Quantum Graphs: 
$\mathcal{PT}$-symmetry and reflection symmetry of the spectrum

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Abstract

Not necessarily self-adjoint quantum graphs – differential operators on metric graphs – are considered. Assume in addition that the underlying metric graph possesses an automorphism (symmetry) $\mathcal{P}$. If the differential operator is $\mathcal{PT}$-symmetric, then its spectrum has reflection symmetry with respect to the real line. Our goal is to understand whether the opposite statement holds, namely whether the reflection symmetry of the spectrum of a quantum graph implies that the underlying metric graph possesses a non-trivial automorphism and the differential operator is $\mathcal{PT}$-symmetric. We give partial answer to this question by considering equilateral star-graphs. The corresponding Laplace operator with Robin vertex conditions possesses reflection-symmetric spectrum if and only if the operator is $\mathcal{PT}$-symmetric with $\mathcal{P}$ being an automorphism of the metric graph.

1 Introduction

Our paper is devoted to spectral theory of quantum graphs – ordinary differential operators on metric graphs. This is one of the most rapidly growing areas of modern mathematical physics due to its important applications in physics and applied sciences as well as interesting mathematical problems that emerge. It appeared that symmetries of the underlying metric graphs play a very important role in constructing counterexamples and proving spectral estimates. If the theory of self-adjoint operators on metric graphs is rather well-understood, the corresponding theory of non-self-adjoint operators is in its incubatory stage. The main subject of our studies is precisely non-self-adjoint quantum graphs.

The main goal of our current paper is to understand connections to the theory of $\mathcal{PT}$-symmetric operators – yet another area of mathematical physics that has got a lot of attention recently. Standard quantum mechanics in one dimension is described by self-adjoint differential operators leading to purely real spectrum. Extending the set of allowed operators by including $\mathcal{PT}$-symmetric ones leads to the spectrum with reflection symmetry with respect to the real axis, not only as a set but also including multiplicities. (In the classical studies $\mathcal{P}$ is the reflection operator $(\mathcal{P}f)(x) = f(-x)$ and $\mathcal{T}$ is the time-reversal operator of complex conjugation $(\mathcal{T}f)(x) = \overline{f(x)}$.) If a metric graph possesses a certain automorphism (symmetry) $\mathcal{P}$, then the corresponding differential operator can be chosen to have $\mathcal{PT}$-symmetry, leading to reflection-symmetric spectrum. We would
like to understand whether this mechanism is unavoidable for a quantum graph to have a reflection-symmetric spectrum.

We consider the case of an equilateral star-graph \( \Gamma \), as the one in Figure 1, formed by \( N \) identical edges joined at the central vertex, together with the Laplace operator acting on it. The metric graph \( \Gamma \) has a rich symmetry group generated by the permutations of the edges. If, the so-called standard vertex conditions (continuity of the function and vanishing of the sum of normal derivatives), are introduced, then the corresponding operator is self-adjoint and the spectrum is real (an infinite set of discrete eigenvalues tending to \(+\infty\)). One may break the self-adjointness by introducing Robin conditions with non-real parameters at the degree-one vertices. It is relatively easy to see that if the set of Robin parameters is invariant under conjugation, then the corresponding Laplace operator is \( PT \)-symmetric with respect to a certain automorphism \( P \) of the underlying metric graph \( \Gamma \). Then the spectrum possesses reflection symmetry with respect to the real axis. Our main question is whether the opposite statement holds, namely, whether the reflection symmetry of the spectrum implies \( PT \)-symmetry of the operator with respect to a certain automorphism \( P \) of the metric graph \( \Gamma \). For an operator with discrete spectrum and eigenfunctions of the operator and its adjoint building a biorthogonal basis, one may easily construct a symmetry operator in the Hilbert space, provided the spectrum is reflection symmetric. Such symmetry operator is defined using the eigenfunctions and there is no guarantee that it comes from an automorphism of the metric graph.

Our main goal is to prove the following theorem:

**Theorem 1** (Main Theorem). Let \( L_h \) be the Laplace operator acting on the equilateral star-graph \( \Gamma \) with the domain given by standard vertex conditions at the internal vertex and Robin conditions including complex valued parameters \( h_i \) at the degree-one vertices. For the spectrum of the operator \( L_h \) to possess reflection symmetry with respect to the real line it is necessary and sufficient that the quantum graph \( L_h \) is \( PT \)-symmetric, where \( P \) is a certain automorphism of the underlying metric star-graph \( \Gamma \).

We doubt that the theorem holds for arbitrary metric graphs, but it might be interesting to characterize the class of graphs and vertex conditions for which a similar statement holds at least for the Laplace operator. In the case under consideration the metric graph \( \Gamma \) is an equilateral star-graph and the group of its automorphisms is clear. Moreover, we do not consider all possible differential operators on \( \Gamma \) but just the family \( L_h \) containing a finite number of (Robin) parameters. Therefore, we are going to prove first a slightly different theorem and obtain the Main Theorem 1 as its corollary:

**Theorem 2.** Let \( L_h \) be the Laplace operator acting on the equilateral star-graph \( \Gamma \) with the domain given by standard vertex conditions at the internal vertex and Robin conditions including complex valued parameters \( h_i \) at the degree-one vertices. For the spectrum of the operator \( L_h \) to possess reflection symmetry with respect to the real line it is necessary and sufficient that the set of Robin parameters \( \{h_i\}_{i=1}^N \) is invariant under conjugation.

Spectral theory of non-self-adjoint operators on the star-graph has already been discussed by one of the co-authors [1]. The main difference to the current paper is that Neumann conditions were assumed at the degree-one vertices, while one considered rotation-invariant conditions at the central vertex. Operators with the Robin conditions at degree-one vertices were considered by M. Žnojil [18, 19]. All these three papers are devoted to the problem of proving that the spectrum of the operator possesses reflection symmetry (with respect to the real or imaginary axis), provided the vertex conditions have a certain special form. Our interest is in proving the opposite statement.

The paper is organized as follows. In Section 2 we describe the model and discuss its elementary spectral properties. Section 3 is devoted to an easier direction of Theorem 2 proving if the set of Robin parameters \( \{h_i\}_{i=1}^N \) is invariant under conjugation, then the spectrum has reflection symmetry.
with respect to the real axis. The opposite (harder) statement is proven in the Section \[3\]. The last section is devoted to the proof of the Main Theorem \[4\]. The proofs of elementary Propositions \[1\] and \[2\] can be found in the Appendix.

2 Description of the Model and Definitions

In this section we define rigorously the Laplace operator on the equilateral star-graph \( \Gamma \), depicted in Figure \( \Gamma \) with complex Robin parameters at the degree one vertices. The operator we define should be consistent with the geometric picture – the vertex conditions should connect together values of the functions at each vertex separately.

Figure 1: Star-graph \( \Gamma \) with \( N \) edges.

More explicitly let us assume that the graph \( \Gamma \) is built of \( N \) edges \( e_1 \) till \( e_N \), each of unit length. We identify each edge with a separate copy of the interval \([0,1]\), where 1 corresponds to the unique internal vertex. Consider the Hilbert space \( \mathcal{H} = L^2((0,1), \mathbb{C}^N) \ni u = (u_1, \ldots, u_N) \) equipped with the inner product:

\[
\langle u, v \rangle := \sum_{i=1}^{N} \int_{0}^{1} \pi_i(x)u_i(x)v_i(x)\,dx.
\]

Let \( h_1 \) till \( h_N \), known as Robin parameters, be given complex numbers and also let \( h := (h_1, \ldots, h_N) \). Consider the Laplace operator \( L_h = -d^2/dx^2 \) with the domain \( \text{Dom}(L_h) \), consisting of all complex-valued functions in the Sobolev space \( W^2_2((0,1), \mathbb{C}^N) \) fulfilling the following vertex conditions:

- **standard** vertex conditions at the internal vertex:

\[
\begin{align*}
  u_1(1) &= u_2(1) = \cdots = u_N(1), \\
  u_1'(1) + u_2'(1) + \cdots + u_N'(1) &= 0;
\end{align*}
\]

- **complex Robin** conditions at the external vertices:

\[
  u_j'(0) = h_j u_j(0), \quad 1 \leq j \leq N.
\]

The reader should note that the operator \( L_h \) is not necessarily self-adjoint. This stems from the fact that complex values for Robin parameters are allowed. To see this, let \( u \) and \( v \) be two
elements of $\text{Dom}(L_h)$. Using integration by parts, we have:

$$\langle L_h u, v \rangle - \langle u, L_h v \rangle = \sum_{i=1}^{N} \left( - \int_0^1 \overline{\pi_i'(x)} v_i(x) \, dx + \int_0^1 \overline{\pi_i(x)} v_i'(x) \, dx \right)$$

$$= \sum_{i=1}^{N} \left( - \overline{\pi_i'(x)} v_i(x) \big|_0^1 + \overline{\pi_i(x)} v_i(x) \big|_0^1 \right)$$

$$= \sum_{i=1}^{N} (\overline{\pi_i} - \pi_i) \overline{v_i(0)} v_i(0) + \sum_{i=1}^{N} [\pi_i'(1) - \pi_i(1)] v_i(1),$$

where Equations (4) are used. From Equations (2) and (3), one can see that the second sum above vanishes and we get:

$$\langle L_h u, v \rangle - \langle u, L_h v \rangle = \sum_{i=1}^{N} (\overline{\pi_i} - \pi_i) \overline{v_i(0)} v_i(0),$$

(5) which does not in general vanish, since we allow for complex Robin parameters. Therefore, the spectrum of $L_h$ might contain complex values.

In what follows, we use a boldface letter to denote an $N$-tuple and the corresponding Roman letter with subscripts, running from 1 till $N$, to denote its components. For instance, $c$ is used to denote the $N$-tuple $(c_1, \ldots, c_N)$. In this context, we use $\overline{c}$ to indicate $(\overline{c_1}, \ldots, \overline{c_N})$ and use $c_i$, $1 \leq i \leq N$, to indicate the $(N-1)$-tuple obtained from $c$ by suppressing its $i$th component. For example, if $c = (-i, 1, 3i, -3i, i)$, then $\overline{c} = (i, 1, -3i, 3i, -i)$ and $c_5 = (-i, 1, -3i, i)$.

**Definition 1.** An $N$-tuple $c$ is called invariant under conjugation, if non-real components of this tuple can be grouped in conjugate pairs.

For example, $c$ introduced above is invariant under conjugation but $d = (1, i, i, -i)$ is not.

**Definition 2.** The time-reversal operator $T$ is an operator defined on $\mathcal{H}$ by

$$Tu = \overline{u}.$$  

(6)

This is an anti-linear operator.

**Definition 3.** Let $i$ and $j$ be integers and $1 \leq i \leq j \leq N$. A linear operator $\mathcal{P}_{i,j}$ acting on $\mathcal{H}$ as follows

$$\mathcal{P}_{i,j} \mathcal{u}_k = \begin{cases} u_k, & k \neq i, j \\ u_j, & k = i \\ u_i, & k = j \end{cases}, \quad 1 \leq k \leq N$$

(7)

is called a permutation operator. Note that, for any $1 \leq i \leq N$, $\mathcal{P}_{i,i}$ is the identity operator id$_{\mathcal{H}}$.

Permutations $\mathcal{P}_{i,j}$ are elements of the automorphism group for the metric star-graph $\Gamma$. This group naturally induces a group of unitary transformations (symmetries) in the Hilbert space $\mathcal{H}$:

$$Sf(x) = f(S^{-1}x)$$

(8)

for any $S$ from the graph automorphism group. If all $h_i$’s are equal then the quantum graph, namely, the operator $L_h$ possesses the same symmetry group as $\Gamma$. This is not the case if $h_i$’s are different.

**Definition 4.** A unitary operator $S$ defined on $\mathcal{H}$ is called a symmetry of the quantum graph $L_h$, if $SL_h = L_hS$. In this case, the quantum graph is called $S$-symmetric. For $S$ to be a symmetry of $L_h$, it is necessary that $S(\text{Dom}(L_h)) \subseteq \text{Dom}(L_h)$.
3 Sufficient Condition for Theorem 2

In this section we prove that the invariance of the $N$-tuple $h = (h_1, \ldots, h_N)$ under conjugation implies that the spectrum of $L_h$ possesses reflection symmetry with respect to the real axis. To establish this, one needs the following proposition whose proof is given in Appendix 1.

Proposition 1. Let $\mathcal{A} \mathcal{T}$, where $\mathcal{A}$ is an invertible linear operator defined on $\mathcal{H}$ and $\mathcal{T}$ is the time-reversal operator, be a symmetry for a linear operator $L$ acting in a Hilbert space $\mathcal{H}$, namely, $\mathcal{A} \mathcal{T}L = L \mathcal{A} \mathcal{T}$. Then if $\lambda$ is an eigenvalue of $L$ with degeneracy $d$, then $\overline{\lambda}$ is also an eigenvalue of $L$ with the same degeneracy $d$.

Lemma 3. If the $N$-tuple $h = (h_1, \ldots, h_N)$, consisting of Robin parameters, is invariant under conjugation, then there exists an automorphism $\mathcal{P}$ of the graph $\Gamma$ and hence an invertible linear operator on $\mathcal{H}$ such that the mentioned quantum graph $L_h$ is $\mathcal{P} \mathcal{T}$-symmetric, that is, $\mathcal{P} \mathcal{T}L_h = L_h \mathcal{P} \mathcal{T}$.

Proof. If all components of $h$ are real, then it is straightforward to see that, say, $\mathcal{P}_{1,1} \mathcal{T} = \text{id}_{\mathcal{H}} \mathcal{T}$ is a symmetry of the quantum graph. Therefore, suppose that this is not the case and, since $h$ is assumed to be invariant under conjugation, suppose that $h$ has at least two non-real components. Let $2m$, for some integer $m$ where $1 \leq m \leq \lfloor N/2 \rfloor$, be the number of non-real components of $h$. Without loss of generality, one can assume that the components of $h$ are coming in an order in which $h_{2j} = \overline{h}_{2j-1}$, for all integers $1 \leq j \leq m$, and all other components (if any) are real.

We now show that $\mathcal{P} \mathcal{T}$, where $\mathcal{P} := \prod_{j=1}^{2m} \mathcal{P}_{2j-1,2j}$, is a symmetry of $L_h$. Expressed in words, $\mathcal{P}$ is the operator that interchanges the $(2j-1)\text{th}$ and $(2j)\text{th}$ $(1 \leq j \leq m)$ components of the $N$-tuple it is acting on, and leaves the rest (if any) of the components unchanged.

First, we show that $\text{Dom}(L_h)$ is invariant under the action of $\mathcal{P} \mathcal{T}$. Let $u$ be in $\text{Dom}(L_h)$ and let $v = \mathcal{P} \mathcal{T}u$. Then, for every integer $j$ in the interval $[1, m]$, $v_{2j-1} = \overline{v}_{2j}$ and $v_{2j} = \overline{v}_{2j-1}$ and, for every integer $j$ in the interval $[2m+1, N]$, $v_j = \overline{v}_j$. Therefore, Equations 2 and 3 are fulfilled for components of $v$, since the corresponding equations for $v$ components are complex conjugates of, at most, a rearrangement of their $u$-component counterparts. To see that Robin vertex conditions are also satisfied for $v$ components, we show that $v_k'(0) = h_k v_k(0)$, for every integer $k$ in the interval $[1, N]$.

If $k = 2j - 1$, for some integer $j$ in the interval $[1, m]$, then $v_k = \overline{v}_{k+1}$ and $h_k = \overline{h}_{k+1}$. Hence $v_k'(0) = h_k v_k(0)$ if and only if $\overline{v}_{k+1}(0) = \overline{h}_{k+1} v_{k+1}(0)$ or, equivalently, $u_{k+1}'(0) = h_{k+1} u_{k+1}(0)$. For even integers $k$ in this interval, the proof is similar. If $k$ is an integer in $[2m + 1, N]$, provided that this interval is non-empty, then $v_k = \overline{v}_k$ and $h_k = \overline{h}_k$. Thus $v_k'(0) = h_k v_k(0)$ is equivalent to $u_k'(0) = h_k u_k(0)$ in this case.

Checking that $L_h \mathcal{P} \mathcal{T}u = \mathcal{P} \mathcal{T}L_h u$, for any $u$ in the domain of $L_h$, is straightforward.

The fact that the invariance of the $N$-tuple of Robin parameters under complex conjugation implies reflection symmetry of the spectrum, follows simply as a combination of Proposition 1 with Lemma 3.

4 Necessary Condition for Theorem 2

In this section we assume that the spectrum of $L_h$ is invariant under complex conjugations and we prove that $h$ is invariant under conjugation. To this end, we start by determining the secular equation for $L_h$.
The Secular Equation

Let $\lambda := z^2$ be a non-zero eigenvalue of $L_h$. Hence, there exists a non-zero $u$ in $\text{Dom}(L_h)$ such that $L_h u = z^2 u$.

In particular, after writing it in component form, we have:

$$-\frac{d^2}{dx^2} u_i(x) = z^2 u_i(x), \quad i = 1, 2, \ldots, N.$$ (9)

The general solutions of Equations (9), for non-zero $z$, have the following form:

$$u_i(x) = A_i \cos zx + B_i \sin zx, \quad i = 1, 2, \ldots, N,$$ (10)

where $A_i$’s and $B_i$’s are complex constants. Taking into account the vertex conditions (11) on them, we obtain $B_i = (h_i A_i)/z$ and

$$u_i(x) = \frac{A_i}{z} \left(z \cos zx + h_i \sin zx\right).$$ (11)

Taking into account the vertex conditions (2) on these functions, one gets:

$$\alpha_{h_1}(z) A_1 = \alpha_{h_2}(z) A_2 = \cdots = \alpha_{h_N}(z) A_N,$$ (12)

where $\alpha_{h_i}(z)$ were introduced in (11). Vertex condition (3) give rise to the following equation:

$$\beta_{h_1}(z) A_1 + \beta_{h_2}(z) A_2 + \cdots + \beta_{h_N}(z) A_N = 0,$$ (13)

where

$$\beta_{h_i}(z) := -z \sin z + h_i \cos z, \quad (i = 1, 2, \ldots, N).$$ (14)

Equations (12) along with Equation (13) form a system of $N$ linear equations for $N$ unknowns $A_1$ till $A_N$. For this system to have a non-trivial solution, it is necessary and sufficient that the determinant of the coefficients vanishes, namely,

$$D_h(z) = 0,$$ (15)

where

$$D_h(z) := \begin{vmatrix}
\alpha_{h_1}(z) & -\alpha_{h_2}(z) & 0 & 0 & \cdots & 0 & 0 \\
0 & \alpha_{h_2}(z) & -\alpha_{h_3}(z) & 0 & \cdots & 0 & 0 \\
0 & 0 & \alpha_{h_3}(z) & -\alpha_{h_4}(z) & \cdots & 0 & 0 \\
0 & 0 & 0 & \alpha_{h_4}(z) & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & \alpha_{h_{N-1}}(z) & -\alpha_{h_N}(z) \\
\beta_{h_1}(z) & \beta_{h_2}(z) & \beta_{h_3}(z) & \beta_{h_4}(z) & \cdots & \beta_{h_{N-1}}(z) & \beta_{h_N}(z)
\end{vmatrix}. \quad (16)$$

Equation (15) is the secular equation of $L_h$. Expanding the determinant above along the last row and noting that each of the $N$ resultant determinants is in triangular form, one gets the following relation for $D_h(z)$:
\[ D_h(z) = \sum_{i=1}^{N} \left( \beta_{h_i}(z) \prod_{\substack{j=1 \atop j \neq i}}^{N} \alpha_{h_j}(z) \right). \]  

(17)

The function \( D_h(z) \) is an entire function, since the functions \( \alpha \) and \( \beta \) are entire. Secondly,

\[ D_h(z) = D_h(z), \]

(18)

since \( \alpha_{h_i}(z) = \alpha_{h_i}(z) \) and \( \beta_{h_i}(z) = \beta_{h_i}(z) \).

**On the Roots of the Secular Equation**

When all the Robin parameters are zero, that is, when \( h = 0 \), Equation (17) reduces to

\[ D_0(z) = -N z^N \sin(z) \cos(z)^{N-1}. \]

(19)

The non-zero roots of \( D_0(z) \) then are \( n\pi \) (for any non-zero integer \( n \)), each of multiplicity one, and \( n\pi + \pi/2 \) (for any integer \( n \)), each of multiplicity \( N - 1 \). We concentrate ourselves here on the former set of roots, which are easier to handle. Now consider the case in which \( h \neq 0 \), and let \( \bar{z}_n(h) \), for some fixed positive integer \( n \), be a root of the secular equation \( D_h(z) = 0 \). Then we write \( \bar{z}_n(h) \) in the following form:

\[ \bar{z}_n(h) = n\pi + \Delta_n(h), \]

(20)

where \( \Delta_n(h) \) denotes the deviation of \( \bar{z}_n(h) \), as a root of equation \( D_h(z) = 0 \), from \( n\pi \). We show that, for sufficiently large \( n \), the correction term \( \Delta_n(h) \) takes the following form:

\[ \Delta_n(h) = \frac{a_1(h)}{n} + \frac{a_3(h)}{n^3} + \frac{a_5(h)}{n^5} + \cdots, \]

(21)

with some coefficients \( a_i(h) \). The general structure of these coefficients will be determined later.

First we engineer a complex-valued function \( K_\epsilon \), in which \( \epsilon \) is a positive real parameter, so that

\[ D_h(n\pi + z) = 0 \iff K_{\frac{1}{n\pi}}(z) = 0, \]

(22)

for any complex number \( z \) and for any positive integer \( n \). Employing the elementary formulas:

\[ \sin(n\pi + z) = (-1)^n \sin z, \]
\[ \cos(n\pi + z) = (-1)^n \cos z, \]

it is straightforward to see that

\[ K_\epsilon(z) := \sum_{i=1}^{N} \left\{ - (1 + \epsilon z) \sin z + \epsilon h_i \cos z \right\} \prod_{\substack{j=1 \atop j \neq i}}^{N} \left\{ (1 + \epsilon z) \cos z + \epsilon h_j \sin z \right\}, \]

(23)

does the job.

We now show that there exists a neighborhood \( \mathcal{N} \) of the origin and a positive number \( \epsilon_0 \) such that for every \( \epsilon \) in the interval \( (0, \epsilon_0) \), the function \( K_\epsilon \) has a unique root \( \Delta(\epsilon) \) in \( \mathcal{N} \). More importantly, we show that the dependence of \( \Delta \) on \( \epsilon \) is analytic. Note that \( \Delta \) is, in general, a complex-valued function of \( \epsilon \).
The equation \( K_\epsilon(z) = 0 \) can be considered as a polynomial equation in \( \epsilon \):

\[
g_0(z) + g_1(z) \epsilon + g_2(z) \epsilon^2 + \cdots + g_N(z) \epsilon^N = 0,
\]

in which the coefficient-functions \( g_i(z) \) are entire trigonometric functions of \( z \). Among all these coefficient-functions, what we actually need is the explicit form of just the first function \( g_0(z) \). It is straightforward to see that

\[
g_0(z) = -N \sin z \cos z^{N-1}.
\]

For this function we have

\[
g_0(0) = 0, \quad g'_0(0) = -N,
\]

and, consequently, the entire function \( g_0 \) is invertible in a neighborhood of the origin, where its first derivative is separated from zero. Using the inverse of \( g_0 \), the Equation (24) can be written in the following manner:

\[
G_\epsilon(z) = z,
\]

where

\[
G_\epsilon(z) := -g_0^{-1}\left(g_1(z) \epsilon + g_2(z) \epsilon^2 + \cdots + g_N(z) \epsilon^N\right).
\]

Of course, \( \epsilon \) in (26) should be chosen sufficiently small. The reader also notes that for any \( z \) in the suitable domain, \( g_0^{-1}(z) = -g_0^{-1}(z) \), since \( g_0 \) itself is an odd function.

We now have:

\[
G'_\epsilon(z) = -\frac{1}{g'_0\left(g_1(z) \epsilon + g_2(z) \epsilon^2 + \cdots + g_N(z) \epsilon^N\right)} \epsilon\left(g'_1(z) + g'_2(z) \epsilon + \cdots + g'_N(z) \epsilon^{N-1}\right),
\]

where prime everywhere denotes the derivative with respect to \( z \). As Equation (27) shows, \(|G'_\epsilon(z)|\) is controlled by \( \epsilon \). In particular, there exists \( \epsilon_0 > 0 \) and there exists a neighborhood \( \mathcal{N} \) such that \(|G'_\epsilon(z)| < 1\), for all \( z \) in \( \mathcal{N} \) and all \( \epsilon \) in the interval \((0, \epsilon_0)\). The fixed-point theorem then implies that the Equation (25), or equivalently, the Equation \( K_\epsilon(z) = 0 \) has a unique root \( \Delta(\epsilon) \) in \( \mathcal{N} \). To see the analytic dependence of \( \Delta \) on \( \epsilon \), note that the solution curve \( \Delta = \Delta(\epsilon) \) can be viewed as the intersection of the following two analytic manifolds:

\[
x = G_\epsilon(\Delta), \quad x = \Delta,
\]

in the three-dimensional space, and therefore it is analytic and one can write:

\[
\Delta(\epsilon) = b_0(h) + b_1(h) \epsilon + b_2(h) \epsilon^2 + \cdots,
\]

with some coefficients \( b_i(h) \). The function \( K_\epsilon(z) \) possesses the property \( K_{-\epsilon}(-z) = -K_\epsilon(z) \) and, consequently, \( \Delta(\epsilon) \) is an odd function of \( \epsilon \). Therefore, all even coefficients in the expansion (28) vanish:

\[
\Delta(\epsilon) = b_1(h) \epsilon + b_3(h) \epsilon^3 + \cdots
\]

Now let \( n \) be a positive integer such that \( 1/(n \pi) \) lies in \((0, \epsilon_0)\). Therefore, the unique root \( \Delta_n(h) \) of \( K_{1/n} \) in \( \mathcal{N} \) or, considering (23), equivalently the unique root of Equation \( D_h(n \pi + z) = 0 \) in \( \mathcal{N} \) is \( \Delta_n(h) = \Delta\left(\frac{1}{n \pi}\right) \), and expansion (21) holds with

\[
a_j(h) := \frac{1}{\pi j} b_j(h),
\]

for all odd positive integers \( j \).

Our next goal is to discuss formulas for the expansion coefficients, this can be done in terms of symmetric polynomials in \( h_i \),
Elementary Symmetric Polynomials

In this subsection, we introduce a special kind of symmetric polynomials that allows us to write Equation (17) in a more flexible form, which fits better to our purpose.

Definition 5. For a non-negative integer $m$, the $m$th elementary symmetric polynomial in $N$ variables $x_1$ till $x_N$ is denoted by $s_m(x_1, \ldots, x_N)$ and it is defined by

$$s_m(x_1, \ldots, x_N) = \begin{cases} 1, & m = 0 \\ \sum x_{i_1} \cdots x_{i_m}, & 1 \leq m \leq N \\ 0, & m \geq N + 1 \end{cases}$$

where the sum above is over all indices $i_1$ till $i_m$ such that $1 \leq i_1 < \cdots < i_m \leq N$.

For instance, the elementary symmetric polynomials in three variables are:

- $s_0(x_1, x_2, x_3) = 1$,
- $s_1(x_1, x_2, x_3) = x_1 + x_2 + x_3$,
- $s_2(x_1, x_2, x_3) = x_1x_2 + x_2x_3 + x_1x_3$,
- $s_3(x_1, x_2, x_3) = x_1x_2x_3$,
- $s_m(x_1, x_2, x_3) = 0, \quad (m \geq 4)$.

It is readily seen that the symmetric polynomial $s_m(x_1, \ldots, x_N), m \leq N$, is homogeneous of degree $m$ in the sense that for any number $\lambda$,

$$s_m(\lambda x_1, \ldots, \lambda x_N) = \lambda^m s_m(x_1, \ldots, x_N).$$

In the coming sections, we make use of the properties of elementary symmetric polynomials mentioned in the following proposition, which proof can be found in Appendix 1.

Proposition 2. Let $c = (c_1, \ldots, c_N)$, and let $i$ and $j$ be integers such that $1 \leq i \leq N$ and $0 \leq j \leq N - 1$. Then

$$c_i s_j(c) = s_{j+1}(c) - s_{j+1}(c_i),$$

$$\sum_{i=1}^{N} s_j(c_i) = (N - j) s_j(c).$$

Moreover, we also make use of the following well-known identity:

$$\prod_{j=1}^{N} (x + c_j) = \sum_{k=0}^{N} s_k(c) x^{N-k}.$$

The following lemma is in some sense the key observation that makes the proof to work.

Lemma 4. An $N$-tuple $c = (c_1, \ldots, c_N)$ of complex numbers is invariant under conjugation if and only if, for all $1 \leq m \leq N$, $s_m(c)$ is real.

Proof. First, suppose that $c$ is invariant under conjugation and let $m, 1 \leq m \leq N$, be a given integer. From Equation (32), we have:

$$s_m(c_1, \ldots, c_N) = \sum c_{i_1} \cdots c_{i_m}.$$
Since \( c \) is invariant under conjugation, for each term in the sum above \( \overline{c_{i_1}} \cdots \overline{c_{i_m}} = c_{j_1} \cdots c_{j_m} \), where \( 1 \leq j_1 < \cdots < j_m \leq N \). Of course, not all of these \( j \) indices are necessarily distinct from their corresponding \( i \) indices. Thus, each term in this sum is either real or its complex conjugate is also a term in this sum and, hence, \( s_m(c_1, \ldots, c_N) \) is real.

Conversely, suppose that \( s_m(c) \)'s, \( 1 \leq m \leq N \), are all real. Consider the following polynomial:

\[
P(z) := \prod_{i=1}^{N} (z - c_i). \tag{37}
\]

Using Equations (36) and (33), \( P(z) \) can be written as follows:

\[
P(z) = z^n + \sum_{m=1}^{N} (-1)^m s_m(c) z^{N-m}, \tag{38}
\]

and, therefore, \( P(z) \) is a polynomial with real coefficients. Consequently, a complex number \( z_0 \) is a root of \( P(z) \) if and only if \( \overline{z_0} \) is a root and, since the roots of \( P \) are \( c_1, c_2, \ldots, \) and \( c_N \). This would then mean that \( c \) is invariant under conjugation.

**The Secular Equation, New Guise**

We are now ready to write Equation (14) in terms of elementary symmetric polynomials. Plugging \( z \cos z \) for \( x \) and \( h_j \sin z \) for \( c_j \) in Equation (36), and using Equation (33), one can write:

\[
\prod_{j=1, j \neq i}^{N} \alpha_{h_j}(z) = \prod_{j=1}^{N} (z \cos z + h_j \sin z) = \sum_{k=0}^{N-1} s_k(h_1 \sin z, \ldots, h_{i-1} \sin z, h_{i+1} \sin z, \ldots, h_N \sin z) (z \cos z)^{N-1-k} = \sum_{k=0}^{N-1} s_k(h_i) z^{N-1-k} (\sin z)^k (\cos z)^{N-1-k}. \]

Hence,

\[
\beta_{h_i}(z) \prod_{j=1, j \neq i}^{N} \alpha_{h_j}(z) = (-z \sin z + h_i \cos z) \sum_{k=0}^{N-1} s_k(h_i) z^{N-1-k} (\sin z)^k (\cos z)^{N-1-k},
\]

and after multiplying the terms, we get:

\[
\beta_{h_i}(z) \prod_{j=1}^{N} \alpha_{h_j}(z) = -\sum_{k=0}^{N-1} s_k(h_i) z^{N-k} (\sin z)^{k+1} (\cos z)^{N-1-k} + \sum_{k=0}^{N-1} h_i s_k(h_i) z^{N-k-1} (\sin z)^k (\cos z)^{N-k}. \tag{39}
\]

The first sum, after the term corresponding to \( k = 0 \) is separated, can be written in the following form:

\[
z^N \sin z (\cos z)^{N-1} + \sum_{k=1}^{N-1} s_k(h_i) z^{N-k} (\sin z)^{k+1} (\cos z)^{N-1-k}. \tag{40}
\]
Using Equation (34), the second sum in Equation (39) can be rewritten as follows:

\[
\sum_{k=0}^{N-1} [s_{k+1}(h) - s_{k+1}(h_i)] z^{N-k-1} (\sin z)^k (\cos z)^{N-k}
\]

\[
= \sum_{k=1}^{N} [s_k(h) - s_k(h_i)] z^{N-k} (\sin z)^{k-1} (\cos z)^{N-k+1}
\]

\[
= \sum_{k=1}^{N-1} \{[s_k(h) - s_k(h_i)] z^{N-k} (\sin z)^{k-1} (\cos z)^{N-k+1}\} + s_N(h) (\sin z)^{N-1} \cos z, \quad (41)
\]

where in the last line, the Nth term of the sum is written separately, and \( s_N(h_i) = 0 \) has been employed. Plugging Equations (40) and (41) back into Equation (39), we obtain:

\[
\beta_{h_i}(z) \prod_{j=1, j \neq i}^{N} \alpha_{h_j}(z) = -z^N \sin z (\cos z)^{N-1}
\]

\[
+ \sum_{k=1}^{N-1} \{ -s_k(h_i) z^{N-k} (\sin z)^{k+1} (\cos z)^{N-k-1}
\]

\[
+ [s_k(h) - s_k(h_i)] z^{N-k} (\sin z)^{k-1} (\cos z)^{N-k+1}\}
\]

\[
+ s_N(h) (\sin z)^{N-1} \cos z. \quad (42)
\]

The summand in the middle term above can be written as:

\[
\{[s_k(h) - s_k(h_i)] \cos^2 z - s_k(h_i) \sin^2 z\} z^{N-k} (\sin z)^{k-1} (\cos z)^{N-k-1},
\]

or

\[
[s_k(h) \cos^2 z - s_k(h_i)] z^{N-k} (\sin z)^{k-1} (\cos z)^{N-k-1}.
\]

Plugging back the last expression into Equation (42), yields:

\[
\beta_{h_i}(z) \prod_{j=1, j \neq i}^{N} s_{h_j}(z) = -z^N \sin z (\cos z)^{N-1}
\]

\[
+ \sum_{k=1}^{N-1} s_k(h) z^{N-k} (\sin z)^{k-1} (\cos z)^{N-k+1}
\]

\[
- \sum_{k=1}^{N-1} s_k(h_i) z^{N-k} (\sin z)^{k-1} (\cos z)^{N-k-1}
\]

\[
+ s_N(h) (\sin z)^{N-1} \cos z.
\]

Finally, summing over \( i \) and using Equation (35), one gets:

\[
D_h(z) = -N z^N \sin z (\cos z)^{N-1}
\]

\[
+ \sum_{k=1}^{N-1} \{ s_k(h) (k - N \sin^2 z) z^{N-k} (\sin z)^{k-1} (\cos z)^{N-k-1}\}
\]

\[
+ N s_N(h) (\sin z)^{N-1} \cos z, \quad (43)
\]

which can be written more compactly as:

\[
D_h(z) = -N z^N \sin z (\cos z)^{N-1} + z^N \sum_{k=1}^{N} \frac{s_k(h)}{z^k} f_k(z), \quad (44)
\]

where

\[
f_k(z) := (k - N \sin^2 z) (\sin z)^{k-1} (\cos z)^{N-k-1}, \quad (k = 1, 2, \ldots, N). \quad (45)
\]
For \( \tilde{\varphi} \tilde{\varphi} \) Equation (44) and plug expansion and then collect the resultant series in terms of different powers of \( z \) with respect to the first term, for all \( a \) the following result for coefficients above, must vanish. Equating all coefficients to zero and solving the equations recursively, we get

\[
D_h(z) = -N \sin(z) \cos(z)^N + \sum_{k=1}^{N} \frac{s_k(h)}{z^k} f_k(z).
\]

For any positive integer \( n \), \( n \pi \) is a root of the first term on the right hand side of Equation (46). As Equation (49) shows, this term actually gives the secular equation when \( h = 0 \) and \( z \neq 0 \).

Let \( C_n \) denote a circle of some \( small \) but fixed radius \( r_n \) centered at \( n \pi \). We have:

\[
\left| \frac{s_k(h)}{z^k} \right| \leq \left( \frac{N}{k} \right) \left( \frac{h}{|z|} \right)^k,
\]

where \( h := \max \{ |h|, \ldots, |h_N| \} \). Thus, for any \( z \) chosen inside \( C_n \) with large \( n \), the expression on the left in Equation (47) becomes small. On the other hand, \( f_k \)'s are all uniformly bounded inside every \( C_n \). To see this, note that all \( f_k \)'s are uniformly bounded inside, say, \( C_1 \) and they are periodic with period \( 2\pi \). Hence, the second term on the right of Equation (49) becomes negligible with respect to the first term, for all \( z \) inside \( C_n \) with large \( n \). Since the second term is continuous inside any of the circles \( C_n \), one then expects the secular equation, when \( h \neq 0 \), has a root that is arbitrary close to \( n \pi \), if \( n \) is sufficiently large.

Structure of the Coefficients \( a_j(h) \)

In this subsection we deal with the practical problem of determining the coefficients \( a_j(h) \), which appear in the expansion of the correction term \( \Delta_n(h) \) in Equation (21). We remind that all even coefficients in the expansion are zero and we employ a recursive calculation to determine the general structure of odd coefficients.

We Taylor expand, around \( z = 0 \), the sine and cosine functions appearing in \( D_h(z) \) given by Equation (44) and plug \( \tilde{\varphi}_n(h) = n \pi + \Delta_n(h) \), with \( \Delta_n(h) \) given by Equation (21), into this Taylor’s expansion and then collect the resultant series in terms of different powers of \( n \). The powers of \( n \) that appear in this expansion are:

\[
n^{N-1}, n^{N-3}, n^{N-5}, n^{N-7}, \ldots = \{n^{N-2i+1}\}_{i \in \mathbb{N}} = \{0, 1, 2, 3, \ldots\}
\]

For \( \tilde{\varphi}_n(h) \) to be a root of the secular equation, all the coefficients of the powers of \( n \) introduced above, must vanish. Equating all coefficients to zero and solving the equations recursively, we get the following result for coefficients \( a_i(h) \) with odd indices:

\[
a_{2i-1}(h) = s_1(h) F_{i}(s_1(h), \ldots, s_{i-1}(h)) + \frac{i}{\pi^2 N N^2} (s_1(h))^{i-1} s_i(h), \quad i = 2, 3, 4, \ldots, \quad (48)
\]

where \( F_i \)'s are some polynomial of degree \( 2i \) in \( i - 1 \) variables. The coefficients of \( F_i \)'s are real-valued rational functions of \( N \). For \( i = 1 \), the corresponding function \( F_1 \) is zero. More explicitly, for instance:

\[
a_1(h) = \frac{1}{\pi N} s_1(h), \quad (49)
\]
and
\[ a_3(h) = s_1(h)F_1((s_1(h)) + \frac{2}{\pi^3 N^2} s_1(h)s_2(h), \]
\[ a_5(h) = s_1(h)F_2(s_1(h), s_2(h)) + \frac{3}{\pi^5 N^3} (s_1(h))^2 s_3(h), \]
where
\[ F_1(x_1) = -\frac{3N - 2}{3\pi^3 N^3} x_1^2 - \frac{1}{\pi^3 N^2} x_1, \]
\[ F_2(x_1, x_2) = \frac{10N^2 - 15N + 6}{5\pi^3 N^3} x_1^4 + \frac{12N - 8}{3\pi^3 N^4} x_1^3 x_2 - \frac{7N - 6}{\pi^3 N^4} x_1^2 x_2^2 + \frac{2}{\pi^3 N^3} x_1^2 x_2 + \frac{4}{\pi^3 N^3} x_2^2. \]

A closer look at Equations (48) reveals that \( s_1(h) \) appears, for the first time, in the equation for \( a_{2i-1}(h) \) and, moreover, it appears there with power equal to one. This we use to prove the main result of this section.

**Necessary Condition, The Proof**

Finally, everything is in order and we finalize the proof for the necessary condition of the main theorem. In fact, here we assume that the eigenvalues of \( L_h \) possess reflection symmetry with respect to the real axis and we prove that the \( N \)-tuple \( h = (h_1, \ldots, h_N) \), consisting of Robin parameters, is invariant under conjugation.

Since the eigenvalues of \( L_h \) possesses reflection symmetry with respect to the real axis, then \( D_h(z) = 0 \) if and only if \( D_h(\overline{z}) = 0 \) and, by Equation (18), this is equivalent to \( D_{\overline{h}}(z) = 0 \). Therefore, \( \bar{z}_n(h) \) introduced in Equation (20), is a root of \( D_{\overline{h}}(z) \) as well. If one uses the same procedure that gave rise to Equation (48), but this time for \( D_{\overline{h}}(z) \), one gets:
\[ a_1(h) = \frac{1}{\pi N} s_1(h), \quad (50) \]
and
\[ a_{2i-1}(h) = s_1(h) F_i(s_1(h), \ldots, s_{i-1}(h)) + i \frac{1}{\pi^{2i-1} N^i} (s_1(h))^{i-1} s_1(h), \quad i = 2, 3, 4, \ldots \quad (51) \]

Here we used \( s_m(h) = s_m(\overline{h}) \) for \( m = 1, \ldots, N \).

Comparing Equations (49) and (50), one finds that \( s_1(h) \) is real. Now assume that \( s_1(h) \) till \( s_{k-1}(h), 1 \leq k \leq N, \) are real. From Equation (51), we have:
\[ a_{2k-1}(h) = s_1(h) F_k(s_1(h), \ldots, s_{k-1}(h)) + \frac{k}{\pi^{2k-1} N^k} (s_1(h))^{k-1} s_1(h), \]
and from Equation (48), we have
\[ a_{2k-1}(h) = s_1(h) F_k(s_1(h), \ldots, s_{k-1}(h)) + \frac{k}{\pi^{2k-1} N^k} (s_1(h))^{k-1} s_k(h). \]
Thus \( s_k(h) \) is also real. Consequently, all polynomials \( s_1(h) \) till \( s_N(h) \) are real and by Lemma 4, \( h \) is invariant under conjugation.
5 Proof of the Main Theorem [1] and perspectives

We need to prove that existence of a certain $\mathcal{PT}$-symmetry is necessary and sufficient for the spectrum of the operator $L_h$ to possess reflection symmetry with respect to the real axis. Sufficiency (it is a general property of $\mathcal{PT}$-symmetric operators) is already proven – it is given by Proposition [1]. Hence it remains to prove the necessity. Theorem [2] implies that the spectrum possesses reflection symmetry only if the set of Robin parameters $\{h_i\}$ is invariant under complex conjugation. Then Lemma [3] implies that there exists an automorphism $\mathcal{P}$ of $\Gamma$ (given by a product of edge permutations) such that the operator $L_h$ is $\mathcal{PT}$-symmetric. It follows that every operator $L_h$ with reflection-symmetric spectrum possesses $\mathcal{PT}$-symmetry with a certain automorphism $\mathcal{P}$ given as a product of permutations. The Main Theorem is proven.

We have already mentioned in the Introduction that we doubt that the statement that reflection symmetry of the spectrum implies $\mathcal{PT}$-symmetry of the quantum graph operator $L$ with respect to a certain automorphism $\mathcal{P}$ of the underlying metric graph holds in full generality. This would imply in particular that all quantum graphs with reflection symmetric spectrum necessarily are defined on symmetric metric graphs. It might happen that this statement holds if one restricts consideration to vertex conditions given only via complex delta interactions. We are planning to return back to this question in one of our future publications.

Note that in the proof of Theorem [2] and therefore in the proof of the Main Theorem we did not use that the multiplicities of the conjugated eigenvalues coincide. The reason is that only a small part of the eigenvalues was used. One may show that the eigenvalues of $L_h$ are situated close to the eigenvalues of the standard Laplace operator $L_0$. More precisely, there is exactly one eigenvalue close to $\pi n$ and $N-1$ eigenvalues close to $\pi(n+1/2)$. In our proof we used just the series of eigenvalues close to $\pi n$ and such a series is invariant under conjugation only if it is real. Such eigenvalues cannot be degenerate. Generalising our results for arbitrary graphs would require to take into account that the multiplicities in the conjugated pairs of eigenvalues coincide.

Researchers working with $\mathcal{PT}$-symmetric operators are often interested when the operator is not self-adjoint, but the spectrum is real anyway. One may study this question for quantum graphs getting explicit examples.

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1 Proofs of Propositions 1 and 2

In this appendix we prove Propositions [1] and [2].

Proof. (Proposition [1] Since $\mathcal{AT}$ is a symmetry of $L$, we have:

$$L \mathcal{AT} = \mathcal{AT} L.$$ \hfill (52)

On the other hand, since $\lambda$ is an eigenvalue of $L$ with degeneracy $d$, there exist $d$ linearly independent functions $u^1, u^2, \ldots, u^d$ in $\text{Dom}(L)$ such that

$$Lu^i = \lambda u^i, \quad (i = 1, \ldots, d).$$
Acting both sides of the equation above by $AT$ and considering that $T$ is anti-linear and $A$ is linear, one gets:

$$ATL_{ii} = \lambda AT_{ii}, \quad (i = 1, \ldots, d).$$

Using Equations (52) and (6) in the equations above, one gets:

$$L(\mathbf{A}u_i) = \lambda (\mathbf{A}u_i), \quad (i = 1, \ldots, d).$$

Now we show that the functions $\mathbf{A}u_1, \mathbf{A}u_2, \ldots,$ and $\mathbf{A}u_d$ are linearly independent. Let $c_1, c_2, \ldots,$ and $c_N$ be complex numbers such that

$$c_1 (\mathbf{A}u^1) + c_2 (\mathbf{A}u^2) + \cdots + c_N (\mathbf{A}u^N) = 0.$$

Then

$$\mathbf{A}(c_1 u^1 + c_2 u^2 + \cdots + c_1 u^N) = 0,$$

and, since $\mathbf{A}$ is invertible, we have:

$$c_1 u^1 + c_1 u^2 + \cdots + c_1 u^N = 0,$$

or

$$c_1 u^1 + \bar{c}_1 u^2 + \cdots + \bar{c}_1 u^N = 0.$$

Therefore, all $c_i$’s vanish, since $u^i$’s are linearly independent.

**Proof.** (Proposition 2) To prove Equation (34), because of symmetry, one can assume that $i = N$ without loss of generality.

In what follows, $\sum^{(1)}$ indicates a sum over all subscripts such that the lowest possible value for subscripts is 1 and the highest possible value for subscripts is $N$, and $\sum^{(2)}$ indicates the same except that the highest possible value for subscripts is $N - 1$ instead.

$$\text{RHS} = \sum^{(1)} c_{i_1} \cdots c_{i_{j+1}} - \sum^{(2)} c_{i_1} \cdots c_{i_{j+1}} = (c_N \sum^{(2)} c_{i_1} \cdots c_{i_{j+1}} + \sum^{(2)} c_{i_1} \cdots c_{i_{j+1}}) - \sum^{(2)} c_{i_1} \cdots c_{i_{j+1}} = c_N s_j(c_N) = \text{LHS}.$$

Equation (34) then follows from Equation (35).

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