e-ISSN 2320 –7876 www.ijfans.org
Research Paper Vol.11, Iss.9, Dec 2022

HIGHER ORDER DIFFERENTIAL OPERATORS ON GRAPHS

KRISHNAMOORTHY. K
Research Scholar
M.Phil Mathematics
Bharath Institute Of Higher Education And Research
Mail Id : karthigame.89@gmail.com
Guide Name: **Dr. N. RAMYA**
Head of the Department, Department Of Mathematics
Bharath Institute Of Higher Education And Research

Address for Correspondence

KRISHNAMOORTHY. K
Research Scholar
M.Phil Mathematics
Bharath Institute Of Higher Education And Research
Mail Id : karthigame.89@gmail.com
Guide Name: **Dr. N. RAMYA**
Head of the Department, Department Of Mathematics
Bharath Institute Of Higher Education And Research

Abstract

In the recent decades, a new frontier has emerged with a similar goal, that is to con-trol the optical properties of materials. If we can engineer materials that prohibit or allow the propagation of light at certain frequencies, or localize it, our technology would benefit greatly. For instance, one envisions optical integrated circuits, which potentially can op- erate faster than our current semiconductor ones. The materials that could lead us to such goal are the so called photonic crystals.Sections B and C of contain an exposition and the proofs of our results concerning existence and confinement of guided waves in photonic crystal waveguides. Namely, we prove existence and confinement of guided waves through a linear defect in a PBG material, provided some "strength" conditions on the defect. The results are obtained both for the scalar (corresponding to acoustic or 2*D* photonic guides) and the full 3*D* Maxwell cases. In the last couple of decades, engineers have been able to produce thin, graph-like structures (quantum wires, mesoscopic systems). The need to study propagation of waves in such structures has lead to the birth of quantumgraph theory. Quantum graphs also arise as simplified model in many areas of science. Besides quantum wires and mesoscopic system already mentioned, quantum

graphs also arise in modelling free-electron theory of conjugated molecules in chemistry, photonic crystals theory, scattering theory, quantum chaos and nanotechnology.

INTRODUCTION

Our current technology trend in electronics seems to gear towards faster and smaller equipment. With the miniaturization scale going towards nano-scale, the theory of quan- tum graphs is indispensable to our understanding and in making breakthrough in some areas of nanotechnology.In sections B and C of we describe and prove our results concerning spec- tral properties of quantum graphs.One of the results concerning quantum graphs that we establish, is validity of the lim- iting absorption principle and thus absence of singular continuous spectrum for scatteringgraphs. The limiting absorption principle is useful for understanding the spectrum of a quantum graph, which in turn gives us information about quantum dynamics on suchobjects.

As in the case of photonic crystal, gaps in the spectrum are essential for quantum graph studies as well. A standard way to create spectral gaps is to make the medium pe- riodic. However, this neither guarantees existence of gaps (except in the one-dimensional case), nor allows easy control over the location of the gaps. We present a novel proceduresof opening spectral gaps in regular finite quantum graphs. This procedure also allows some control over the location of the gaps.

SPECTRAL PROPERTIES OF PHOTONIC WAVE GUIDES*

One could think of a photonic crystal as a block of a dielectric medium (e.g., GaAs) withholes within its structure arranged in a periodic manner. These holes are filled with adifferent dielectric material (e.g., air). Photonic crystals play the role of optical analogs of semiconductors. In a semiconductor, its atoms are arranged in a periodic lattice. This periodic structure prohibits electrons to have certain values of energies. These forbidden energy values form the so-called gaps in the energy spectrum of a semiconductor and theycorrespond to values in the spectral gaps of Schrödinger operator $H = -\Delta + V(x)$ with a periodic potential $V(x)$. Allowed energy values form the spectral bands. Thus, the energy spectrum of a semiconductor has a band-gap structure (see Fig. 1). Existence of theseenergy gaps is what makes semiconductors so useful.

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e-ISSN 2320 –7876 www.ijfans.org
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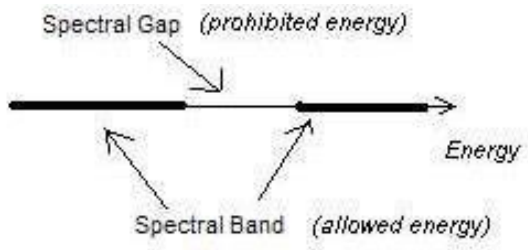

Fig. 1. Spectral Band-Gap

In the case of a photonic crystal, propagation of monochromatic electromagnetic waves (instead of electrons) through a block of dielectric material containing holes dis-tributed periodically and filled with air (or other dielectric material) is studied. See Fig. 2.

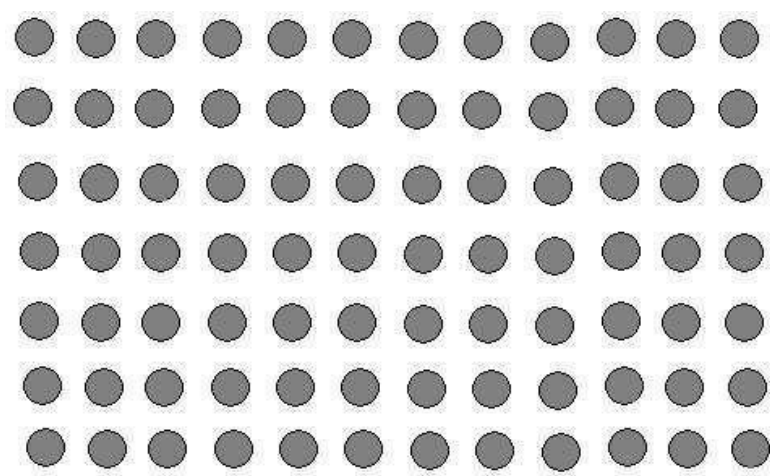

Fig. 2. PBG Material

Photonic crystals were first suggested in 1987, see **[25, 62]** . Analogously to the semiconductor case, frequency spectrum of a photonic crystal has a band-gap structure. Ifa frequency gap does indeed exist, waves with frequencies within the gap cannot exist inthe medium. Photonic crystals with gaps in their spectra need to be manufactured.

Photonic crystals offer great promises in lasers, high-speed computers and in the area of telecommunications. Already, fiber-optic cables, which guide light, have revolutionized the telecommunications industry. Photonic crystals provide potentially better means of guiding and localizing light than current optical materials. There exist several books and surveys about both physics

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and mathematics, as well as possible applications of photoniccrystals. See for example.

A linear photonic band-gap (PBG) waveguide is a linear "defect" introduced into

photonic crystal that destroys its periodicity. This could change the spectrum in such a way that allows waves of certain frequencies, which were originally prohibited from existing in the "defect-less" bulk, to propagate within the defect. This suggests that such linear defects can possibly be used as efficient optical waveguides. Below is a picture of amore general PBG waveguide (Fig. 3).

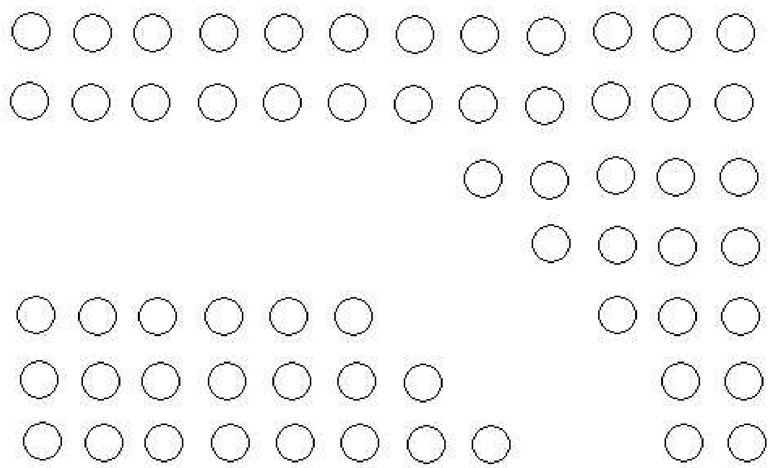

Fig. 3. A PBG Waveguide

Current fiber optic cables use total internal reflection to guide light. However, when the cable is bent past a certain critical angle, total internal reflection fails and significant amount of light escapes from the cable. A waveguide carved out of a photonic crystal does not use the law of total internal reflection. Light of frequencies prohibited in the bulk is confined to the waveguide due to the periodic arrangement of holes surrounding the waveguide. Hence light is still guided along bends in photonic waveguides.

In order to study propagation of electromagnetic waves in photonic crystal, we must turn to Maxwell equations. In cgs units (centimeter, gram, second), they are

$$\nabla \cdot B = 0 \qquad \nabla \times E + \frac{1}{c}\frac{\partial B}{\partial t} = 0$$

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$$\nabla\cdot D = 4\pi\rho \qquad \nabla\times H - \frac{1}{c}\frac{\partial D}{\partial t} = \frac{4\pi}{c} J$$

where E and H are the electric and magnetic fields respectively, D and B are the dis- placement and magnetic induction fields respectively and ρ and J are the free charges andcurrents. The constant c is the speed of light.

SPECTRAL PROPERTIES OF QUANTUM GRAPHS*

A. Quantum Graphs - An Introduction

We first start with defining what a graph is. A graph Γ consists of a set $V(\Gamma)$ of points called vertices together with a set $E(\Gamma)$ that consists of pairs of vertices. The elements of $E(\Gamma)$ are called edges. We will also denote them as $V := V(\Gamma)$ and $E := E(\Gamma)$ if there isno ambiguity about which graphs we are referring to.

Loops and multiple edges between vertices are allowed. If V and E are finite sets, we said Γ is a finite graph. If either V or E is (countably) infinite then Γ is an infinite graph. The degree d_v of a vertex v is the number of edges incident to v. We will assume that d_v is positive and finite. Due to positivity of d_v, there are no isolated vertices.

A metric graph is a graph Γ such that each edge e is assigned a positive length $l_e \in (0, \infty]$ and a coordinate x_e along the edge. The subscript e will be dropped if there is no ambiguity. A metric graph is considered to be a one-dimensional variety. With thecoordinate system x_e, the standard notions of analysis like metric, measure, integration, limit and differentiation along the edges can be employed. Function spaces such as $L^2(\Gamma)$, where the function belongs to $L^2(e)$ on each edge e in Γ can also be introduced.

A *quantum graph* is a metric graph equipped with a self-adjoint differential operator.

In defining a differential operator on graph, one needs to impose some “boundary” conditions at the vertices. The simplest of such examples is the operator that acts as $-\frac{d^2}{dx_e^2}$ along

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the edges on functions that are continuous and such that at each vertex v the sum of thederivatives along the edges emanating from v is zero. This vertex condition is commonly

*Part of this chapter is reprinted with permission from *On the limiting absortionprinciple and spectra of quantum graphs* by B. S. Ong, *Quantum Graphs and Their Applications*, Contemp. Math. **415** (2006). © 2006 by AMS.

known as Kirchhoff, Neumann, or zero flux condition.

Quantum graphs naturally arise as simplified models in mathematics, physics, chem- istry, and engineering. There are systems that have some dimensions too small to be stud- ied using classical physics, while too large to be considered on the quantum level only. Such systems are called *mesoscopic* and may look like surfaces (*quantum walls*), wires (*quantum wires*) or dots (*quantum dots*). See **[22]** for more details. Some models of mesoscopic systems and nanotechnology involve quantum graph theory.

The most important reason for considering quantum graphs is studying propagation of waves through media that resemble thin neighborhoods of graphs, such as circuits of quantum wires. Applications also include thin acoustic, quantum and optical waveguides.Quantum graphs model arising in photonic crystal theory were obtained and studied in **[41, 42]** . Further applications of quantum graphs can be found in **[36]** .

1. More on Graphs and Metric Graphs

Let $\Gamma = (V, E)$ be a graph. If $e = xy$ is an edge formed by joining two nonadjacent vertices $x, y \in \Gamma$ then we will denote by $\Gamma + e$ the graph $(V, E \cup \{e\})$. If $e \in E$, then $\Gamma - e$is the graph $(V, E \setminus \{e\})$.

We will sometimes consider metric graphs Γ with infinite leads. An infinite lead is an edge of infinite length with one vertex. One can naturally identify such edge with the half-axis $\mathbb{R}^+$. Infinite leads are not edges described in $E(\Gamma)$. Hence one can assume that each element of $E(\Gamma)$ has finite length. We also make the following assumption:

Assumption 1: The lengths of all edges e are uniformly bounded from below:

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$$0 < c \leq l_e \leq \infty, \tag{3.1}$$

where c is a positive constant. In the case of a finite graph, this is naturally true.

Functions on a metric graph Γ are defined along the edges. A function is said to be

continuous on Γ if it is continuous along all edges in Γ and at each vertex the function values from different edges insident to that vertex agree. As mentioned before, with the edges being identified with segments of the real line, one can define Lebesgue measure along the edges of Γ. Thus one can define in a natural way some function spaces on Γ.

Definiton 1. *1. The space $L^2(\Gamma)$ on Γ consists of functions f that are measurable and square integrable on each edge e and satisfy*

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

In other words, $L^2(\Gamma)$ is the orthogonal direct sum of spaces $L^2(e)$.

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

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

There is no natural way to define Sobolev spaces $H^k(\Gamma)$ of order $k > 1$.

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2. Operators on Graphs

A quantum graph is a metric graph equipped with a self-adjoint differential operator. Someof the simplest operators frequently encountered in quantum graph theory act on the edges as the negative second derivative

$$f(x) \to -\frac{d^2 f}{dx^2}(x) \qquad (3.2)$$

or more general Schrödinger type operator

$$f(x) \to \left(i\frac{d}{dx} + A(x)\right)^2 f(x) + V(x)f(x).$$

Here x denotes the coordinate x_e along the edge e. Higher order differential and even pseudo-differential operators can arise as well. For the remainder of this chapter, we willonly be considering operator that acts as negative second derivative on each edge.

Besides specifying the differential expression of the operator on the edges, we would also need to describe the operator's domain, which involves prescribing some "boundary" conditions at the vertices. We will only deal with local vertex conditions. In particular, we are interested in all local vertex conditions that lead to a self-adjoint realization of operatorwith differential expression such as (3.2).

In considering local vertex conditions, it suffices to address the problem of self-adjointness at a single vertex v with degree d_v. For functions in H^1 on each edge, let F be the vector $(f_1(v), \ldots, f_d(v))^t$ of the vertex values of the function along each edge adjacent to v (so there are d_v edges) and $F^J = (f_1^J(v), \ldots, f_d^J(v))^t$ is the vector of the derivatives at v taken along the edges in the outgoing directions from v. Then the most general form of such a (homogeneous) condition is

$$A_v F + B_v F^J = 0 \qquad (3.3)$$

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Here A_v and B_v are $d_v \times d_v$ matrices. The rank of $d_v \times 2d_v$ augmented matrix $[A_v|B_v]$ must equal to d_v in order to ensure the correct number of independent conditions. The following theorem from **[28]** gives necessary and sufficient conditions on the matrices A_v and B_v that lead to the resulting operator being self-adjoint. We state the theorem without proof,which can be found in **[28]** .

2. Proof of the Main Result

The proof of Theorem 16 will use the Dirichlet-to-Neumann map to rewrite the spectral problem on Γ as a vector valued spectral problem on a half-line with a general Robin condition at the origin.

First of all, Lemma 15 implies that it is sufficient to prove absence of singular continu- ous spectrum on the positive half-axis only. Then the statement about absolute continuousspectrum would follow as well by the same Lemma.

Let $R(\lambda)$ be the resolvent of H. The first statement of Theorem 16 is established inthe following

Lemma 18. *Let f be a compactly supported function on* Γ *which is smooth on each edge and satisfies the vertex conditions (3.3). Then for any interval* $[a, b] \subset \mathbb{R}^+$ *that does not intersect* $\sigma(H_0)$ *one has*

$$\sup_{\substack{a \le \lambda \le b \\ 0 < \epsilon < 1}} |(R(\lambda + i\epsilon)f, f)| < \infty. \tag{3.14}$$

In fact, the expression $(R(\lambda)f, f)$ *can be analytically continued through such intervals* $[a, b]$.

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So, now our task is to prove Lemma 18. This will be done using the Dirichlet-to- Neumann operator to reduce the spectral problem for H on Γ to a vector one on the half- line.

At this point it will be beneficial to have in mind a different geometric picture of Γ than in Fig. 5. Namely, imagine that all the n infinite rays e_v, $v \in B$ are stretched along the positive half-axis in parallel, being connected at the origin by the finite graph Γ_0 attachedto the rays at the vertices of B (see Fig. 6). Any function u on Γ can now be viewed as the

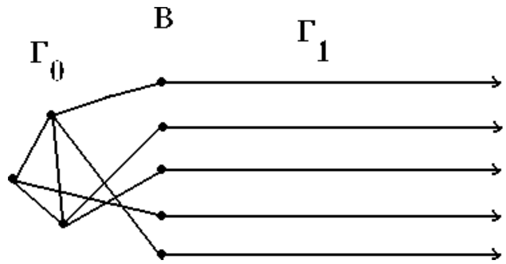

Fig. 6. A Different Visualization of Γ.

pair (u_0, u_1), where $u_j = u|_{\Gamma_j}$. Functions defined on the part Γ_1 of Γ (in particular, u_1) can be interpreted as vector-valued functions on $\mathbb{R}^+$ with values in $\mathbb{C}^n$ (recall that $n = |B|$). In particular, interpreting u_1 as such, we can write $u|_B = u_1|_B = u(0)$, where 0 is the origin in $\mathbb{R}^+$.

Let now $f = (f_0, f_1)$ be as in Lemma 18. Then $u = R(\lambda)f$ is a function that belongs to H^2_{loc} on each edge and satisfies vertex conditions (3.3) and the equation

$$Hu - \lambda u = f. \tag{3.15}$$

Here u naturally depends on λ. The quantity we need to estimate in (3.14) is now theinner product $(u, f) = (u_0, f_0) + (u_1, f_1)$. Let us write (3.15) and the vertex conditions

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separately for u_0 on Γ_0 and u_1 on Γ_1. On the finite graph Γ_0 we get

$$\left(-\frac{d^2}{dx^2}-\lambda\right)u_0 = f_0 \qquad (3.16)$$

(3.3) satisfied on vertices of Γ_0 except those in $B u_0|_B = u_1(0)$

Similarly, on Γ_1 we have

$$\left(-\frac{d^2}{dx^2}-\lambda\right)u_1 = f_1 \text{ on } \mathbb{R}^+ \qquad (3.17)$$

$$u'_1(0) = Nu_0$$

Here N is the previously introduced "normal derivative at B" operator on Γ_0 and functions

u_1, f_1 are interpreted as functions on $\mathbb{R}^+$ with values in $\mathbb{C}^n$.

Notice that the boundary conditions on B in (3.16) and at zero in (3.17) are just the vertex conditions (3.3) on B rewritten[2].

If now we are able to express Nu_0 in terms of $u_1(0)$ and f_0, we will essentially separate problems on Γ_0 and Γ_1. This can easily be done due to Lemma 17. Indeed, if $R_0(\lambda)$ is the resolvent of the operator H_0 studied in the previous section, then clearly one has

$$u_0 = R_0(\lambda)\left(\frac{d^2}{dx^2}+\lambda\right)E(u_1(0)) + R_0(\lambda)f_0 \qquad (3.18)$$

and thus

$$Nu_0 = \Lambda(\lambda)u_1(0) + NR_0(\lambda)f_0 = \Lambda(\lambda)u_1(0) + g(\lambda). \qquad (3.19)$$

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Here, for a given f_0 of the considered class, $g(\lambda) = NR_0(\lambda)f_0$ is a known meromorphicvector function of λ in C with singularities only at points of $\sigma(H_0)$.

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[2] When we need to remember that $u_j(\cdot)$ also depends on λ, we will write it as $u_j(\cdot, \lambda)$.

Now the problem (3.17) can be rewritten as

$$(-\frac{d^2}{dx^2} - \lambda)u_1 = f_1 \text{ on } \mathbb{R}^+ \qquad (3.20)$$

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$$u_1'(0) = \Lambda(\lambda)u_1(0) + g(\lambda).$$

By the construction, $\Lambda(\lambda)$ is a meromorphic matrix function in C with self-adjointvalues along the real axis. We also observe that the only memory of the finite part of the graph is confined to the vector-function $g(\lambda)$. We also need to remember that u_1 mustbelong to $L^2(\mathbb{R}^+, \mathbb{C}^n)$.

If we now show that both expressions $(u_1(\cdot, \lambda), f_1(\cdot))$ and $u_1(0, \lambda)$ continue analytically through the real axis except a discrete set, then according to (3.18) the same will hold for $(u_0(\cdot, \lambda), f_0(\cdot))$, and thus the Lemma and the main Theorem will be proven. Hence, we only need to concentrate on the vector problem (3.20) on the positive half-axis.

Let us consider the self-adjoint operator P in $L^2(\mathbb{R}^+)$ naturally corresponding to $-\frac{d^2}{dx^2}$ with ~~the N~~eumann condition at the origin. Let also $r(\lambda)$ be its resolvent. We sketch below the proof of the following well known limiting absorption result:

Lemma 19. *For any smooth compactly supported function f on* $\mathbb{R}^+$ *and any interval* $(a, b) \subset \mathbb{R}^+$, *the inner product* $(r(\lambda)f, f)$ *as a function of* λ *can be analytically continued through* (a, b) *from the upper half-plane Im* $\lambda > 0$.

Let us chose in the upper half-plane the branch of $\sqrt{\lambda}$ that has positive imaginary part. The above lemma then follows immediately from the explicit formula for $r(\lambda)$:

$$(r(\lambda)f)(x) = \frac{i}{2}\int_0^\infty \frac{e^{i\sqrt{\lambda}(x+s)} + e^{i\sqrt{\lambda}|x-s|}}{\sqrt{\lambda}} f(s)\, ds. \tag{3.21}$$

This formula also implies that the value $(r(\lambda)f)(0)$ has the same analyticity property.

In what follows we will abuse notations using $r(\lambda)$ where in fact one should use $r(\lambda) \bigotimes I$ (here I is the unit $n \times n$ matrix).

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It is not hard to solve (3.17) now. Indeed, after a simple computation one arrives tothe formula for the solution that one can check directly when $\mathrm{Im}\sqrt{\lambda} > 0$:

$$u_1(x,\lambda) := (r(\lambda)f_1)(x) - ie^{i\sqrt{\lambda}x}A(\lambda) \tag{3.22}$$

where the vector $A(\lambda)$ is:

$$A(\lambda) = \Lambda(\lambda)[\sqrt{\lambda} + i\Lambda(\lambda)]^{-1}\left((r(\lambda)f_1)(0) + \frac{g(\lambda)}{\sqrt{\lambda}}\right) \tag{3.23}$$

Notice that the matrix function $\sqrt{\lambda} + i\Lambda(\lambda)$ is meromorphic on the Riemann surface of $\sqrt{\lambda}$. Due to self-adjointness of $\Lambda(\lambda)$, the values of that function for non-zero real λ are invertible. Hence, the matrix function $\left(\sqrt{\lambda} + i\Lambda(\lambda)\right)^{-1}$ is meromorphic on the sameRiemann surface.

Now the quantity of interest becomes

$$(u_1(\cdot,\lambda), f_1(\cdot)) = (r(\lambda)f_1, f_1) - i(e^{i\sqrt{\lambda}x}A(\lambda), f_1(x)). \tag{3.24}$$

Lemma 19 implies the needed analyticity of the first term in the sum. Since $\mathrm{Im}\sqrt{\lambda} > 0$, according to the remarks after (3.21), $(r(\lambda)f_1)(0)$ is analytic hence $e^{i\sqrt{\lambda}x}A(\lambda)$ is analytic through (a, b) as well save for a discrete set of λ. Thus the final term in the sum can also be analytically continued through (a, b) as well outside of a discrete set of λ.

This finishes the proof of Lemma 18. □

Since the space of functions f as above is dense in $L^2(\Gamma)$, it is well known that (3.14) implies absence of the singular continuous spectrum (e.g., Proposition 2 and (18) in Section 1.4.5 of **[63]** or pp. 136-139 in Section XIII.6 of **[53]**) and thus proves Theorem 16.

e-ISSN 2320 –7876 www.ijfans.org
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SUMMARY

In this dissertation, we described our results concerning two areas of applied spectral the-ory.

Photonic crystals offer great promises in lasers, high-speed computers and in the area of telecommunications. Already, fiber-optic cables, which guide light, have revolutionized the telecommunications industry. Photonic crystals provide potentially better means of guiding and localizing light than current optical materials.

In the area of photonic crystal waveguides (PBG waveguides), we proved existence and confinement of guided waves through a linear defect in a PBG material, provided some "strength" conditions on the defect. The results are obtained both for the scalar (corresponding to 2*D* photonic or any dimension acoustic guides) and the full 3*D* Maxwellcases. See **[43, 44]** .

The most important reason for considering quantum graphs is studying propagationof waves through media that resemble thin neighborhoods of graphs, such as circuits ofquantum wires. Applications also include thin acoustic, quantum and optical waveguides.One of the results in quantum graphs that we have is establishing a limiting absorption principle and thus absence of singular continuous spectrum for scattering graphs. Thelimiting absorption principle is useful in understanding the spectrum of a quantum graph which in turn gives us information about quantum dynamics on such objects. See **[49]** .

As we have seen in the case of photonic crystal, gaps in the spectrum are essential for guiding and localizing light. A standard way to create spectral gaps is to make the medium periodic. Unfortunately, this neither guarantees existence of gaps (except in the one-dimensional case), nor allows easy control over the location of the gaps. We present a novel procedures of opening spectral gaps in regular finite quantum graphs. This procedure also allows some control over the location of the gaps. See **[45]** .

The work done in this dissertation clearly can and needs to be continued further. For instance, concerning photonic crystal waveguides, one would like to show that the spectraof Maxwell and Acoustic operators are absolutely continuous (i.e., that no bound states can arise). Propagation of guided waves in bent waveguides are very important in applicationand thus would be a natural choice for the next project.

In quantum graph theory, the resonant gap opening procedure is very important for applications and thus the technique needs to be extended to any graph (finite or infinite). Also one needs to obtain weaker conditions on the scatters that ensure that gaps can be opened.

e-ISSN 2320 –7876 www.ijfans.org
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The results are published in one paper **[44]** , one more paper is accepted for publica-tion **[49]** , and two more are in preparation **[43, 45]** .

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