{sk\mu} := \{\lambda_{lsk\mu}\}_{l\geq 1}$, for $s = 1,\dots,E-1; k = 1,\dots,n_s - 1; \mu = k,\dots,n_s$. Always from [13] we have a theorem of reconstruction of the potential Q.

Theorem 5.2. *Let Γ be a metric star-graph with a loop in the internal vertex. Consider the equations (15) with associated $L_{sk\mu}$ problems, $s = 1,\dots,E-1; k = 1,\dots,n_s - 1; \mu = k,\dots,n_s$ on the graph. Then from the knowledge of $\Lambda_{sk\mu}$, for every s,k,μ, it is possible to recover the unknown potential Q.*

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