SPECTRAL PROBLEMS OF OPTICAL WAVEGUIDES AND QUANTUM GRAPHS

A Dissertation

by

BENG SEONG ONG

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

August 2006

Major Subject: Mathematics

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Approved by:

Chair of Committee,	Peter Kuchment
Committee Members,	Joseph Ward
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ABSTRACT

Spectral Problems of Optical Waveguides and Quantum Graphs. (August 2006)

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Chair of Advisory Committee: Dr. Peter Kuchment

In this dissertation, we consider some spectral problems of optical waveguide and quantum graph theories.

We study spectral problems that arise when considerating optical waveguides in photonic band-gap (PBG) materials. Specifically, we address the issue of the existence of modes guided by linear defects in photonic crystals. Such modes can be created for frequencies in the spectral gaps of the bulk material and thus are evanescent in the bulk (i.e., confined to the guide).

In the quantum graph part we prove the validity of the limiting absorption principle for finite graphs with infinite leads attached. In particular, this leads to the absence of a singular continuous spectrum.

Another problem in quantum graph theory that we consider involves opening gaps in the spectrum of a quantum graph by replacing each vertex of the original graph with a finite graph. We show that such "decorations" can be used to create spectral gaps.

To my dear mother

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I would also like to thank the mathematics department at Texas A&M University for their generosity; otherwise it would be impossible to get this far. I would like to thank my committee members for their support and valuable suggestions. Many of my colleagues' discussions have also benefitted me.

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During my time here, I have also learned the extremely fast and addictive sport of badminton. It has provided me with an outlet for stress and kept me sane. I owe it to these elderly gentlemen, Jim Melton and Edward McWilliams, who first taught me the basic strategies of the game.

I am eternally grateful and indebted to my dissertation advisor, Prof. Peter Kuchment, for his advice, care, suggestions, guidance and most of all, his great patience with me. Without his help, both academic and financial, this dissertation would never have been realized.

All of my family, parents, brother and sister have also encouraged and supported me in my studies. In particular, my mother has been my pillar of strength. Through her prayers and emotional support, I have been able to overcome some really difficult and trying times.

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CHAPTER I

INTRODUCTION

This dissertation addresses two areas of spectral theory. One deals with the so called photonic crystal waveguides. The other comes from quantum graph theory.

Chapter II starts with the introduction to the wonders of photonic crystals. Throughout history, mankind has made many technological leaps as a result of deeper understanding and/or modifying of material properties. Starting from the Iron Age, humans have learned how to modify mechanical properties of existing materials by combining them to form new materials, such as alloys, plastic and ceramics. In the last century, we learned how to control electrical properties of materials. Transistor is one of such technological advances that have revolutionized the world of electronics. With computers and other electronic equipments widely available and very much depended upon, their impacts are tremendous in our everyday life.

In the recent decades, a new frontier has emerged with a similar goal, that is to control 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 operate 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 chapter II 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

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obtained both for the scalar (corresponding to acoustic or $2D$ photonic guides) and the full $3D$ Maxwell cases. See **[43, 44]** .

Chapter III concerns quantum graphs. 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 quantum graph 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.

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 quantum graphs is indispensable to our understanding and in making breakthrough in some areas of nanotechnology.

In sections B and C of chapter III we describe and prove our results concerning spectral properties of quantum graphs.

One of the results concerning quantum graphs that we establish, is validity of the limiting absorption principle and thus absence of singular continuous spectrum for scattering graphs **[49]** . The limiting absorption principle is useful for understanding the spectrum of a quantum graph, which in turn gives us information about quantum dynamics on such objects.

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 periodic. 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 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 results are presented in one paper published **[44]** , one more accepted for publication **[49]** , and two more in preparation **[43, 45]** .

CHAPTER II

SPECTRAL PROPERTIES OF PHOTONIC WAVE GUIDES*

A. Introduction to PBG Waveguides

One could think of a photonic crystal as a block of a dielectric medium (e.g., GaAs) with holes within its structure arranged in a periodic manner. These holes are filled with a different 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 they correspond 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 these energy gaps is what makes semiconductors so useful.

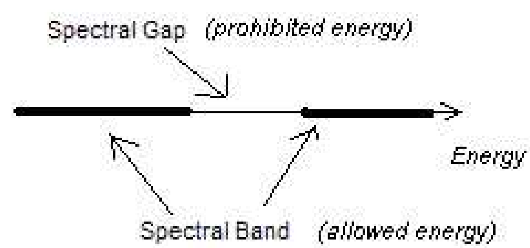

Fig. 1. Spectral Band-Gap

In the case of a photonic crystal, propagation of monochromatic electromagnetic

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waves (instead of electrons) through a block of dielectric material containing holes distributed periodically and filled with air (or other dielectric material) is studied. See Fig. 2.

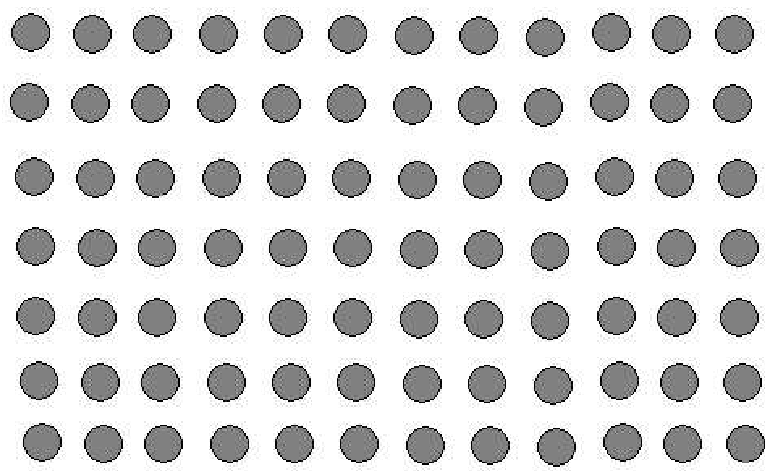

Fig. 2. PBG Material

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. If a frequency gap does indeed exist, waves with frequencies within the gap cannot exist in the 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 and mathematics, as well as possible applications of photonic crystals. See for example, **[24, 26, 40]** .

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 a more general PBG waveguide (Fig. 3).

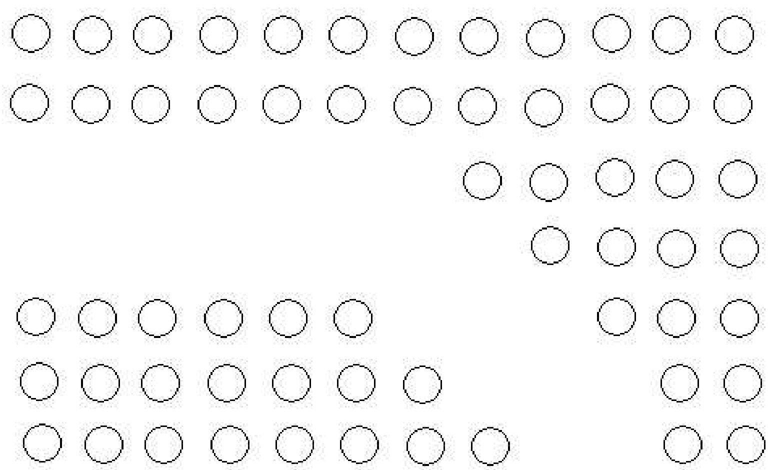

Fig. 3. A PBG Waveguide

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

$$\nabla \cdot \mathbf{B} = 0 \qquad \nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = 0$$
$$\nabla \cdot \mathbf{D} = 4\pi\rho \qquad \nabla \times \mathbf{H} - \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} = \frac{4\pi}{c}\mathbf{J}$$

where $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic fields respectively, $\mathbf{D}$ and $\mathbf{B}$ are the displacement and magnetic induction fields respectively and ρ and $\mathbf{J}$ are the free charges and currents. The constant c is the speed of light.

In studying photonic crystals, we will only be concerned with a mixed dielectric medium, a composite of regions of homogeneous dielectric materials, with no free charge or currents. This means that $\rho = 0$ and $\mathbf{J} = 0$. In linear media, we can use the constitutive relation $\mathbf{D}(x) = \varepsilon(x)\mathbf{E}(x)$ where $\varepsilon(x)$ here is the scalar real dielectric constant (i.e., we assume the material to be lossless). See **[23]** for an explanation of this relation. There is also a similar relation for $\mathbf{B}$ and $\mathbf{H}$, namely $\mathbf{B} = \mu(x)\mathbf{H}$. However, for most dielectric materials of interest, the magnetic permeability $\mu(x)$ is constant and we may set $\mathbf{B} = \mathbf{H}$. So, we restrict ourselves to linear lossless non-magnetic materials.

Substituting all the above relations into the Maxwell equations, we obtain

$$\nabla \cdot \mathbf{H}(x,t) = 0 \qquad \nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{H}(x,t)}{\partial t} = 0$$
$$\nabla \cdot \varepsilon(x)\mathbf{E}(x,t) = 0 \qquad \nabla \times \mathbf{H}(x,t) - \frac{\varepsilon(x)}{c}\frac{\partial \mathbf{E}(x,t)}{\partial t} = 0$$

where $x \in \mathbb{R}^3$ and $t \in \mathbb{R}$.

We restrict ourselves to monochromatic electromagnetic waves and thus we can write $\mathbf{H}(x,t)$ and $\mathbf{E}(x,t)$ (with some abuse of notation) as

$$\mathbf{H}(x,t) = \mathbf{H}(x)e^{i\omega t} \quad \mathbf{E}(x,t) = \mathbf{E}(x)e^{i\omega t} \tag{2.1}$$

where ω is the frequency of the monochromatic wave.

Inserting (2.1) into Maxwell equations, the two divergence equations give conditions

$$\nabla \cdot \mathbf{H}(x) = 0, \quad \nabla \cdot \mathbf{D}(x) = 0$$

These equations show that there are no point sources or sinks in the displacement and magnetic fields in the medium. If $\mathbf{H}(x) = \mathbf{a}e^{i\mathbf{k}\cdot x}$ is a plane wave, then the zero divergence condition above requires that $\mathbf{a} \cdot \mathbf{k} = 0$.

The two curl equations relating $\mathbf{E}(x)$ to $\mathbf{H}(x)$ are now reduced to the following

$$\nabla \times \mathbf{E}(x) + \frac{i\omega}{c}\mathbf{H}(x) = 0 \tag{2.2}$$

$$\nabla \times \mathbf{H}(x) + \frac{i\omega}{c}\varepsilon(x)\mathbf{E}(x) = 0 \tag{2.3}$$

We can decouple these equations in the following way, divide the second equation above by $\varepsilon(x)$ and then take the curl on both sides. Use the first equation above to eliminate $\mathbf{E}(x)$. The resulting equation entirely in $\mathbf{H}(x)$ is

$$\nabla \times \frac{1}{\varepsilon(x)}\nabla \times \mathbf{H}(x) = \left(\frac{\omega}{c}\right)^2 \mathbf{H}(x). \tag{2.4}$$

Along with the $\nabla \cdot \mathbf{H}(x) = 0$, this determines $\mathbf{H}(x)$. The above is an eigenvalue problem for the eigenvalue $\lambda = \left(\frac{\omega}{c}\right)^2$. By studying the above spectral problem, we gain understanding of propagation of monochromatic waves in photonic crystals.

Although there is essentially no difference mathematically in studying (2.4) or a similar equation in terms of $\mathbf{E}(x)$, we have opted to go with (2.4).

There are three questions that we would want to address about linear PBG waveguides.

1. Under what conditions on the defect will new spectrum arise in the "defect-less" medium's spectral gap (assuming there is a gap)? The next two sections will show that under some conditions about the defect, creation of new spectrum within the gap of the "defect-less" medium is ensured.

2. There are no hard walls to confine waves in photonic waveguides. Will the waves still be confined within the guides ? The waves are confined because their frequencies are prohibited to exist outside the defect. So, confinement in this situation means that waves must decay exponentially away from the defect, i.e., are evanescent into the bulk. The next two sections will answer affirmatively this question.

3. Lastly, if there are waves that exist and are confined within the defect, will they propagate ? Or will the waves "stuck" somewhere within the defect ? This corresponds to proving that the operators we consider have no bound states (or L^2 eigenfunctions). It has been known that operators of the above type have no singular continuous spectrum. Thus this is equivalent to proving that the spectra of the above operators are absolutely continuous. This problem is still unresolved, albeit absence of bound states is expected.

B. Existence and Confinement of Guided Modes. Scalar Model

If we assume that the photonic crystal is homogeneous in one direction, say in the direction of z-axis for example, then the eigenvalue problem (2.4) for Maxwell operator can be simplified. In this situation, the dielectric constant $\varepsilon(x,y)$ depends only on $(x,y) \in \mathbb{R}^2$ rather than on $(x,y,z) \in \mathbb{R}^3$. In this case every eigenfunction of (2.4) can be classified into two distinct modes (polarizations). These modes have either the magnetic or the electric field perpendicular to the plane of periodicity, see **[24]** . The mode, where the magnetic field is perpendicular to the plane of periodicity, has nonzero field components (E_x, E_y, H_z) and is called TE (transverse-electric) mode. The other mode in which the magnetic field is parallel to the plane of periodicity is called TM (transverse-magnetic) mode.

We start with TE mode and show that (2.4) can be reduced to a scalar problem. Let $\mathbf{H} = (0, 0, H)$, divergence free condition for $\mathbf{H}$ shows that H does not depends on z. By a direct calculation,

$$\nabla \times \frac{1}{\varepsilon} \nabla \times \mathbf{H} = (\frac{\partial}{\partial z}\left(\frac{-1}{\varepsilon}\frac{\partial H}{\partial x}\right), \frac{\partial}{\partial z}\left(\frac{-1}{\varepsilon}\frac{\partial H}{\partial y}\right), -\nabla_{(x,y)} \cdot \frac{1}{\varepsilon}\nabla_{(x,y)} H).$$

Since ε and H do not depend on z, the first two components vanish. Thus the eigenvalue problem in the vector case (2.4) can be reduced to a scalar one, namely

$$-\nabla \cdot \frac{1}{\varepsilon(x,y)} \nabla H = \left(\frac{\omega}{c}\right)^2 H$$

where $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y})$.

Before we consider the TM mode, we first have to derive an equation similar to (2.4) but for $\mathbf{E}$. We take the curl of (2.2) and then use (2.3) to eliminate $\mathbf{H}$. After dividing by ε, the resulting equation entirely in $\mathbf{E}$ is

$$-\frac{1}{\varepsilon}\Delta\mathbf{E} = \left(\frac{\omega}{c}\right)^2 \mathbf{E} \tag{2.5}$$

With TM mode, we have $\mathbf{E} = (0, 0, E)$. The condition $\nabla \cdot \varepsilon\mathbf{E} = 0$ and that ε does not depend on z imply that E also does not depend on z. By direct calculation, we obtain

$$-\Delta\mathbf{E} = (0, 0, -\Delta E).$$

Hence the eigenvalue problem in the vector case (2.5) boils down to a scalar case for TM mode, namely

$$-\frac{1}{\varepsilon(x)}\Delta E = \left(\frac{\omega}{c}\right)^2 E.$$

We will consider in this section the existence and confinement of guided modes for scalar operators:

$$A_1 := -\nabla \cdot \frac{1}{\varepsilon(x)}\nabla$$

or

$$A_2 := -\frac{1}{\varepsilon(x)}\Delta$$

where $\varepsilon(x)$ is a bounded positive function. The operators A_1 and A_2 correspond to the case of TE and TM modes respectively.

We now describe the mathematical model studied in this section that will encompass both cases above. This operator also arises in studying acoustic waves in the so called phononic crystals (or acoustic band-gap structures). Let $\varepsilon_0(x)$ and $\rho_0(x)$ be bounded positive measurable functions in $\mathbb{R}^d$ separated from zero, i.e. $0 < c_0 \leq \varepsilon_0(x),\ \rho_0(x) \leq c_1 < \infty$. It is usually assumed in the photonic crystal theory that both functions are periodic with respect to a lattice $\Gamma \subset \mathbb{R}^d$, but this is not required for the basic results we obtain in this chapter.

One can think that the whole space $\mathbb{R}^d$ is filled with a dielectric or acoustic material with properties described by the functions ε_0 and ρ_0 (the physical interpretation of these functions depends on whether one deals with electromagnetic or acoustic case, but this will be of no importance for our study). In the case of periodic functions this models a photonic or phononic crystal. This is our un-perturbed (bulk) medium.

The operator A_0 is the self-adjoint realization of

$$A_0 := -\frac{1}{\rho_0(x)}\nabla \cdot \frac{1}{\varepsilon_0(x)}\nabla \tag{2.6}$$

in $L_2(\mathbb{R}^d, \rho_0(x)\, dx)$ defined by means of its quadratic form

$$\int \varepsilon_0^{-1}|\nabla u|^2 dx \tag{2.7}$$

with the domain $H^1(\mathbb{R}^d)$.

We will consider a "defect" strip

$$\mathcal{S}_l = \{x = (x_1, x') \in \mathbb{R}^d \,|\, x \in \mathbb{R},\ x' \in l\Omega\},$$

where Ω is a domain in $\mathbb{R}^{d-1}$ (e.g., the unit ball centered at the origin) and $l\Omega$ is the domain Ω scaled with factor l. Below is an example of $\mathcal{S}_l$ (Fig. 4).

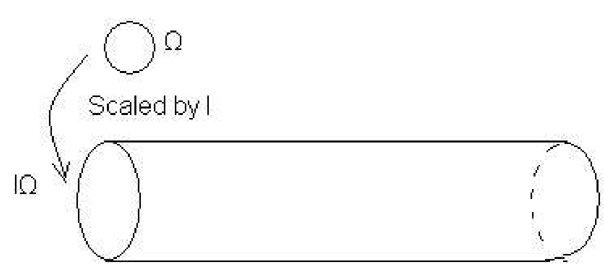

Fig. 4. $\mathcal{S}_l$

We now introduce the perturbed medium, for which

$$\varepsilon(x) = \begin{cases} \varepsilon > 0 & \text{for } x \in \mathcal{S}_l \\ \varepsilon_0(x) & \text{for } x \notin \mathcal{S}_l \end{cases}, \quad \rho(x) = \begin{cases} \rho > 0 & \text{for } x \in \mathcal{S}_l \\ \rho_0(x) & \text{for } x \notin \mathcal{S}_l \end{cases}.$$

Physically, a linear homogeneous defect $\mathcal{S}_l$ is introduced into the original medium.

We define the perturbed operator

$$A := -\frac{1}{\rho(x)}\nabla \cdot \frac{1}{\varepsilon(x)}\nabla \tag{2.8}$$

that corresponds to the modified medium analogously to the background operator A_0. This operator is self-adjoint in the weighted L_2-space $L_2(\mathbb{R}^d, \rho(x)\,dx)$, which will from now on be denoted $L_{2,\rho}$. Operator A here can be seen to include both cases of the scalar operators A_1 and A_2.

Our goal is to show that for any gap (α, β) in the spectrum $\sigma(A_0)$ of the unperturbed medium and under appropriate conditions on the parameters l, ρ, and ε of the line defect, spectrum of the perturbed medium arises in the gap.

One naturally wants to interpret this as existence of guided waves in the "photonic waveguide" $\mathcal{S}_l$, while this would require proving some additional properties. These are first of all confinement of the wave to the guide (i.e., evanescence into the bulk), which is also proven below, and non-existence of bound states (i.e., the fact that the wave is actually propagating along the waveguide), which we have not been able to prove yet, although there is little doubt that this is true. Some initial results in this direction have been obtained in **[12, 14, 15]** .

The results in this section is contained in **[44]** . One should mention paper **[1]** by H. Ammari and F. Santosa, where spectral properties of the TM mode in a 2D PBG waveguides were studied in the special case of a linear defect aligned with a periodicity axis of an otherwise periodic medium (and hence Floquet theory **[34, 53]** was applicable).

In particular, exponential confinement of the guided modes (if they exist) for this particular case was proven there. Existence of guided modes was not established. Some of the constructions presented here are similar to the ones used in **[11]** for localized defects.

1. Formulation of the Results

Our main results are the following theorems.

Theorem 1. *Let $G = (\alpha, \beta)$ be a non-empty finite gap in the spectrum of the "background medium" operator A_0 (in particular, $\alpha > 0$). Assume that for some $\delta \in (0, \dfrac{\beta - \alpha}{2})$ the following inequality is satisfied:*

$$l^4 \delta^2 \rho^2 \varepsilon^2 > \nu_{d-1}, \tag{2.9}$$

where $\nu_{d-1} > 0$ is the lowest eigenvalue of the bi-harmonic operator Δ^2 in Ω with Dirichlet boundary conditions.

Then any interval of length 2δ in the gap G contains at least one point of the spectrum $\sigma(A)$ of the perturbed operator.

This theorem guarantees that when (2.9) is satisfied, defect modes in the spectral gaps of the background medium exist, and the corresponding spectrum forms a δ-net in the gap.

Before formulating the next theorem, we remind the reader about existence of the so called generalized eigenfunction expansions. Generalized eigenfunction u of A is a function that satisfies $Au = zu$ for some z in a distributional sense. Generalized eigenfunctions do not have to belong to the domain of A or even to L_2 space. In the case of the operators we consider, for almost all points $z \in \mathbb{R}$ with respect to the spectral measure, there is a complete family of generalized eigenfunctions $\mathcal{A}$ for operator A. Each $u \in \mathcal{A}$ is in H^1_{loc} and has the properties

$$(1 + |x|)^{-N} u(x) \in L_2(\mathbb{R}^d) \text{ and } (1 + |x|)^{-N} \nabla u(x) \in L_2(\mathbb{R}^d) \tag{2.10}$$

for some $N > 0$. This is a well known fact for elliptic operators with smooth coefficients **[4]** , while for operators of the type we study one can find the corresponding results in **[27]** . We will use the polynomial boundedness condition (2.10) in the following form:

$$\|u\|_{L_2(K+x)} + \|\nabla u\|_{L_2(K+x)} \leq C_K(1+|x|)^N \tag{2.11}$$

for any compact K and $x \in \mathbb{R}^d$. We summarize (2.11) as *polynomial boundedness of order N.*

Theorem 2. *If u is a polynomially bounded generalized eigenfunction of A that corresponds to a value z in a gap G of $\sigma(A_0)$, then it decays exponentially away from the defect strip $\mathcal{S}_l$.*

The exact meaning of the exponential decay will be provided in the reformulation of Theorem 2 given in Theorem 3 of the next subsection.

2. Proofs of the Results

We adopt the following notations: the norm and inner product in $L_2(\mathbb{R}^d)$ will be denoted by $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ respectively, while those in the weighted space $L_2(\mathbb{R}^d;\, \rho(x)dx)$ will be denoted with the subscript ρ: $\|\cdot\|_\rho$, $\langle\cdot,\cdot\rangle_\rho$. Notice that the norms $\|\cdot\|$, $\|\cdot\|_\rho$, and $\|\cdot\|_{\rho_0}$ are equivalent.

a. Proof of Theorem 1

Let $(\mu-\delta, \mu+\delta)$ be a sub-interval of the gap G. The idea of the proof is that under the conditions of the theorem one is able to provide an approximate eigenfunction $u(x)$ for the operator A, such that $\|u\|_\rho = 1$ and

$$\|Au - \mu u\|_\rho^2 < \delta^2. \tag{2.12}$$

Finding such an approximate eigenfunction would imply immediately the statement of the theorem. This is because showing $\sigma(A) \cap (\mu-\delta, \mu+\delta) \neq \emptyset$ is equivalent to showing $\text{dist}(\mu, \sigma(A)) < \delta$. If $\mu \in \sigma(A)$ then we are done and $\text{dist}(\mu, \sigma(A)) < \delta$ trivially. If $\mu \notin \sigma(A)$ then $A_\mu := A - \mu I$ has an inverse. Due to self-adjointness of A in $L_{2,\rho}$, we have $\| (A-\mu)^{-1} \|_\rho \leq \text{dist}(\mu, \sigma(A))^{-1}$. Suppose a function u has $\| u \|_\rho = 1$, then $1 \leq \|A_\mu u\|_\rho \|A_\mu^{-1}\|_\rho$. It follows that (2.12) implies

$$\frac{1}{\delta} < \frac{1}{\|A_\mu u\|_\rho} \leq \|A_\mu^{-1}\|_\rho \leq \frac{1}{\text{dist}(\mu, \sigma(A))}$$

$$\Rightarrow \quad \text{dist}(\mu, \sigma(A)) < \delta.$$

For functions u supported in the defect strip, where $\rho(x) = \rho$, then

$$\rho \, \|Au - \mu u\|^2 = \|Au - \mu u\|_\rho^2 < \delta^2 \, \|u\|_\rho^2 = \rho\delta^2 \, \|u\|^2$$

which is equivalent to

$$\|Au - \mu u\|^2 < \delta^2 \, \|u\|^2 \, .$$

Thus for a function u supported in the defect strip, (2.12) is equivalent to finding a function u such that $\|u\| = 1$ and

$$\|Au - \mu u\|^2 < \delta^2. \tag{2.13}$$

So, let us construct such a function.

Let $\phi(x') \in C_0^\infty(\Omega)$ and $\psi(x_1) \in C_0^\infty(\mathbb{R})$ be functions of unit L_2-norm on Ω and $\mathbb{R}$ respectively. Then for $l, n > 0$, define $\phi_l(x') := l^{(1-d)/2}\phi(x'/l)$ and $\psi_n(x_1) := n^{-1/2}\psi(x_1/n)$ which also have unit L_2-norms in the corresponding spaces. Indeed, by change of variables $y' = x'/l$ and $y_1 = x_1/n$, one obtains

$$\int_{l\Omega} |\phi_l(x')|^2 \; dx' = \int_\Omega l^{1-d} |\phi(y')|^2 \; l^{d-1} dy' = \int_\Omega |\phi(y')|^2 \; dy' = 1$$

$$\int_{\mathbb{R}} |\psi_n(x_1)|^2 \ \ dx_1 = \int_{\mathbb{R}} n^{-1}|\psi(y_1)|^2 \ n^1 dy_1 = \int_{\mathbb{R}} |\psi(y_1)|^2 \ dy_1 = 1.$$

Introducing $k = \sqrt{\mu\rho\varepsilon}$, we consider the function

$$u_{l,n}(x) = \phi_l(x')\psi_n(x_1)e^{ikx_1}, \tag{2.14}$$

which will be our candidate for an approximate eigenfunction.

Instead of estimating the left hand side of (2.13), we will estimate $\|\varepsilon\rho\,(Au - \mu u)\|^2$. Since $\varepsilon(x)$ and $\rho(x)$ are positive constants inside the defect, (2.13) is equivalent to

$$\|\varepsilon\rho(Au - \mu u)\|^2 < \delta^2\rho^2\varepsilon^2. \tag{2.15}$$

The left hand side can be further simplified to

$$\|\varepsilon\rho(Au - \mu u)\|^2 = \|\varepsilon\rho(-\frac{1}{\rho}\nabla \cdot \frac{1}{\varepsilon}\nabla u - \mu u)\|^2 = \|-\Delta u - k^2 u\|^2$$

Thus the needed inequality (2.15) can be also rewritten as

$$\|\Delta u + k^2 u\|^2 < \delta^2\rho^2\varepsilon^2. \tag{2.16}$$

Let us calculate directly the left hand side of (2.16) for the function u introduced above. We start by calculating $-\Delta u$:

$$\Delta u = \nabla \cdot ((\psi_n' + ik\psi_n)\phi_l e^{ikx_1}, \ \psi_n e^{ikx_1}\nabla_{x'}\phi_l)$$

$$= (\psi_n'' + 2ik\psi_n' - k^2\psi_n)\phi_l e^{ikx_1} + \psi_n e^{ikx_1}\Delta_{x'}\phi_l$$

$$= (\psi_n'' + 2ik\psi_n')\phi_l e^{ikx_1} - k^2 u + \psi_n e^{ikx_1}\Delta_{x'}\phi_l$$

Understanding that all norms appearing below as the norms in L_2, (2.16) expands to

$$\begin{aligned} \|\Delta u + k^2 u\|^2 &= \|(\Delta_{x'}\phi_l)\psi_n + \phi_l\psi_n'' + 2ik\phi_l\psi_n'\|^2 \\ &= \|(\Delta_{x'}\phi_l)\psi_n + \phi_l\psi_n''\|^2 + 4k^2 \ \|\phi_l\psi_n'\|^2 \ . \end{aligned} \tag{2.17}$$

We used the condition that functions ϕ and ψ are real valued and Pythagorean theorem for L_2-norm .

Let $\gamma > 0$. Using the inequality

$$(a+b)^2 \leq (1+\gamma)\, a^2 + \left(1 + \frac{1}{\gamma}\right) b^2$$

and normalization of the functions, we can estimate the last expression from above to get the following upper bound for the expression in question:

$$\begin{aligned} \|\Delta u + k^2 u\|^2 \leq & \frac{1+\gamma}{l^{d+3}} \; \|\Delta\phi\left(\frac{x'}{l}\right)\|^2_{L_2(l\Omega)} \\ & + \frac{1+\frac{1}{\gamma}}{n^5} \; \|\psi''\left(\frac{x_1}{n}\right)\|^2_{L_2(\mathbb{R})} + \frac{4k^2}{n^3} \; \|\psi'\left(\frac{x_1}{n}\right)\|^2_{L_2(\mathbb{R})} \end{aligned} \tag{2.18}$$

where we used

$$\|(\Delta_{x'}\phi_l)\psi_n\|^2 = \|\Delta\phi_l\|^2_{L_2(l\Omega)}\|\psi_n\|^2_{L_2(\mathbb{R})} = \|\Delta\phi_l\|^2_{L_2(l\Omega)} = \frac{1}{l^{d+3}} \; \|\Delta\phi\left(\frac{x'}{l}\right)\|^2_{L_2(l\Omega)}$$

$$\|\phi_l\psi''_n\|^2 = \|\phi_l\|^2_{L_2(l\Omega)}\|\psi''_n\|^2_{L_2(\mathbb{R})} = \|\psi''_n\|^2_{L_2(\mathbb{R})} = \frac{1}{n^5} \; \|\psi''\left(\frac{x_1}{n}\right)\|^2_{L_2(\mathbb{R})}$$

$$\|\phi_l\psi'_n\|^2 = \|\phi_l\|^2_{L_2(l\Omega)}\|\psi'_n\|^2_{L_2(\mathbb{R})} = \|\psi'_n\|^2_{L_2(\mathbb{R})} = \frac{1}{n^3} \; \|\psi'\left(\frac{x_1}{n}\right)\|^2_{L_2(\mathbb{R})} \; .$$

All of the above equalities follow directly from definition of L_2-norm, separability of the integrands and chain rule.

By changing variables to $(x_1/n, x'/l)$, this expression reduces to

$$\frac{1+\gamma}{l^4} \; \|\Delta\phi(x')\|^2_{L_2(\Omega)} + \frac{1+\frac{1}{\gamma}}{n^4} \; \|\psi''(x_1)\|^2_{L_2(\mathbb{R})} + \frac{4k^2}{n^2} \; \|\psi'(x_1)\|^2_{L_2(\mathbb{R})} \; . \tag{2.19}$$

Since n can be chosen arbitrarily large (without changing the defect strip), the last two terms can be made arbitrarily small (uniformly with respect to k on any finite interval). Hence, one needs to control only the first term by an appropriate choice of a test function

ϕ. In other words, one is interested in

$$\nu_{d-1} = \inf \, \|\Delta\phi(x')\|^2_{L_2(\Omega)},$$

where the $infimum$ is taken over real functions in $C_0^\infty(\Omega)$ of unit L_2-norm. This is then the lowest eigenvalue of the bi-harmonic operator Δ^2 with Dirichlet boundary conditions in Ω. In particular, $\nu_{d-1} > 0$. Now, due to arbitrariness of $\gamma > 0$, our condition boils down to

$$\frac{\nu_{d-1}}{l^4} < \delta^2\rho^2\varepsilon^2 \tag{2.20}$$

or

$$l^4\delta^2\rho^2\varepsilon^2 > \nu_{d-1}, \tag{2.21}$$

which proves the statement of the theorem.

b. Proof of Theorem 2

Let G be a spectral gap of A_0 and $z \in \sigma(A) \cap G$. Let also $u(y)$ be a polynomially growing generalized eigenfunction for the operator A that corresponds to z (in the meaning explained in the introduction). Let $x = (x_1, x') \in \mathbb{R}^d$ and $\chi_x(y)$ be the characteristic function of the cube $\{y \,|\, |y_j - x_j| \leq 1\}$ centered at x.

We now give a more precise formulation of Theorem 2:

Theorem 3. *There exist positive constants C_1 and $C(z)$ such that*

$$\|\chi_x u\| \leq C_1 \left(1 + |x_1|\right)^N e^{-C(z)dist(x,\, S_l)}, \tag{2.22}$$

where N is the order of polynomial boundedness of u.

Remark 4. *One might be concerned with the fact that albeit the eigenfunction decays exponentially away from the defect strip, the factor in front of the expression grows polynomially along the strip. However, for a generalized eigenfunction that grows polynomially* *one cannot expect anything better. In the periodic situation, using Floquet-Bloch theory, one can guarantee absence of this growth. Details of this claim will be provided at the end of this section.*

Proof. Define the sesqui-linear form

$$Q[\varphi, w] := \langle \nabla\varphi, \frac{1}{\varepsilon_0}\nabla w\rangle - z\langle \varphi, w\rangle_{\rho_0}$$

with the domain $H^1(\mathbb{R}^d)$.

Let $R(z) = (A_0 - z)^{-1}$ and $\varphi := R(z)\chi_x u$. We use here that z is not in the spectrum of A_0. Note that $\varphi \in D(A_0)$.

Let $p = \max(2\text{dist}(x, S_l), 1)$ and $\xi_x(y)$ be a nonnegative smooth cutoff function that depends on y_1 only, is supported in $(x_1 - (p+1), x_1 + (p+1))$ and such that it is equal to 1 on $[x_1 - p, x_1 + p]$. We assume further that $\xi_x(y) \le 1$ and $|\nabla\xi_x(y)| = |\xi_x'(y_1)| \le C$ for some constant C and all $x, y \in \mathbb{R}^d$. For simplicity of notation, we drop the subscript x in $\xi = \xi_x$. Note that $\xi u \in H^1(\mathbb{R}^d)$. Using $w = \xi u$, one gets

$$Q[\varphi, \xi u] = \langle A_0\varphi, \xi u\rangle_{\rho_0} - \langle z\varphi, \xi u\rangle_{\rho_0} = \langle \chi_x u, \xi u\rangle_{\rho_0} = \|\chi_x u\|^2_{\rho_0} \ .$$

This means that our goal should be to estimate $Q[\varphi, \xi u]$ from above. On the other hand, using the equality $Au = zu$, one gets

$$Q[\varphi, \xi u] = \langle \nabla\varphi, \frac{1}{\varepsilon_0}\nabla(\xi u)\rangle - \langle \varphi, \xi z u\rangle_{\rho_0}$$

$$= \langle \nabla\varphi, \frac{1}{\varepsilon_0}\nabla(\xi u)\rangle - \langle \varphi, \xi A u\rangle_{\rho_0} + \langle \varphi, \frac{\rho}{\rho_0}\xi A u\rangle_{\rho_0} - \langle \varphi, \frac{\rho}{\rho_0}\xi A u\rangle_{\rho_0} \tag{2.23}$$

Before proceeding further, we introduce these two functions

$$\tilde{\epsilon}(x) = \frac{1}{\varepsilon_0(x)} - \frac{1}{\varepsilon(x)}, \ \tilde{\rho}(x) = \frac{1}{\rho_0(x)} - \frac{1}{\rho(x)}.$$

Notice that both these functions are supported inside the strip $\mathcal{S}_l$.

Returning to (2.23), combine the second and third terms together, we get $\langle \varphi, \xi\rho\tilde{\rho}Au\rangle_{\rho_0}$. Performing integration by parts on the fourth term of (2.23),

$$-\langle \varphi, \frac{\rho}{\rho_0}\xi Au\rangle_{\rho_0} = \langle \varphi, \xi\nabla\cdot\frac{1}{\varepsilon}\nabla u\rangle = -\langle \nabla(\xi\varphi), \frac{1}{\varepsilon}\nabla u\rangle$$
$$= -\langle \xi\nabla\varphi, \frac{1}{\varepsilon}\nabla u\rangle - \langle \varphi\nabla\xi, \frac{1}{\varepsilon}\nabla u\rangle \tag{2.24}$$

By expanding the first term of (2.23) and add both (2.24) and $\langle \varphi, \xi\rho\tilde{\rho}Au\rangle_{\rho_0}$ to it, (2.23) can be rewritten as

$$\langle \nabla\varphi, \xi\tilde{\epsilon}\nabla u\rangle + \langle \varphi, \xi\rho\tilde{\rho}Au\rangle_{\rho_0} + \langle \nabla\xi, \frac{u}{\varepsilon_0}\nabla\varphi - \frac{\varphi}{\varepsilon}\nabla u\rangle. \tag{2.25}$$

Our last task in proving the theorem is to estimate from above the terms in (2.25). In order to do so, we need an auxiliary statement concerning the exponential decay of the resolvent, which is a result of **[3, 9]** :

Lemma 5. [3, 9] *There exist a positive number m_z that depends only on the distance of the point z from the gap edges, such that for a positive constant C the following estimates hold for the local $L_2(\mathbb{R}^d)$-norm of the resolvent $R(z)$:*

$$\begin{aligned} \|\chi_u R(z)\chi_v\| &\leq Ce^{-m_z|u-v|} \\ \|\chi_u \nabla R(z)\chi_v\| &\leq Ce^{-m_z|u-v|} \end{aligned} \tag{2.26}$$

for any u, $v \in \mathbb{R}^d$. Here the norms in the left hand side are the operator norms in $L_2(\mathbb{R}^d)$.

We can now get the needed estimates. Let $V = [x_1 - p - 1, x_1 + p + 1] \times l\Omega$. This is a compact domain that can be covered by the union of p fixed size domains $V_j = [a_j, a_j + 2] \times l\Omega$ and which contains the supports of $(\xi\tilde{\epsilon})$ and $(\xi\tilde{\rho})$. Also note that $\text{dist}(x, V_j) \geq \text{dist}(x, S_l)$. Now using the lemma above and (2.11) we get

$$\begin{aligned} |\langle \nabla\varphi, \xi\tilde{\epsilon}\nabla u\rangle| &\leq \|\chi_V\nabla\varphi\| \, \|\xi\tilde{\epsilon}\nabla u\| \leq C \, \|\sum_j \chi_{V_j}\nabla R(z)\chi_x u\| \|\sum_j \chi_{V_j}\nabla u\| \\ &\leq Cp^2(|x_1| + p + 1)^{2N} e^{-m_z \text{dist}(x,\mathcal{S}_l)} \leq C(|x_1| + 1)^{2N} e^{-(m_z - \eta)\text{dist}(x,\mathcal{S}_l)} \end{aligned} \tag{2.27}$$

We used here that $p = \max(2\text{dist}(x, \mathcal{S}_l), 1)$. We also denoted by C different constants.

Analogously,

$$|\langle \varphi, \xi\rho\tilde{\rho}Au\rangle_{\rho_0}| \leq C|z| \sum_j \|\chi_{V_j}\varphi\| \, \|\xi\tilde{\rho}u\| \leq C(1+|x_1|)^{2N} e^{-(m_z-\eta)\text{dist}(x,\mathcal{S}_l)} \tag{2.28}$$

Let us move now to estimating the last term in (2.25). Denote by $a > 0$ a number such that shifts of $l\Omega$ by vectors aj with $j \in \mathbb{Z}^{d-1}$ cover the whole space $\mathbb{R}^{d-1}$. We denote

$$W_j := ([x_1 - p - 1, x_1 - p] \cup [x_1 + p, x_1 + p + 1]) \times (l\Omega + aj)\,.$$

Then $W_j = W_0 + (0, aj)$. Notice that $W = \cup_j W_j$ covers $\text{supp}\,\nabla\xi$ and $\text{dist}(x, W_j) \geq C_1(p + |j|) - C_2$.

We are now ready to estimate the last term of (2.25) from above. We proceed as before, using the lemma, the polynomial growth of u, and uniform boundedness of $\nabla\xi$.

$$\begin{aligned} |\langle \nabla\xi, \frac{u}{\varepsilon_0}\nabla\varphi\rangle| &\leq C\sum_j \|\chi_{W_j}u\| \|\chi_{W_j}\nabla R(z)\chi_x u\| \\ &\leq C\sum_j (|x_1| + p + |j| + 1)^{2N} e^{-m_z \text{dist}(x,W_j)} \\ &\leq C(|x_1| + p + 1)^{2N} e^{-m_z^1 \text{dist}(x,\mathcal{S}_l)} \sum_j (1 + |j|)^{2N} e^{-m_z^2|j|} \\ &\leq C(|x_1| + 1)^{2N} e^{-(m_z^1 - \eta)\text{dist}(x,\mathcal{S}_l)} \end{aligned} \tag{2.29}$$

where m_z^1 and m_z^2 are positive constants.

The expression $|\langle \nabla\xi, \dfrac{\varphi}{\varepsilon}\nabla u\rangle|$ is estimated analogously. Combining the above estimates, we get

$$\|\chi_x u\|^2 \leq C\, \|\chi_x u\|^2_{\rho_0} = Q[\varphi, \xi u] \leq C_\eta (1 + |x_1|)^{2N} e^{-m_z^1 \text{dist}(x,\mathcal{S}_l)}.$$

This finishes the proof of the theorem.

If we assume that $\varepsilon_0(x)$ and $\rho_0(x)$ are periodic in the x_1-direction with period a, we can remove the polynomial growth of the eigenfunction along the strip. In the periodic situation, operator A has a complete set of generalized eigenfunctions that do not grow in the direction of periodicity, namely x_1-direction in this case. Indeed, suppose u is a generalized eigenfunction of A corresponding to z which satisfies (2.10). According to Bloch-Floquet theory, $u(x)$ can be chosen as $\tilde{u}(x)e^{ikx_1}$ where $\tilde{u}(x)$ is periodic in x_1-direction with period a and $k = 2\pi/a$, then u satisfies:

$$\|u\|_{L_2(K+x)} + \|\nabla u\|_{L_2(K+x)} \leq C_K(1 + |x'|)^N \tag{2.30}$$

for any compact K and x in $\mathbb{R}^d$.

Theorem 6. *If $\varepsilon_0(x)$ and $\rho_0(x)$ are periodic with the same period in the x_1-direction then one can find a complete family of generalized eigenfunctions that satisfies (2.30), in which case*

$$\|\chi_x u\| \leq Ce^{-C(z)dist(x,\mathcal{S}_l)} \tag{2.31}$$

for some constants C, $C(z)$ and generalized eigenfunction u of A with eigenvalue z.

Proof. Due to periodicity of operator and Bloch-Floquet theory, there exists a complete set of generalized eigenfunctions that do not grow in the waveguide's axial direction. Then repeating the previous proof one comes up with the estimate (2.31).

C. Existence and Confinement of Guided Modes. Maxwell Equation

We now consider the case of the full Maxwell operator. The results in this section are contained in **[43]** . Most of the notations from previous section are employed here as well with a few differences. Throughout this section, we assume $d = 3$, i.e., $x \in \mathbb{R}^3$. The dielectric properties of the materials are still represented by $\varepsilon_0(x)$ (unperturbed) or $\varepsilon(x)$ (perturbed) with upper and lower bounds as in previous section. Periodicity of bulk PBG material is still not assumed. The defect strip $\mathcal{S}_l$ is defined in the same way as before with Ω a unit disc centered at the origin in $\mathbb{R}^2$ and $\mathcal{S}_l$ now lives in $\mathbb{R}^3$.

We use the notation

$$\nabla^\times u = \nabla \times u = \text{curl}\, u.$$

The operator M_0 is the self-adjoint realization of

$$M_0 := \nabla^\times \frac{1}{\varepsilon_0(x)} \nabla^\times \tag{2.32}$$

in $L_2(\mathbb{R}^3; \mathbb{C}^3)$ defined by means of its quadratic form

$$\int \varepsilon_0^{-1} |\nabla^\times u|^2 dx \tag{2.33}$$

with the domain $H^1(\mathbb{R}^3; \mathbb{C}^3)$.

The perturbed operator is

$$M := \nabla^\times \frac{1}{\varepsilon(x)} \nabla^\times, \tag{2.34}$$

which corresponds to the modified medium. It is defined analogously as the background operator M_0. This operator is self-adjoint in $L_2(\mathbb{R}^3; \mathbb{C}^3)$.

From the (2.4), we should be considering the spectrum of the following operator

$$\nabla^\times \frac{1}{\varepsilon(x)} \nabla^\times$$

on the space $\mathbb{S}$, where $\mathbb{S}$ is the closure in $H^1(\mathbb{R}^3; \mathbb{C}^3)$ of the linear subset $\{\mathbf{H} \in C_0^1(\mathbb{R}^3; \mathbb{C}^3) | \nabla \cdot \mathbf{H} = 0\}$. However, the spectra of these two operators differ only at $\lambda = 0$. Since any gap in the spectrum occurs above zero, it is therefore sufficient to consider the unrestricted operator M.

Our goal is still the same as in previous section, which is to show that for any gap (α, β) in the spectrum $\sigma(M_0)$ of the unperturbed medium and under appropriate conditions on the parameters l and ε of the line defect, spectrum of the perturbed medium arises in the gap. In addition, we want to show confinement of the wave to the guide (i.e., evanescence into the bulk). The non-existence of bound states has not been established yet but is generally believed to be true.

1. Formulation of the Results

Our main results are the following theorems.

Theorem 7. *Let $G = (\alpha, \beta)$ be a non-empty finite gap in the spectrum of the "background medium" operator M_0 (in particular, $\alpha > 0$). Assume that for some $\delta \in (0, \dfrac{\beta - \alpha}{2})$ and μ is the center of any interval of length 2δ the following inequality is satisfied:*

$$l^4 \delta^2 \varepsilon^2 > \nu, \tag{2.35}$$

where $\nu > 0$ is lowest eigenvalue of the bi-harmonic operator Δ^2 acting on a divergence free $\mathbb{R}^2$-valued vector fields on Ω with Dirichlet boundary conditions on $\partial\Omega$.

Then any interval of length 2δ in the gap G contains at least one point of the spectrum $\sigma(M)$ of the perturbed operator.

This theorem guarantees that when (2.35) is satisfied, eigenmodes of the perturbed medium arise in the spectral gaps of the background medium and furthermore, the corresponding spectrum forms a δ-net in the gap. Before one can fully associate these modes with the guided waves, one needs to establish their confinement to the waveguide (i.e., their evanescent nature in the bulk of the material). This is achieved in the next result.

We will once again need to use generalized eigenfunction expansions. From **[27]** , for the operator of the type we considered, there is a complete family of generalized eigenfunction of the operator M corresponding to $z \in \mathbb{R}$ (for almost all such z) with respect to the spectral measure. Each generalized eigenfunction $u \in H^1_{loc}(\mathbb{R}^3, \mathbb{C}^3)$ from this family has the properties that

$$(1+|x|)^{-N} u(x) \in L_2(\mathbb{R}^3; \mathbb{C}^3) \text{ and } (1+|x|)^{-N}\, \nabla^{\times} u(x) \in L_2(\mathbb{R}^3; \mathbb{C}^3) \tag{2.36}$$

for some $N > 0$. The eigenvalue problem $Mu = zu$ is satisfied in the distributional sense. Analogous to the previous section, we will use the polynomial bounded-ness condition in following form:

$$\|u\|_{L_2((K+x);\mathbb{C}^3)} + \|\nabla^{\times} u\|_{L_2((K+x);\mathbb{C}^3)} \leq C_K (1+|x|)^N \tag{2.37}$$

for any compact set $K \subset \mathbb{R}^3$ and $x \in \mathbb{R}^3$. We said (2.37) as *polynomial bounded-ness of order* N.

Recall that G is a spectral gap of M_0 . Let $x = (x_1, x') \in \mathbb{R}^3$ and $\chi_x(y)$ be the characteristic function of the cube $\{y||y_j - x_j| \leq 1\}$ centered at x.

Theorem 8. *Let u be a polynomially bounded generalized eigenfunction of M corresponding to $z \in G \cap \sigma(M)$, then there exist positive constants C_1 and $C(z)$ such that*

$$\|\chi_x u\| \leq C_1 \,(1+|x_1|)^N \, e^{-C(z) dist(x,\, S_l)}, \tag{2.38}$$

where N is the order of polynomial bounded-ness of u.

When the bulk medium is assumed to be periodic in the x_1-direction, the polynomial growth in (2.38) disappears:

Theorem 9. *If $\varepsilon_0(x)$ is periodic in the x_1-direction then one can find a complete family of generalized eigenfunctions that satisfies*

$$\|u\|_{L_2((K+x);\mathbb{C}^3)} + \|\nabla^\times u\|_{L_2((K+x);\mathbb{C}^3)} \le C_K(1+|x'|)^N \tag{2.39}$$

for any compact set $K \subset \mathbb{R}^3$, $x \in \mathbb{R}^3$ and generalized eigenfunction u in the said family. In this case, we have

$$\|\chi_x u\| \le Ce^{-C(z)dist(x,\mathcal{S}_l)} \tag{2.40}$$

for some constants C, $C(z)$ and generalized eigenfunction u of M with eigenvalue z.

2. Proofs of the Results

We adopt the following notations: the norm and inner product in $L_2(\mathbb{R}^n;\mathbb{C}^3)$ will be denoted by $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ respectively.

a. Proof of Theorem 7

Let $(\mu-\delta,\mu+\delta)$ be a sub-interval of the gap G. To show $\sigma(M)\cap(\mu-\delta,\mu+\delta)\neq\emptyset$ is equivalent to showing dist$(\mu,\sigma(M))<\delta$. If $\mu\in\sigma(M)$ then dist$(\mu,\sigma(M))<\delta$ trivially and we are done. If $\mu\notin\sigma(M)$ then $M_\mu := M-\mu I$ has an inverse. Due to self-adjointness of M in $L_2(\mathbb{R}^3,\mathbb{C}^3)$, we have $\|(M-\mu)^{-1}\| = \text{dist}(\mu,\sigma(M))^{-1}$. Suppose function w has unit norm, then $1 \le \|M_\mu w\|\|M_\mu^{-1}\|$, then

$$1 \le \|M_\mu w\| \text{ dist}(\mu,\sigma(M))^{-1}$$

$$\Rightarrow \text{dist}(\mu,\sigma(M)) \le \|M_\mu w\| \ .$$

So, if $\|M_\mu w\| < \delta$ then dist$(\mu,\sigma(M))<\delta$.

So the idea of the proof is to find a function $w(x)$ with $\|w\|=1$ for the operator M

such that

$$\|Mw - \mu w\|^2 < \delta^2. \tag{2.41}$$

So, let us construct such a function.

Let g be a smooth divergence free real vector field on $\mathbb{R}^2$ with compact support in Ω and has unit L^2-norm, i.e, $g(y,z) = (\phi(y,z), \zeta(y,z))$ where ϕ, $\zeta \in C_0^\infty(\Omega)$ and div $g = 0$. We define $\phi_l(x') := l^{-1}\phi(x'/l)$ and $\zeta_l(x') := l^{-1}\zeta(x'/l)$ where $(x' = (y,z))$. Let $g_l := (\phi_l, \zeta_l)$ and the following are true of g_l

i) $\|g_l\|$ =1

$$\int_{l\Omega} |g_l(x')|^2 dx' = \int_{l\Omega} |\phi_l(x')|^2 + |\zeta_l(x')|^2 dx'$$

By a change of variable $y' = x'/l$ the above becomes

$$\int_{\Omega} (|l^{-1}\phi(y')|^2 + |l^{-1}\zeta(y')|^2) l^2 dy' = \int_{\Omega} |\phi(y')|^2 + |\zeta(y')|^2 dy' = \int_{\Omega} |g(y')|^2 dy' = 1.$$

ii) div $g_l = 0$

$$\text{div } g_l = l^{-2}\left(\frac{\partial \phi}{\partial y}(x'/l) + \frac{\partial \zeta}{\partial z}(x'/l)\right) = l^{-2}\text{div } g(x'/l) = 0.$$

Let $\psi(x_1) \in C_0^\infty(\mathbb{R})$ with a unit L_2-norm and define $\psi_n(x_1) = n^{-1/2}\psi(x_1/n)$ for $n > 0$. By a change of variable $y_1 = x_1/n$, we see that

$$\int_{\mathbb{R}} |\psi_n(x_1)|^2 \ dx_1 = \int_{\mathbb{R}} n^{-1}|\psi(y_1)|^2 \ n^1 dy_1 = \int_{\mathbb{R}} |\psi(y_1)|^2 \ dy_1 = 1.$$

Introducing $k = \sqrt{\mu\varepsilon}$, the following function be will our candidate for an approximate eigenfunction

$$w_{l,n}(x) = \psi_n(x_1)e^{ikx_1}\begin{pmatrix} 0 \\ \phi_l(x') \\ \zeta_l(x') \end{pmatrix}, \tag{2.42}$$

The function $w_{l,n}$ has unit norm in L_2 over $\mathbb{R} \times l\Omega$. Indeed,

$$\int_{\mathbb{R}}\int_{l\Omega} |w_{l,n}|^2 dx' dx_1 = \int_{\mathbb{R}} |\psi_n(x_1)|^2 dx_1 \int_{l\Omega} |g_l(x')|^2 dx' = 1$$

Instead of estimating the left hand side of (2.41), we will estimate $\|\varepsilon\,(Mw - \mu w)\|^2$. Taking into account that the function w is supported inside the defect, the needed inequality (2.41) can be also rewritten as

$$\|\varepsilon\,(Mw - \mu w)\|^2 < \delta^2\varepsilon^2$$

$$\Rightarrow \|\nabla^\times\nabla^\times w - k^2 w\|^2 < \delta^2\varepsilon^2. \tag{2.43}$$

Using the identity

$$\nabla^\times\nabla^\times w = -\Delta w + \nabla(\nabla\cdot w)$$

and that g_l is divergence free, we obtain

$$\|\nabla^\times\nabla^\times w - k^2 w\|^2 = \left\|\begin{pmatrix} 0 \\ -(\psi_n'' + 2ik\psi_n')\phi_l - \psi_n\Delta\phi_l \\ -(\psi_n'' + 2ik\psi_n')\zeta_l - \psi_n\Delta\zeta_l \end{pmatrix}\right\|^2$$

understanding that all of the above norms are in $L_2(\mathbb{R}^3;\mathbb{C}^3)$.

Using the definition of the L_2-norm for vector functions and the condition that functions ϕ, ζ and ψ are real valued and also through normalization of the functions and change of variables, the above expression is equal to

$$\frac{1}{n^4}\,\|\psi''\|^2_{L_2(\mathbb{R})} + \frac{4k^2}{n^2}\,\|\psi'\|^2_{L_2(\mathbb{R})} + \frac{1}{l^4}\,\|\Delta\phi\|^2_{L_2(\Omega)} + \frac{1}{l^4}\,\|\Delta\zeta\|^2_{L_2(\Omega)}$$

$$+\frac{2}{n^2l^2}\langle\psi'',\psi\rangle_{L_2(\mathbb{R})}\left(\langle\Delta\phi,\phi\rangle_{L_2(\Omega)}+\langle\Delta\zeta,\zeta\rangle_{L_2(\Omega)}\right)$$

Since n can be chosen arbitrarily large (without changing the defect strip), the terms with the factor $1/n$ can be made arbitrarily small (uniformly with respect to k on any finite interval). Hence, one needs to control only the remaining terms by an appropriate choice of a divergence free vector field g. In other words, one is interested in

$$\frac{1}{l^4}\ \|\Delta\phi\|^2_{L_2(\Omega)}+\frac{1}{l^4}\ \|\Delta\zeta\|^2_{L_2(\Omega)}<\delta^2\varepsilon^2 \tag{2.44}$$

or

$$\|\Delta g\|^2_{L_2(\Omega;\mathbb{R}^2)}<l^4\delta^2\varepsilon^2 \tag{2.45}$$

Let

$$\nu=\inf\ \|\Delta g\|^2_{L_2(\Omega;\mathbb{R}^2)}$$

where the *infimum* is taken over real vector fields in $C_0^\infty(\Omega;\mathbb{R}^2)$ with $\|g\|_{L^2(\Omega;\mathbb{R}^2)}=1$ and $\nabla\cdot g=0$. This is then the lowest eigenvalue of bi-harmonic operator Δ^2 with Dirichlet boundary conditions in Ω on a divergence free subspace. In particular, $\nu>0$. Hence our condition boils down to

$$l^4\delta^2\varepsilon^2>\nu \tag{2.46}$$

which proves the statement of the theorem.

b. Proof of Theorem 8

Define the sesqui-linear form

$$Q[\varphi,w]:=\langle\nabla^\times\varphi,\frac{1}{\varepsilon_0}\nabla^\times w\rangle-z\langle\varphi,w\rangle$$

with the domain $H^1(\mathbb{R}^3;\mathbb{C}^3)$.

Let $R(z)=(M_0-z)^{-1}$ and $\varphi:=R(z)\chi_x u$. Here, we use that z is not in the spectrum of M_0. Note that $\varphi \in D(M_0)$.

Let $p = \max(2\text{dist}(x, S_l), 1)$ and $\xi_x(y)$ be a nonnegative smooth cutoff function that depends on y_1 only, is supported in $(x_1 - (p+1), x_1 + (p+1))$ and such that it is equal to 1 on $[x_1 - p, x_1 + p]$. We assume further that $\xi_x(y) \leq 1$ and $|\nabla \xi_x(y)| = |\xi_x'(y_1)| \leq C$ for some constant C and all $x, y \in \mathbb{R}^3$. For simplicity of notation, we drop the subscript x in $\xi = \xi_x$. Note that $\xi u \in H^1(\mathbb{R}^3; \mathbb{C}^3)$. Using $w = \xi u$, one gets

$$Q[\varphi, \xi u] = \langle M_0 \varphi, \xi u \rangle - \langle z\varphi, \xi u \rangle = \langle \chi_x u, \xi u \rangle = \|\chi_x u\|^2 .$$

This means that our goal should be to estimate $Q[\varphi, \xi u]$ from above. On the other hand, using the equality $Mu = zu$ and easily justifiable integration by parts, one gets

$$Q[\varphi, \xi u] = \langle \nabla^\times \varphi, \frac{1}{\varepsilon_0} \nabla^\times (\xi u) \rangle - \langle \varphi, \xi z u \rangle$$

$$= \langle \nabla^\times \varphi, \tilde{\epsilon} \nabla^\times (\xi u) \rangle + \langle \nabla^\times \varphi, \frac{1}{\varepsilon} \nabla^\times (\xi u) \rangle - \langle \varphi, \xi M u \rangle$$

$$= \langle \nabla^\times \varphi, \tilde{\epsilon} \nabla^\times (\xi u) \rangle + \langle \nabla^\times \varphi, \frac{1}{\varepsilon} \nabla^\times (\xi u) \rangle - \langle \nabla^\times (\xi \varphi), \frac{1}{\varepsilon} \nabla^\times u \rangle$$

where

$$\tilde{\epsilon}(x) = \frac{1}{\varepsilon_0(x)} - \frac{1}{\varepsilon(x)}.$$

Notice that this function is supported inside the strip $\mathcal{S}_l$. Using the identity $\nabla^\times (\xi u) = \xi \nabla^\times u + \nabla \xi \times u$, the first two terms above can be combined to obtain

$$\langle \nabla^\times \varphi, \tilde{\epsilon}(\xi \nabla^\times u + \nabla \xi \times u) \rangle + \langle \nabla^\times \varphi, \frac{1}{\varepsilon}(\xi \nabla^\times u + \nabla \xi \times u) \rangle$$

$$= \langle \nabla^\times \varphi, \xi \tilde{\epsilon} \nabla^\times u \rangle + \langle \nabla^\times \varphi, (\tilde{\epsilon} + \frac{1}{\varepsilon}) \nabla \xi \times u \rangle + \langle \nabla^\times \varphi, \frac{1}{\varepsilon} \xi \nabla^\times u \rangle$$

The term $-\langle \nabla^\times (\xi \varphi), \frac{1}{\varepsilon} \nabla^\times u \rangle$ can be expanded to

$$-\langle \xi \nabla^\times \varphi, \frac{1}{\varepsilon} \nabla^\times u \rangle - \langle \nabla \xi \times \varphi, \frac{1}{\varepsilon} \nabla^\times u \rangle$$

Combining the last two expressions, we get

$$\langle \nabla^\times \varphi, \xi\tilde{\epsilon}\nabla^\times u\rangle + \langle \nabla^\times \varphi, \frac{1}{\varepsilon_0}\nabla\xi \times u\rangle - \langle \nabla\xi \times \varphi, \frac{1}{\varepsilon}\nabla^\times u\rangle \tag{2.47}$$

Our last task in proving the theorem is to estimate from above the terms in (2.47). In order to do so, we need an auxiliary statement concerning the exponential decay of the resolvent, which is a result of **[10]** :

Lemma 10. **[10]** *There exist a positive number m_z that depends only on the distance of the point z from the gap edges, such that for a positive constant C the following estimates hold for the local $L_2(\mathbb{R}^3;\mathbb{C}^3)$-norm of the resolvent $R(z)$:*

$$\begin{aligned} \|\chi_u R(z)\chi_v\| &\le Ce^{-m_z|u-v|} \\ \|\chi_u \nabla^\times R(z)\chi_v\| &\le Ce^{-m_z|u-v|} \end{aligned} \tag{2.48}$$

for any $u, v \in \mathbb{R}^3$. Here the norms in the left hand side are the operator norms in $L_2(\mathbb{R}^3;\mathbb{C}^3)$.

We can now get the needed estimates. Let $V = [x_1 - p - 1, x_1 + p + 1] \times l\Omega$. This is a compact domain that can be covered by the union of p fixed size domains $V_j = [a_j, a_j + 2] \times l\Omega$ and which contains the supports of $(\xi\tilde{\epsilon})$. Also note that $\text{dist}(x, V_j) \ge \text{dist}(x, S_l)$. Now using the lemma above and (2.37) we get

$$\begin{aligned} |\langle \nabla^\times \varphi, \xi\tilde{\epsilon}\nabla^\times u\rangle| &\le \|\chi_V \nabla^\times \varphi\| \, \|\xi\tilde{\epsilon}\nabla^\times u\| \le C \, \|\sum_j \chi_{V_j}\nabla^\times R(z)\chi_x u\| \|\sum_j \chi_{V_j}\nabla^\times u\| \\ &\le Cp^2(|x_1| + p + 1)^{2N} e^{-m_z \text{dist}(x,\mathcal{S}_l)} \le C(|x_1| + 1)^{2N} e^{-(m_z - \eta)\text{dist}(x,\mathcal{S}_l)} \end{aligned} \tag{2.49}$$

We used here that $p = \max(2\text{dist}(x, \mathcal{S}_l), 1)$. We also denoted by C different constants.

Let us move now to estimating the last term in (2.47). Denote by $a > 0$ a number such that shifts of $l\Omega$ by vectors aj with $j \in \mathbb{Z}^2$ cover the whole space $\mathbb{R}^2$. We denote

$$W_j := ([x_1 - p - 1, x_1 - p] \cup [x_1 + p, x_1 + p + 1]) \times (l\Omega + aj) \, .$$

Then $W_j = W_0 + (0, aj)$. Notice that $W = \cup_j W_j$ covers $\operatorname{supp} \nabla\xi$ and $\text{dist}(x, W_j) \geq C_1(p + |j|) - C_2$.

We are now ready to estimate the last term of (2.47) from above. We proceed as before, using the lemma, the polynomial growth of u, and uniform boundedness of $\nabla\xi$.

$$
\begin{aligned}
|\langle \nabla^\times \varphi, \frac{1}{\varepsilon_0} \nabla\xi^\times u\rangle| &\leq C \sum_j \|\chi_{W_j} u\| \|\chi_{W_j} \nabla^\times R(z) \chi_x u\| \\
&\leq C \sum_j (|x_1| + p + |j| + 1)^{2N} e^{-m_z \text{dist}(x, W_j)} \\
&\leq C(|x_1| + p + 1)^{2N} e^{-m_z^1 \text{dist}(x, \mathcal{S}_l)} \sum_j (1 + |j|)^{2N} e^{-m_z C_1 |j|} \\
&\leq C(|x_1| + 1)^{2N} e^{-(m_z^1 - \eta) \text{dist}(x, \mathcal{S}_l)}
\end{aligned}
\tag{2.50}
$$

where m_z^1 is a positive constant.

The expression $|\langle \nabla\xi^\times \varphi, \frac{1}{\varepsilon} \nabla^\times u\rangle|$ is estimated analogously. Combining the above estimates, we get

$$
\|\chi_x u\|^2 \leq C \ \|\chi_x u\|^2_{\rho_0} = Q[\varphi, \xi u] \leq C_\eta (1 + |x_1|)^{2N} e^{-m_{z,\eta} \text{dist}(x, \mathcal{S}_l)}.
$$

where $m_{z,\eta}$ is a positive constant. This finishes the proof of the theorem.

c. Proof of Theorem 9

In this periodic situation, operator M has a complete family of generalized eigenfunctions that do not grow in the direction of periodicity, namely x_1-direction in this case. Indeed, suppose u is a generalized eigenfunction of M corresponding to z which satisfies (2.36). According to Bloch-Floquet theory, $u(x)$ can be chosen as $\tilde{u}(x) e^{ikx_1}$ where $\tilde{u}(x)$ is periodic in x_1-direction with period a and $k = 2\pi/a$, then u satisfies (2.39). Then repeating the previous proof, one comes up with the estimate (2.40).

Remark 11. *Just like in the scalar case, one needs to show that the discovered modes do not correspond to bound states. This problem is still open.*

CHAPTER III

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 is no 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 the coordinate 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 $-\dfrac{d^2}{dx_e^2}$ along the edges on functions that are continuous and such that at each vertex v the sum of the derivatives along the edges emanating from v is zero. This vertex condition is commonly

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known as Kirchhoff, Neumann, or zero flux condition.

Quantum graphs naturally arise as simplified models in mathematics, physics, chemistry, and engineering. There are systems that have some dimensions too small to be studied 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:

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

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 $k > 1$.

2. Operators on Graphs

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

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

or more general Schrödinger type operator

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

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 will only 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 operator with 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 $(f_1(v), \dots, f_d(v))^t$ of the vertex values of the function along each edge adjacent to v (so there are d_v edges) and $F' = (f_1'(v), \dots, f_d'(v))^t$ 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

$$A_v F + B_v F' = 0 \tag{3.3}$$

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]** .

Theorem 12. *Let Γ be a metric graph with finitely many edges. Consider the operator H acting as $-\dfrac{d^2}{dx_e^2}$ on each edge e, with the domain consisting of functions that belong to $H^2(e)$ on each edge e and satisfy the boundary conditions (3.3) at each vertex. Here $\{A_v, B_v | v \in V\}$ is a collection of matrices of sizes $d_v \times d_v$ such that each matrix $[A_v|B_v]$*

has the maximal rank. In order for H to be self-adjoint, the following condition at each vertex is necessary and sufficient:

$$\textit{for any vertex } v\textit{, the matrix } A_v B_v^* \textit{ is self adjoint.} \tag{3.4}$$

For the remainder of this chapter, we always assume that A_v and B_v in (3.3) satisfy (3.4).

Let P_v and $P_{1,v}$ be the orthogonal projections in $\mathbb{C}^d$ onto the kernels kerB_v and kerB_v^* respectively. The complementary orthogonal projectors onto the ranges $R := R(B_v^*)$ and $R_1 := R(B_v)$ are denoted as Q_v and $Q_{1,v}$ respectively.

Suppose $[A_v|B_v]$ is of maximal rank and $A_v B_v^*$ is self-adjoint, then $Q_1 B_v Q : R \to R_1$ is invertible and its inverse is denoted by $B_v^{(-1)}$. Also $L_v := B_v^{(-1)} A_v$ is self adjoint in $Q\mathbb{C}^{d_v}$. Then the condition (3.3) is equivalent to

$$\begin{aligned} &P_v F(v) = 0 \\ &Q_v F'(v) + L_v Q_v F(v) = 0 \end{aligned} \tag{3.5}$$

The proof of conditions (3.5) can be found in **[37]** . They are more convenient for quadratic forms and also in proving self-adjointnes of the operator.

In the case of an infinite graph, we also make an additional assumption:

Assumption 2: The following estimate holds uniformly for all vertices v:

$$\|L_v\|_{\mathbb{C}^{d_v}} \leq S < \infty,$$

or equivalently $\|B_v^{(-1)} A_v Q_v\|_{\mathbb{C}^{d_v}} \leq S < \infty$.

We now define the operator H more precisely:

Definiton 2. *The unbounded operator H in $L^2(\Gamma)$ which acts as the negative second derivative along the edges, is defined on domain $\mathcal{D}(H)$ consisting of functions f such that*

1. *$f \in H^2(e)$ for each edge e,*

2. $\sum_e \|f\|^2_{H^2(e)} < \infty$

3. *for each vertex v, conditions (3.5) are satisfied.*

We describe the corresponding quadratic form

Definiton 3. *The quadratic form h is defined as*

$$h[f,f] := \sum_{e \in E} \int_e \left| \frac{df}{dx} \right|^2 dx - \sum_{v \in V} \langle L_v F, F \rangle \tag{3.6}$$

where $\langle , \rangle$ denotes the standard inner product in $\mathbb{C}^{d_v}$.

The domain of this form consists of all functions f that belongs to $H^1(e)$ for each edge e and satisfy at each vertex the condition $P_v F = 0$, and such that

$$\sum_e \|f\|^2_{H^1(e)} < \infty \tag{3.7}$$

Remark 13. *The first sum in the definition of h is finite due to Cauchy-Schwartz inequality and (3.7). Assumption 1, (3.7) and Sobolev trace theorem show that the trace $F(v)$ is bounded uniformly for all v. Furthermore,*

$$\sum_v \|F(v)\|^2 \leq C \sum_e \|f\|^2_{H^1(e)} < \infty.$$

Using this inequality and assumption 2, we conclude that the second sum in (3.6) is finite, i.e.,

$$\sum_{v \in V} \langle L_v F, F \rangle \leq \sum_{v \in V} \|L_v\| \|F(v)\|^2 < \infty$$

Thus the quadratic form h (3.6) is well defined.

Theorem 14. *Let Γ be a quantum graph. Under the definitions given above for the quadratic form h and operator H, the following statements hold.*

1. *The operator H is self-adjoint and its quadratic form is h.*

2. *Let H_0 be the restriction of H onto the sub-domain consisting of all functions from $\mathcal{D}(H)$ with compact support. Then H_0 is symmetric, essentially self-adjoint, and its closure is H.*

Proof of the Theorem 14 can be found in **[37]** . As it was noticed in **[57]** , when the assumptions 1 and 2 do not hold, the operatorH_0 might not be essentially self-adjoint and thus some "conditions at infinity" are needed.

3. Examples of Vertex Conditions

One of the most common vertex condition is the Neumann (Kirchhoff) vertex condition. It is defined as follows

$$f(x) \text{ is continuous on } \Gamma \text{ and at each vertex } \sum_{v \in e} \frac{df}{dx_e}(v) = 0 \tag{3.8}$$

We can express the above in the form of (3.3) as

$$A_v = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 \\ 0 & 1 & -1 & \cdots & 0 \\ \cdots & \cdots & 0 & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

and

$$B_v = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 1 & \cdots & 1 \end{bmatrix}.$$

The augmented matrix $[A_v|B_v]$ has full rank and $A_v B_v^* = 0$, so (3.4) is satisfied. One can also find the orthogonal projection P_v onto the kernel of B_v and $L_v = B_v^{(-1)} A_v Q_v$ to cast the vertex condition in the form (3.5).

A generalization of the above vertex condition can be defined as above

$$f(x) \text{ is continuous on } \Gamma \text{ and at each vertex } \sum_{v \in e} \frac{df}{dx_e}(v) = \alpha_v f(v) \tag{3.9}$$

for some fixed numbers α_v's. We can express the above in the form of (3.3) as well. Matrix B_v in this case is still same as the above and

$$A_v = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 \\ 0 & 1 & -1 & \cdots & 0 \\ \cdots & \cdots & 0 & 1 & -1 \\ -\alpha_v & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

The rank of the augmented matrix $[A_v|B_v]$ is d_v. Since

$$A_v B_v^* = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & -\alpha_v \end{bmatrix},$$

the above is self-adjoint if and only if α_v is real.

Another vertex condition is *vertex Neumann condition* where the derivative along each edge at each vertex v is required to be zero, i.e. $f_e'(v) = 0$. There are no restrictions placed on the function value. In this case one obtains a Neumann boundary value problem on each edge. The *vertex Dirichlet condition* is when the function value at each vertex is zero and no restriction is placed on the derivatives of the function. For this vertex condition, the operator also decouples but into a Dirichlet boundary value problem on each edge.

B. On the Limiting Absorption Principle and Spectra of Quantum Graphs

Consider a finite graph Γ_0, whose edges are equipped with coordinates (called x, or x_e, if we need to specify the edge e) that identify them with segments of the real axis. A finite set B of vertices of cardinality $|B| = n$, which we will call the *boundary of* Γ_0 is assumed to be fixed. Each vertex $v \in B$ has an infinite edge (*lead*) e_v attached, which is equipped with a coordinate that identifies it with the positive semi-axis. Thus an infinite graph Γ is formed (see Fig. 5).

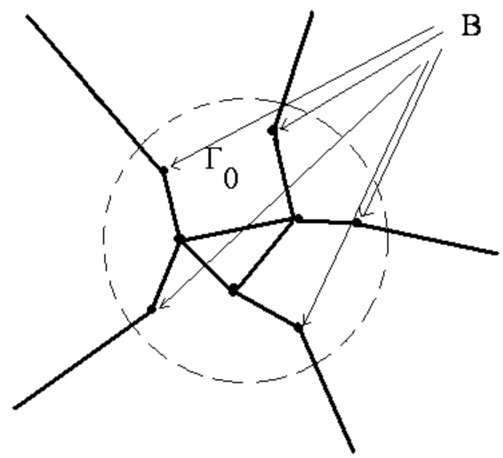

Fig. 5. Graph Γ.

This graph is turned into a quantum graph by equipping it with a self-adjoint differential operator H defined in (2).

We will assume that all "boundary" vertices $v \in B$ have degree two and that the boundary conditions at any such v are "Neumann":

$$\begin{array}{ll} i) & f \text{ is continuous at each vertex } v \in B \\ ii) & \text{at each vertex } v \in B, \ \sum\limits_{v \in e} \dfrac{df}{dx_e}(v) = 0. \end{array} \quad (3.10)$$

Here $\sum_{v\in e} \frac{df}{dx_e}(v)$ is the sum of the derivatives of f in the outgoing directions along all edges emanating from v. In fact, these conditions simply mean that the function and its derivative are both continuous at $v \in B$.

This assumption on the degrees of boundary vertices and on how the conditions look like at the boundary B, in fact does not reduce the generality. Indeed, one can always introduce "fake" boundary vertices a little bit further away along the infinite edges and consider them as the new boundary. Then our assumptions are automatically satisfied, and the operator does not change at all.

It is well known (e.g., **[28, 37]** and references therein), that the operator H is self-adjoint, bounded below, and in the case of a finite graph (which Γ is not, but Γ_0 is) has compact resolvent and thus discrete spectrum. The structure of the spectrum of the operator H on graphs Γ of the type described above has been studied for quite a while (e.g., **[8, 20, 28, 29, 30, 31, 32, 33, 39, 47, 48, 52, 51]**). It is a common knowledge that it possesses continuous part filling the nonnegative half-axis, as well as possibly point spectrum consisting of isolated eigenvalues accumulating at infinity. For completeness, we provide a proof of the following standard statement here (a variation of this proof would use Krein's resolvent formula) that claims that the continuous part of the spectrum does not depend on a finite part of the graph.

Lemma 15. *In the presence of infinite leads (i.e., if $n > 0$), the continuous spectrum of H coincides with the nonnegative half-axis. Eigenvalues of finite multiplicity (including those embedded into the continuous spectrum) accumulating at infinity might be present.*

The proof of the lemma uses Glazman's splitting technique **[21]** . Let us choose coordinates on each of the infinite leads e_v, $v \in B$ that identify the leads with the nonnegative half axis. We identify the point v with the coordinate $x = 0$. So we have $\Gamma = \Gamma_0 \cup \Gamma_1$ where Γ_1 is the disjoint union of n copies of half-axes $[0, \infty)$. Consider the symmetric operator Q that is the restriction of H on the set of those functions $f \in D(H)$ that vanish with their first derivative at all points v. Then Q naturally splits into the orthogonal sum of two minimal operators $Q_0 \bigoplus Q_1$ defined on Γ_0 and Γ_1 respectively. Since Q_0 acts on a finite graph Γ_0 and Q_1 is just the direct sum of n copies of minimal operators corresponding to $-\dfrac{d^2}{dx^2}$ on the half-axis, we conclude that the continuous spectrum of the closure of Q is the same as that of Q_1. Noticing that H is a finite dimensional extension of Q, one can employ Theorems 4 and 11 of Chapter I from **[21]** to imply the statements of the lemma.

The goal of this section is to prove a limiting absorption principle.

Theorem 16. *Let $R(\lambda)$ be the resolvent of H and f be any function from the domain of H that is compactly supported and smooth on each edge. Then the function $(R(\lambda)f, f)$ can be analytically continued from the upper half-plane through $\mathbb{R}^+$, except for a discrete subset of $\mathbb{R}^+$.*

Corollary 1. *The singular continuous spectrum of H is empty and the absolutely continuous spectrum coincides with the nonnegative half axis.*

The results in this section is contained in **[49]** .

1. Dirichlet-to-Neumann Map and Other Auxiliary Considerations

Let us consider the finite part Γ_0 of our graph Γ and treat the vertex set B as its "boundary." We need to define some auxiliary objects related to Γ_0.

First of all, we will consider the operator H_0 on $L_2(\Gamma_0)$ that acts as the negative second derivative along each edge, and whose domain $D(H_0)$ consists of those functions from the Sobolev space $H^2(e)$ on each edge e of Γ_0 that satisfy Neumann conditions on B and satisfy conditions (3.3) at all vertices of Γ_0 except those in B. It is standard **[37]** that this operator is self-adjoint, bounded below, and has compact resolvent, and thus discrete spectrum $\sigma(H_0) = \{\lambda_1, ..., \lambda_n, ...\}$ accumulating to infinity. We will denote by $R_0(\lambda)$ the resolvent of this operator.

One can also define a linear extension operator E acting from functions defined on the (finite) set B into the domain of H_0

$$E : \mathbb{C}^n \mapsto D(H_0),$$

such that $(Ef)(v) = f(v)$ for all $v \in B$ and the derivative of Ef at each $v \in B$ along any edge of Γ_0 entering v is equal to zero[1]. Such an operator is indeed easy to construct. For instance, for any $v \in B$ one may define a function g_v which is equal to 1 in a neighborhood of v, is smooth on each edge entering v, and is supported inside the ball of radius $l_0/2$ centered at v, where l_0 is the smallest length of an edge of Γ_0. Then one can define $Ef(x) = \sum\limits_{v \in B} f(v)g_v(x)$.

Another operator N that we need is an analog of the "normal derivative at the boundary B of Γ_0." It acts as follows: for any function f on Γ_0 that belongs to $H^2(e)$ on any edge e, one can define the value $Nf(v)$ for $v \in B$ as the derivative of f at v (taken in the direction towards v):

$$Nf(v) = \frac{df}{dx_e}(v),$$

where x_e is the coordinate along e that increases towards v We remind the reader that each vertex in B has only degree two and only one of the edges connected to each vertex in B belongs to Γ_0. Hence there is no ambiguity in defining N as above.

The main technical tool that we will use is the so called Dirichlet-to-Neumann operator, very popular in inverse problems **[51, 60, 61]** , spectral theory **[13, 17]** , and recently in quantum graph theory **[6, 13, 38]** as well. It is a linear operator $\Lambda(\lambda)$ (in our case finite-dimensional) acting on functions defined on B, i.e. $\Lambda(\lambda) : \mathbb{C}^n \mapsto \mathbb{C}^n$. It is defined

[1] We remind the reader that $n = |B|$.

as follows. Given a function ϕ on B, one solves the following problem on Γ_0:

$$\begin{cases} -\dfrac{d^2u}{dx^2} - \lambda u = 0 \text{ on } \Gamma_0 \\ \text{conditions (3.3) are satisfied at all vertices of } \Gamma_0 \text{ except those in } B \\ u|_B = \phi \end{cases} \tag{3.11}$$

One now defines the *Dirichlet-to-Neumann map* as follows:

$$\Lambda(\lambda)\phi = Nu, \tag{3.12}$$

which justifies the name of the operator. The validity of this definition depends upon (unique) solvability of the problem (3.11), which holds unless $\lambda \in \sigma(H_0)$.

Lemma 17. *1. The following operator relation holds:*

$$\Lambda(\lambda) = NR_0(\lambda)(\frac{d^2}{dx^2} + \lambda)E \tag{3.13}$$

2. *The Dirichlet-to-Neumann map $\Lambda(\lambda)$ is a meromorphic matrix valued function of λ with poles on the spectrum of H_0.*

3. *For real values $\lambda \in \mathbb{R} - \sigma(H_0)$ the matrix $\Lambda(\lambda)$ is Hermitian.*

Proof of the Lemma. Let us introduce a new function $g = u - E\phi$ on Γ_0. By the construction of the extension operator E, g clearly satisfies the same vertex conditions (3.3) on $\Gamma_0 - B$, as well as the zero Dirichlet conditions on the boundary $g|_B = 0$. We also note that $Ng = Nu$, since $NE\phi = 0$ for any ϕ. This means that (3.11) can be equivalently rewritten as

$$\begin{cases} -\dfrac{d^2g}{dx^2} - \lambda g = \left(\dfrac{d^2}{dx^2} + \lambda\right) E\phi \in L^2(\Gamma_0) \text{ on } \Gamma_0 \\ \text{conditions (3.3) are satisfied at all vertices of } \Gamma_0 \text{ except those in } B \\ g|_B = 0 \end{cases} .$$

In other words, $(H_0 - \lambda)g = \left(\frac{d^2}{dx^2} + \lambda\right) E\phi$, which together with the definition of the Dirichlet-to-Neumann map proves the first statement of the Lemma.

The second statement of the lemma immediately follows from the first one together with the discreteness of the spectrum of H_0 and standard analyticity properties of the resolvent.

The third statement is well known (e.g., **[13]**) and can be checked by straightforward calculation. □

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 continuous spectrum on the positive half-axis only. Then the statement about absolute continuous spectrum would follow as well by the same Lemma.

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

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

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

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 attached to the rays at the vertices of B (see Fig. 6). Any function u on Γ can now be viewed as the

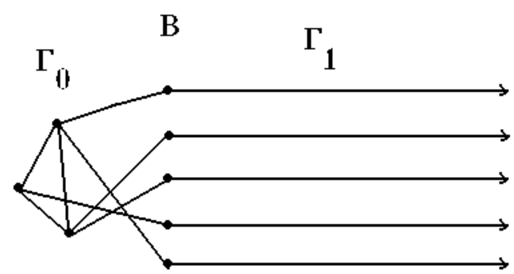

Fig. 6. A Different Visualization of Γ.

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 the inner product $(u, f) = (u_0, f_0) + (u_1, f_1)$. Let us write (3.15) and the vertex conditions separately for u_0 on Γ_0 and u_1 on Γ_1. On the finite graph Γ_0 we get

$$\begin{cases} (-\frac{d^2}{dx^2} - \lambda)u_0 = f_0 \\ \text{(3.3) satisfied on vertices of } \Gamma_0 \text{ except those in } B \\ u_0|_B = u_1(0) \end{cases} \tag{3.16}$$

Similarly, on Γ_1 we have

$$\begin{cases} (-\frac{d^2}{dx^2} - \lambda)u_1 = f_1 \text{ on } \mathbb{R}^+ \\ u_1'(0) = Nu_0 \end{cases} \tag{3.17}$$

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

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

and thus

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

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

[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

$$\begin{cases} (-\frac{d^2}{dx^2} - \lambda)u_1 = f_1 \text{ on } \mathbb{R}^+ \\ u_1'(0) = \Lambda(\lambda)u_1(0) + g(\lambda). \end{cases} \tag{3.20}$$

By the construction, $\Lambda(\lambda)$ is a meromorphic matrix function in $\mathbb{C}$ with self-adjoint values 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 must belong 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 Neumann 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).

It is not hard to solve (3.17) now. Indeed, after a simple computation one arrives to the formula for the solution that one can check directly when 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:

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

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 same Riemann 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 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.

C. Resonant Gap Opening in Quantum Graphs

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.

In this section we present a method of opening gaps in the spectrum of a finite quantum graph by inserting a finite graph (scatterer) to each vertex of the original graph. The gaps are opened around the eigenvalues of the attached graphs. This is so called resonant gap opening (vs. the Bragg scattering gaps in photonic crystals). The results in this section are contained in **[45]** .

The resonant method of opening gaps has been studied before **[2, 50, 55]** . In the case of combinatorial graphs, J. Schenker and M. Aizenman showed in **[55]** that a simple method of "decorating" a graph leads to a very controllable gap structure. In **[38]** , it was shown that similar procedure also works for quantum graphs. This "decoration" procedure uses graphs that attach "sideways" to the original graph (Fig. 7).

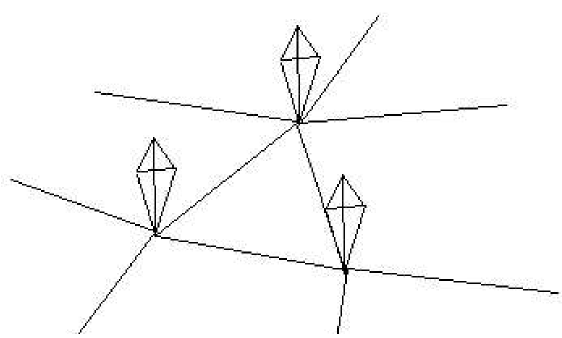

Fig. 7. Decorations Used by Schenker and Aizenman

However, it is often more convenient to incorporate an internal structure into each vertex of the original graph rather than attaching it (Fig. 8). This is the case, for instance, in thin photonic crystals structures. We will describe this internal structures as “spiders” inside vertices of the original graph. We will show that spectral gaps can sometimes be opened using “spider” decorations.

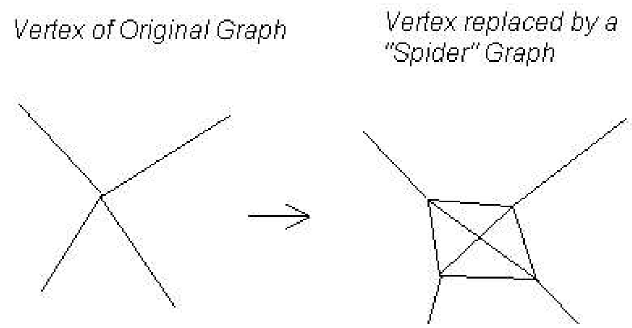

Fig. 8. “Spider” Decoration

Let Γ_0 be a finite regular metric graph. Regularity means that the degree $n > 0$ of each vertex v is the same.

A *path* is a non-empty graph $P = (V, E)$ of the form

$$V(P) = \{v_0, v_1, \dots, v_l\}, \quad E(P) = \{v_0v_1, v_1v_2, \dots, v_{l-1}v_l\}$$

where vertices v_i are all distinct. Hence a path does not contain loops. A path is usually denoted by listing its consecutive vertices as $v_0v_1 \dots v_l$. The length of a path is the number of its edges, i.e. $|E(P)|$. One can also say P is a path from v_0 to v_l or $v_0 - v_l$ path. Of course, a $v_0 - v_l$ path is also a $v_l - v_0$ path. If $P = v_0 \dots v_l$ is a path with $l \geq 2$, then the graph $C := P + v_lv_0$ is a called a *cycle*. Analogous to paths, we describe C by its sequence of vertices. The above cycle could be written as $v_0 \dots v_lv_0$. The length of a cycle is the number of its edges.

We define the *Dirichlet spectrum* $\sigma_D(\Gamma_0)$ *of* Γ_0 as the union over all edges e of spectra of the operators $-\dfrac{d^2}{dx^2}$ on $[0, l_e]$ with zero Dirichlet conditions at the endpoints 0 and l_e. In other words,

$$\sigma_D(\Gamma_0) = \{\left(\frac{n\pi}{l_e}\right)^2 \mid e \in E(\Gamma_0), n \in \mathbb{N}\}.$$

An odd (even) Dirichlet eigenvalue is a Dirichlet eigenvalue $(n\pi l_e^{-1})^2$ with an odd (even) n.

We will describe now the procedure of inserting a "spider" into each vertex of Γ_0. Let G be a finite graph (spider) with $|V(G)| \geq n$. We assume that a subset $B \subset V(G)$ is selected such that $|B| = n$, say $B = \{v_1, \ldots, v_n\}$. We replace each vertex v in Γ_0 with G and then connect each of the edges in Γ_0 incident to v to one of the vertices in B, see fig. 9 below. This must be done in one-to-one fashion, which is possible since $|B| = n = deg(v)$. Any vertices of G that are not in B will be called *internal*, and

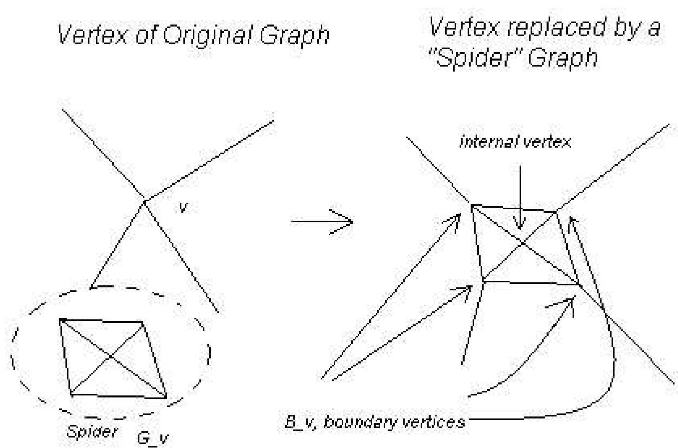

Fig. 9. Replacing Vertex with "Spider" Decoration

correspondingly B will be considered as the *boundary of* G.

This new "decorated" graph will be denoted by Γ. Its set of vertices can be naturally identified with $V(G)\times V(\Gamma_0)$. Its set of edges is correspondingly $E(\Gamma_0)\cup(E(G) \times V(\Gamma_0))$. We will also use the notation B_v for $B \times \{v\} \subset V(\Gamma)$, i.e. for the boundary of the spider embedded into the vertex v.

We also equip this graph Γ with the operator $\mathcal{H}$ which acts as $-\dfrac{d^2}{dx^2}$ along its edges and whose domain consists of functions f on Γ such that:

1. $f \in H^2(e)$ on each edge e in Γ,
2. f is continuous and satisfies the Neumann condition (3.10) at each vertex in $B \times V(\Gamma_0)$,
3. at vertices of Γ that are not in $B \times V(\Gamma_0)$ (i.e., the internal vertices of all spiders), f satisfies self-adjoint vertex conditions (3.3):

$$\mathbf{A}_v \mathbf{F}(v) + \mathbf{B}_v \mathbf{F}'(v) = 0 \quad , v \in \cup_{v\in\Gamma_0}(V(G) \setminus B_v). \tag{3.25}$$

   where $\mathbf{F}(v)$ 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 $\mathbf{F}'(v) = (f_1'(v), \ldots, f_d'(v))^t$ is the vector of the derivatives at v taken along the edges in the outgoing directions from v. The matrices $\mathbf{A}_v$ and $\mathbf{B}_v$ are of size $n \times n$ and satisfy the conditions in Theorem 12 from section A of chapter III.

The spectrum of this operator will be denoted $\sigma(\mathcal{H})$.

1. Auxiliary Dirichlet-to-Neumann Operators

Let H be the operator in $L_2(G)$ that acts as $-\dfrac{d^2}{dx^2}$ on edges with zero Dirichlet conditions imposed on B and conditions (3.25) at the internal vertices of G. We denote by $\sigma(H)$ its spectrum. It is clear, for instance, that when $B = V(G)$ (i.e., when there are no internal vertices in G), $\sigma(H) = \sigma_D(H)$, and thus the spectrum depends on the edges lengths only.

Let now ϕ be a function defined on vertices of B. Consider the following problem on

G:

$$\begin{cases} -u'' = \lambda u \text{ for each edge } \ e \in G \\ \text{conditions } (3.25) \text{ are satisfied on } V(G) \setminus B \\ u|_B = \phi \end{cases} \tag{3.26}$$

If $\lambda \notin \sigma(H)$, then (3.26) can be solved uniquely. For such λ, exactly like it is done in Section B of this chapter, we can introduce the Dirichlet-to-Neumann operator $\Lambda(\lambda)$. It acts as follows: for a given $\phi \in L_2(B) = \mathbb{C}^n$, one finds the solution u of (3.26) and then computes the function Nu on B, where N, as before, denotes the sum of outgoing derivatives of u along edges at each vertex in B. Then one defines $\Lambda(\lambda)\phi := Nu$. Properties of this matrix-function of λ have already been discussed in the Section B of this chapter, see in particular Lemma 17 and considerations before it.

As it was described in Lemma 17, $\Lambda(\lambda)$ is a meromorphic matrix function with poles only in $\sigma(H)$. We are interested now in the situation of a pole λ_0 such that the norm of the inverse matrix to $\Lambda(\lambda)$ tends to zero when $\lambda \to \lambda_0$. To put it differently, we need that $\|\Lambda(\lambda)\phi\| \geq C(\lambda)\|\phi\|$ when $\lambda \to \lambda_0$, with $C(\lambda) \to \infty$. Let us discuss how and when this can happen.

Let us return to the problem (3.26) for some non-zero vector ϕ, considered for a pole $\lambda = \lambda_0$ of $\Lambda(\lambda)$. In this case, since $\lambda_0 \in \sigma(H)$, the problem does not have to have a solution. The first result we have shows that if it does have a solution, then $\Lambda(\lambda)\phi$ has no singularity at λ_0.

Theorem 20. *Let $\lambda_0 \in \sigma(H)$ and $\phi \in S$, where S is the unit sphere in $\mathbb{C}^n$.*

1. *If (3.26) for $\lambda = \lambda_0$ has a solution, then $\| \Lambda(\lambda)\phi \| < C < \infty$ when $\lambda \to \lambda_0$.*
2. *If (3.26) for $\lambda = \lambda_0$ has no solution for any $\phi \in S$, then $\lim\limits_{\lambda \to \lambda_0} \| \Lambda(\lambda)\phi \| = \infty$ for all*

$\phi \in S$. Moreover, the following estimate holds for λ sufficiently close to λ_0:

$$\| \Lambda(\lambda)\phi \| \geq \frac{C_1}{|\lambda - \lambda_0|} \| \phi \|, \tag{3.27}$$

where the positive constant C_1 is independent of ϕ.

The proof is presented in the sub-section 3 below.

2. Spectral Gap Opening. Main Results.

We are now ready to state and prove the main result of this section.

Theorem 21. *Let $\lambda_0 \notin \sigma_D(\Gamma_0)$ be a pole of $\Lambda(\lambda)$ such that the case 2 of Theorem 20 holds. Let also δ be the distance from λ_0 to the set $\sigma_D(\Gamma_0)$. Then there exists $\varepsilon > 0$, depending on the G, B, and δ only, such that there is no spectrum of the operator $\mathcal{H}$ on Γ inside the punctured ε-neighborhood of λ_0:*

$$\{|\lambda - \lambda_0| < \varepsilon, \lambda \neq \lambda_0\}.$$

So far, we have only stated results involving $\Lambda(\lambda)$, one would like to know directly some sufficient conditions on the graph G itself that would lead to (3.26) for $\lambda = \lambda_0$ having no solution for any $\phi \in S$.

Unfortunately we do not have sufficient conditions on any finite graph G yet but we do have a result for graph G without any internal vertices, i.e. $V(G) = B$. Hence $\sigma(H)$ on such graph is the Dirichlet spectrum of G. We assume that $\lambda_0 = \left(\frac{n_0\pi}{l_0}\right)^2 \in \sigma(H) \setminus \sigma_D(\Gamma_0)$ and for some $n_0 \in \mathbb{N}$.

A l_0-*path* refers to a path made up of edges with edge length l_0. A l_0-*cycle* in G is a cycle which every edge in it has length l_0. Now we are ready to introduce this condition on G,

(G1) There exists an odd l_0-cycle in G and all vertices in this cycle belong to B. (there can be elements of B not in the cycle). For every vertex in B, there is a l_0-path from that vertex to a vertex belonging to an odd l_0-cycle.

The following is a theorem about graph G that guarantees gap can be opened at λ_0.

Theorem 22. *Assume that $|V(G)| \geq 3$, condition (G1) are satisfied and $\lambda_0 = (n\pi/l_0)^2$ is an odd eigenvalue. Then the problem (3.26) with $\lambda = \lambda_0$ has no solution for any $\phi \in S$.*

The last two theorems imply the following

Corollary 2. *Under the conditions of Theorem 22, the conclusion of Theorem 21 about spectral gaps holds.*

3. Proofs of the Results

a. Proof of Theorem 20 - Case 1

We start by proving the first part of Theorem 20. Let $\lambda \neq \lambda_0$. We want to solve the following spectral problem

$$\begin{cases} -u'' = \lambda u \text{ on each edge } e \in G \\ \text{conditions } (3.25) \text{ are satisfied on } V(G) \setminus B \\ u|_{\partial G} = \phi \end{cases}$$

Suppose we have a function $\tilde{\phi}$ on G which is twice differentiable on each edge, satisfies vertex conditions (3.25) at the internal vertices of G, and such that $\tilde{\phi}|_{\partial G} = \phi$. Then $w = u - \tilde{\phi}$ solves the following problem:

$$\begin{cases} -w'' - \lambda w = \tilde{\phi}'' + \lambda\tilde{\phi} \text{ on each edge } e \in G \\ \text{conditions } (3.25) \text{ are satisfied on } V(G) \setminus B \\ w|_{\partial G} = 0 \end{cases} \tag{3.28}$$

By assumption that (3.26) for $\lambda = \lambda_0$ has a non-trivial solution, we can choose a $\tilde{\phi}$ that satisfies (3.26) for $\lambda = \lambda_0$. Then solution of (3.28) can be written as

$$w = R(\lambda)(\lambda - \lambda_0)\tilde{\phi} = (\lambda - \lambda_0)R(\lambda)\tilde{\phi}, \tag{3.29}$$

where $R(\lambda)$ is the resolvent for H. Since $\lambda_0 \in \sigma(H)$ and H is self-adjoint, $R(\lambda)$ has a pole of order one at λ_0. Then formula (3.29) proves the first part of the theorem, since the factor $\lambda - \lambda_0$ eliminates the pole.

b. Proof of Theorem 20 - Case 2

Let $\{\psi_j\}_{j\in\mathbb{N}}$ be a complete set of orthonormal eigenfunctions of H corresponding to eigenvalues $\{\lambda_j\}_{j\in\mathbb{N}}$. We denote by $\Psi_j(v_i)$ the sum of the outgoing derivatives of ψ_j at v_i along all edges in G connected to v_i. We also use $\Psi_j := (\Psi_j(v_1), \ldots, \Psi_j(v_n))^T$.

Suppose $\lambda \neq \lambda_0$. Let ϕ be any vector in S. Let $\tilde{\phi}$ be a smooth function on each edge of G, $\tilde{\phi}|_{\partial G} = \phi$ and satisfy condition (3.25) on internal vertices of G. As in proof of case 1 of the theorem, $u = w + \tilde{\phi}$ where w satisfies (3.28). We write w in terms of its Fourier series.

$$\begin{aligned} w &= R(\lambda)(\tilde{\phi}'' + \lambda\tilde{\phi}) \\ &= \sum_j \langle R(\lambda)(\tilde{\phi}'' + \lambda\tilde{\phi}), \psi_j\rangle_{L^2(G)}\psi_j \\ &= \sum_j \langle \tilde{\phi}'' + \lambda\tilde{\phi}, R(\overline{\lambda})\psi_j\rangle_{L^2(G)}\psi_j \\ \\ &= \sum_j \frac{1}{\lambda - \lambda_j}\langle \tilde{\phi}'' + \lambda\tilde{\phi}, \psi_j\rangle_{L^2(G)}\psi_j \\ &= \sum_j \frac{1}{\lambda - \lambda_j}\langle \tilde{\phi}'' + \lambda\tilde{\phi}, \psi_j\rangle_{L^2(G)}\psi_j \end{aligned}$$

We will drop the $L^2(G)$ subscript for now. Applying integration by parts twice to the integral term above, we have

$$
\begin{aligned}
&= \sum_j \frac{1}{\lambda-\lambda_j} \sum_{i=1}^{n} \sum_{v_i \in e} \tilde{\phi}(v_i) \frac{d\psi_j}{dx_e}(v_i)\psi_j + (\lambda-\lambda_j)\langle \tilde{\phi}, \psi_j \rangle \psi_j \\
&= \left(\sum_{\lambda_j=\lambda_0} \frac{1}{\lambda-\lambda_0} \sum_{i=1}^{n} \sum_{v_i \in e} \phi_i \frac{d\psi_j}{dx_e}(v_i) + \sum_{\lambda_j \neq \lambda_0} \frac{1}{\lambda-\lambda_j} \langle \tilde{\phi}, \psi_j \rangle \right) \psi_j + \sum_j \langle \tilde{\phi}, \psi_j \rangle \psi_j \\
&= \frac{1}{\lambda-\lambda_0} \sum_{\lambda_j=\lambda_0} \sum_{i=1}^{n} \phi_i \Psi_j(v_i)\psi_j + \sum_{\lambda_j \neq \lambda_0} \frac{1}{\lambda-\lambda_j} \langle \tilde{\phi}, \psi_j \rangle \psi_j + \sum_j \langle \tilde{\phi}, \psi_j \rangle \psi_j
\end{aligned}
$$

Clearly $\sum_{v_k \in e, e \in G} \frac{d\tilde{\phi}}{dx_e}(v_k)$ is analytic with respect to λ for any v_k, hence it suffice to only consider $\sum_{v_k \in e, e \in G} \frac{dw}{dx_e}(v_k)$. Computing $\sum_{v_k \in e, e \in G} \frac{dw}{dx_e}(v_k)$, we get

$$
\frac{1}{\lambda-\lambda_0} \sum_{\lambda_j=\lambda_0} \langle \phi, \Psi_j \rangle_{\mathbb{C}^n} \Psi_j(v_k) + \sum_{\lambda_j \neq \lambda_0} \frac{1}{\lambda-\lambda_j} \langle \tilde{\phi}, \psi_j \rangle \Psi_j(v_k) + \sum_j \langle \tilde{\phi}, \psi_j \rangle \Psi_j(v_k) \quad (3.30)
$$

The last two terms are both analytic on a small neighborhood around λ_0. If the sum in the first term is nonzero at some v_k then $\Lambda(\lambda)\phi$ has a non-removable singularity at λ_0 for all nonzero ϕ.

To complete the proof, we need the following lemma to show that if (3.26) for $\lambda = \lambda_0$ has no solution for all nonzero ϕ, then

$$
\sum_{\lambda_j=\lambda_0} \langle \phi, \Psi_j \rangle_{\mathbb{C}^n} \Psi_j \neq 0
$$

holds for all $\phi \in S$.

Lemma 23. *If (3.26) for $\lambda = \lambda_0$ has no solution for all nonzero $\phi \in \mathbb{C}^n$ then $\sum_{\lambda_j=\lambda_0} \langle \phi, \Psi_j \rangle_{\mathbb{C}^n} \Psi_j \neq 0$ for all nonzero $\phi \in \mathbb{C}^n$.*

Proof: Let $\tilde{\phi}$ be a smooth function and $\tilde{\phi}|_{\partial G} = \phi$. We express the solution as $u =$

$w + \tilde{\phi}$ where w satisfies

$$Hw - \lambda_0 w = \tilde{\phi}'' + \lambda_0 \tilde{\phi} \tag{3.31}$$

By hypothesis of the lemma, (3.31) has no solution for $\phi \neq 0$. By Fredholm alternative, there exists ψ_j with $\lambda_j = \lambda_0$ such that

$$\langle \tilde{\phi}'' + \lambda_0 \tilde{\phi}, \psi_j \rangle_{L^2(G)} \neq 0$$

but

$$\langle \tilde{\phi}'' + \lambda_0 \tilde{\phi}, \psi_j \rangle_{L^2(G)} = \sum_{i=1}^{n} \tilde{\phi}(v_i) \Psi_j(v_i) = \langle \phi, \Psi_j \rangle_{\mathbb{C}^n}$$

Next, we consider

$$\langle \phi, \sum_{\lambda_j = \lambda_0} \langle \phi, \Psi_j \rangle \Psi_j \rangle = \sum_{\lambda_j = \lambda_0} |\langle \phi, \Psi_j \rangle|^2 > 0 \ \ , \forall \phi \neq 0.$$

Hence $\sum_{\lambda_j = \lambda_0} \langle \phi, \Psi_j \rangle_{\mathbb{C}^n} \Psi_j \neq 0$ for $\forall \ \phi \neq 0$. In particular there exist v_i such that $\sum_{\lambda_j = \lambda_0} \langle \phi, \Psi_j \rangle_{\mathbb{C}^n} \Psi_j(v_i) \neq 0$. □

This completes the proof of the first statement of case 2 of theorem 20.

We now prove the inequality (3.27). Firstly, from the proof of lemma 23, we know that $\sum_{\lambda_j = \lambda_0} |\langle \phi, \Psi_j \rangle|^2 > 0$, $\forall \phi \in S$. Since the above sum of squares is a continuous positive function on the compact set S, there exists a positive constant C_1 such that

$$\sum_{\lambda_j = \lambda_0} |\langle \phi, \Psi_j \rangle|^2 \geq C_1 > 0 \ \ \forall \phi \in S. \tag{3.32}$$

Secondly, $\sum_j |\langle \Psi_j, \phi \rangle|$ is also a continuous positive function on the compact set S, so there exists a positive constant C_2 such that

$$\sum_j |\langle \Psi_j, \phi \rangle| \leq C_2 \ \ \forall \phi \in S.$$

Define

$$f_j(\lambda) = \begin{cases} 1 & \text{if } \lambda_j = \lambda_0 \\ 1 + \dfrac{1}{\lambda - \lambda_j} & \text{if } \lambda_j \neq \lambda_0 \end{cases}$$

Clearly $f_j(\lambda)$ is analytic on some small neighborhood $N(\lambda_0)$ not containing any λ_j. If $\lambda_j \neq \lambda_0$ the let $C_3 := \min_{\lambda \in \overline{N(\lambda_0)}} |\lambda - \lambda_j| > 0$. Then clearly for $\lambda \in N(\lambda_0)$,

$$|f_j(\lambda)| \leq \frac{1}{|\lambda - \lambda_j|} + 1 \leq \frac{1}{C_3} + 1 \quad , \forall\, j \in \mathbb{N} \text{ such that } \lambda_j \neq \lambda_0$$

Next, assuming $\phi \in S$, we estimate the following:

$$\sum_j |f_j(\lambda)||\langle \tilde{\phi}, \psi_j \rangle_{L^2(G)}||\langle \Psi_j, \phi \rangle| \leq C_3 \, \|\tilde{\phi}\|_{L^2(G)} \sum_j |\langle \Psi_j, \phi \rangle| \leq C_2 C_3 \, \|\tilde{\phi}\|_{L^2(G)} \, . \tag{3.33}$$

Using the (3.30) and that $u = w + \tilde{\phi}$,

$$|\langle \Lambda(\lambda)\phi, \phi \rangle| \geq \frac{1}{|\lambda - \lambda_0|} \sum_{\lambda_j = \lambda_0} |\langle \phi, \Psi_j \rangle|^2 - \sum_j |f_j(\lambda)||\langle \tilde{\phi}, \psi_j \rangle_{L^2(G)}||\langle \Psi_j, \phi \rangle|$$

$$-|\langle \Phi, \phi \rangle|$$

where $\Phi = \left(\sum_{v_1 \in e, e \in G} \frac{d\tilde{\phi}}{dx_e}(v_1), \ldots, \sum_{v_n \in e, e \in G} \frac{d\tilde{\phi}}{dx_e}(v_n) \right)^T$.

Using (3.32) and (3.33), we obtain

$$|\langle \Lambda(\lambda)\phi, \phi \rangle| \geq \frac{C_1}{|\lambda - \lambda_0|} - C_2 C_3 \, \|\tilde{\phi}\|_{L^2(G)} - \|\Phi\| \, .$$

Since $\tilde{\phi}$ is assumed to be smooth on each edge, it is in $H^2(e)$ for each edge e in G. By using Sobolev trace theorem on each edge, both $\|\tilde{\phi}\|_{L^2(G)}$ and $\|\Phi\|$ can be bounded above by $C_4 \, \|\phi\|$ for some positive constant C_4. Thus we obtained

$$|\langle \Lambda_v(\lambda)\phi, \phi \rangle| \geq \frac{C_1}{|\lambda - \lambda_0|} - (C_2 C_3 + C_4).$$

Finally, for λ sufficiently close to λ_0, i.e., $|\lambda - \lambda_0| < \frac{C_1}{2C_5}$ then

$$\frac{1}{|\lambda - \lambda_0|}(C_1 - C_5|\lambda - \lambda_0|) > \frac{C_1}{2|\lambda - \lambda_0|}$$

where $C_5 = C_2C_3 + C_4$. The theorem then follows since $|\langle \Lambda(\lambda)\phi, \phi\rangle| \leq \|\Lambda(\lambda)\phi\|$.

c. Proof of Theorem 21

Suppose that $\lambda_0 \in \sigma(H) \setminus \sigma_D(\Gamma_0)$. Let $u(x)$ be an eigenfunction of $\mathcal{H}$ corresponding to an eigenvalue λ. Suppose also that $0 < |\lambda - \lambda_0| < \dfrac{\delta}{2}$, then $\lambda \notin \sigma_D(\Gamma_0)$. The spectral problem $\mathcal{H}u = \lambda u$ on Γ can be rewritten on edges of Γ_0 and vertices in B_v, through the use of the Dirichlet-to-Neumann operator as follows:

$$\begin{cases} -u'' = \lambda u \text{ on each edge of } \Gamma_0 \\ u \text{ is continuous at each vertex in } \bigcup_{v\in\Gamma_0} B_v \\ \phi'_v = -\Lambda(\lambda)\phi_v \text{ at each vertex } v \in \Gamma_0 \end{cases} \tag{3.34}$$

where $\phi_v = (u(v_1), \ldots, u(v_n))^T$, $\phi'_v = (\dfrac{du}{dx_e}(v_1), \ldots, \dfrac{du}{dx_e}(v_n))^T$, and $\{v_i\} \subset B_v$.

We have three cases depending on λ.

Case (i): Suppose $\lambda > 0$. On each edge e in Γ_0 we have $\sin\sqrt{\lambda}l_e \neq 0$ because $\lambda \notin \sigma_D(\Gamma_0)$. Thus the solution of $-u'' = \lambda u$ on e has the following form:

$$u_e(x) = \frac{u(0)\sin\sqrt{\lambda}(l_e - x) + u(l_e)\sin\sqrt{\lambda}x}{\sin\sqrt{\lambda}l_e} \tag{3.35}$$

where we assume e has coordinate x_e in which $x = 0$ and $x = l_e$ are the coordinates of the endpoints of e. Then

$$\frac{du_e}{dx}(x) = \frac{-u(0)\cos\sqrt{\lambda}(l_e - x) + u(l_e)\cos\sqrt{\lambda}x}{\sin\sqrt{\lambda}l_e}\sqrt{\lambda}$$

and

$$\begin{aligned}\|u\|^2_{H^2(e)} &= \int_e (1+|\lambda|^2)|u|^2 dx + \int_e |u'|^2 dx \\ &\leq \frac{2(1+|\lambda|)^2 l_e}{\sin^2 \sqrt{\lambda} l_e} \sum_{v_i \in e} |u(v_i)|^2.\end{aligned}$$

Summing the above over all edges in Γ_0, we have

$$\sum_{e\in\Gamma_0} \|u\|^2_{H^2(e)} \leq \sum_{e\in\Gamma_0} \frac{2(1+|\lambda|)^2 l_e}{\sin^2 \sqrt{\lambda} l_e} \sum_{v_i \in e} |u(v_i)|^2.$$

By our assumption that $|\lambda - \lambda_0| < \frac{\delta}{2}$, it follows that $(1+|\lambda|)^2 \leq (|\lambda_0| + 1 + \frac{\delta}{2})^2$. As for the estimating $\sin \sqrt{\lambda} l_e$ term, we can inscribe a triangle inside each hump of $|\sin \sqrt{\lambda} l_e|$ with vertices of triangle at $((n-1)\pi, 0)$, $(n\pi, 0)$ and $(n\pi/2, 1)$, $n \in \mathbb{N}$, then it follows that

$$|\sin \sqrt{\lambda} l_e| \geq \frac{2l_e}{\pi} \min_n |\sqrt{\lambda} - \frac{n\pi}{l_e}|$$

There exists a positive constant C depending on λ_0 and δ only, such that

$$\frac{2l_e}{\pi} \min_n |\sqrt{\lambda} - \frac{n\pi}{l_e}| \geq \frac{2l_e C_{\lambda_0,\delta}}{\pi} \min_n |\lambda - \left(\frac{n\pi}{l_e}\right)^2|.$$

By triangle inequality,

$$\min_n |\lambda - \left(\frac{n\pi}{l_e}\right)^2| \geq \min_n |\lambda_0 - \left(\frac{n\pi}{l_e}\right)^2| - |\lambda - \lambda_0| \geq \frac{\delta}{2}.$$

Thus, we have

$$|\sin \sqrt{\lambda} l_e| \geq C_{\lambda_0,\delta} l_e \tag{3.36}$$

Since Γ_0 is finite and using (3.36), we can estimate

$$\sum_{e\in\Gamma_0} \|u\|^2_{H^2(e)} \leq C_{\lambda_0,\delta} \sum_{v\in\Gamma_0} \sum_{v_i \in B_v} |u(v_i)|^2. \tag{3.37}$$

Case (ii): If $\lambda = 0$, then solution of $-u'' = \lambda u$ on each e has the following form:

$$u_e(x) = \frac{u(0)(l_e - x) + u(l_e)x}{l_e}. \tag{3.38}$$

Since Γ_0 is finite, we have

$$\sum_{e\in\Gamma_0} \|u\|^2_{H^2(e)} = 2\sum_{e\in\Gamma_0} \frac{2+l_e^3}{l_e} \sum_{v_i\in e} |u(v_i)|^2 \le C \sum_{v\in\Gamma_0}\sum_{v_i\in B_v} |u(v_i)|^2. \tag{3.39}$$

Case (iii): If $\lambda < 0$ then solution of $-u'' = \lambda u$ on each e has the following form:

$$u_e(x) = \frac{u(0)\sinh\sqrt{-\lambda}(l_e - x) + u(l_e)\sinh\sqrt{-\lambda}x}{\sinh\sqrt{-\lambda}l_e}. \tag{3.40}$$

From **[53]** , $\|u\|_{H^2(e)}$ is equivalent to the norm defined by $(\|u\|^2_{L_2(e)} + \|u''\|^2_{L_2(e)})^{1/2}$.

$$\sum_{e\in\Gamma_0} \|u\|^2_{H^2(e)} \le C \int_e (1+|\lambda|^2)|u|^2 dx$$

$$= C\sum_{e\in\Gamma_0}(|\lambda_0| + 1 + \frac{\delta}{2})^2 l_e \sum_{v_i\in e} |u(v_i)|^2 \le C_{\lambda_0,\delta} \sum_{v\in\Gamma_0}\sum_{v_i\in B_v} |u(v_i)|^2. \tag{3.41}$$

Hence from (3.37), (3.39) or (3.41), we end up with

$$\sum_{e\in\Gamma_0} \|u\|^2_{H^2(e)} \le C_{\lambda_0,\delta} \sum_{v\in\Gamma_0} \|\phi_v\|^2 \tag{3.42}$$

The Sobolev trace theorem then implies that

$$\sum_{v\in\Gamma_0}\sum_{v_i\in B_v, v_i\in e} \left|\frac{du}{dx_e}(v_i)\right|^2 \le C \sum_{e\in\Gamma_0} \|u\|^2_{H^2(e)} \tag{3.43}$$

Combining (3.42), (3.43) and using the vertex condition of (3.34) we obtain

$$\sum_{v\in\Gamma_0} \|\Lambda(\lambda)\phi_v\|^2 = \sum_{v\in\Gamma_0} \|\phi_v'\|^2 \le \tilde{C}_{\lambda_0,\delta} \sum_{v\in\Gamma_0} \|\phi_v\|^2 \tag{3.44}$$

If $\phi_v = 0$ for each $v \in \Gamma_0$ and with $\lambda \notin \sigma_D(\Gamma_0)$ then $u = 0$ contradicting that u is an eigenfunction. So there are $\phi_v \neq 0$ for some v.

If now $\lim_{\lambda \to \lambda_0} \|\Lambda(\lambda)\phi_v\| = \infty$ for all $v \in \Gamma_0$, then we will get a contradiction in (3.44) when λ and λ_0 are sufficiently close. More specifically, let $\varepsilon = \frac{C_1^2}{2\tilde{C}_{\lambda_0,\delta}}$ where C_1 is the constant in (3.27). Hence ε depends only on G, B and δ. If $0 < |\lambda - \lambda_0| < \min\{\varepsilon, \frac{\delta}{2}\}$, then

$$\frac{C_1}{|\lambda - \lambda_0|} \sum_{v \in \Gamma_0} \|\phi_v\|^2 \leq \tilde{C}_{\lambda_0,\delta} \sum_{v \in \Gamma_0} \|\phi_v\|^2 \tag{3.45}$$

The term $\sum_{v \in \Gamma_0} \|\phi_v\|^2$ is nonzero and can be cancelled, we then have

$$2\tilde{C}_{\lambda_0,\delta} < \frac{C_1}{|\lambda - \lambda_0|} \leq \tilde{C}_{\lambda_0,\delta}$$

contradicting (3.44).

d. Proof of Theorem 22

Assume that there exist $\phi \in S$ such that (3.26) for $\lambda = \lambda_0$ has a solution.

First we consider a special case. Suppose there is an odd l_0 cycle that contains all vertices in B_v. Denote the cycle as $v_1, \ldots, v_n v_1$. On each edge connecting v_i to v_{i+1} the solution has the form $c_i \cos(\sqrt{\lambda_0} x) + b_i \sin(\sqrt{\lambda_0} x)$ with $x = 0$ representing v_i and $x = l_i$ representing v_{i+1}. Then $u(0) = c_i = \phi_i$ and $u(l_0) = -c_i = \phi_{i+1}$ since λ_0 is an odd eigenvalue and thus $\cos(\sqrt{\lambda_0} l_0) = \cos(n_0 \pi) = -1$. Hence $\phi_i = -\phi_{i+1}$.

Since there is an odd number of vertices in G_v, we have $\phi_1 = -\phi_2 = \cdots = \phi_n = -\phi_1$ which forces $\phi_1 = 0$ and thus $\phi = 0$. Contradicting that $\phi \neq 0$.

Now, we consider the general case. Suppose at v_{J_0}, $\phi_{J_0} \neq 0$. If v_{J_0} belongs to an odd l_0-cycle, then by argument similar to the special case above, we arrive at a contradiction. So we assume that v_{J_0} does not belong to an odd l_0-cycle. Then by condition (G1), there is a l_0-path that connects to a vertex v_c belonging to an odd l_0-cycle. By arguments similar to the special case above, ϕ_c must be zero, otherwise there is no solution to (3.26) for $\lambda = \lambda_0$. We denote the sequence of the vertices in the l_0-path as $v_{J_0} v_{J_1} \ldots v_{J_k},\ (v_{J_k} := v_c)$ and e_{J_i}

as the edge connecting v_{J_i} to $v_{J_{i+1}}$ for $i = 0, \dots, k-1$. On each edge e_{J_i}, the solution of (3.26) for $\lambda = \lambda_0$ has the form $c_i \cos(\sqrt{\lambda_0}x) + b_i \sin(\sqrt{\lambda_0}x)$ with $x = 0$ representing v_{J_i} and $x = l_0$ representing $v_{J_{i+1}}$. Hence, we have

$$\phi_{J_0} = -\phi_{J_1} = \cdots = (-1)^{k-1}\phi_{J_{k-1}} = (-1)^k \phi_{J_k} = 0.$$

Thus $\phi = 0$ contradicting that $\phi \neq 0$. Hence a solution for (3.26) for $\lambda = \lambda_0$ for $\phi \neq 0$ cannot exist.

4. Some Remarks and Examples

We provide now some examples. Example 1 shows that when λ_0 is not an odd eigenvalue, then there might exist $\phi \neq 0$ such that $\lim_{\lambda \to \lambda_0} \| \Lambda(\lambda)\phi \| < \infty$ or equivalently (3.26) for $\lambda = \lambda_0$ has solution for ϕ. On the other hand, example 2 shows that the same might happen when there is no odd cycle (G1 is not satisfied). Finally, example 3 shows that when second statement of (G1) is not satisfied, the same situation might also happen. Example 4 provides a situation when our technique does work and gaps do open.

Example 1: Suppose G is an equilateral triangle with edge length $l_e := l$ and λ_0 is an even Dirichlet eigenvalues, i.e. $\lambda_0 = \frac{n_0^2 \pi^2}{l^2}$ where n_0 is even, then (3.26) for $\lambda = \lambda_0$ has solution for $\phi = (1, \dots, 1)^T$, i.e. $u(x) = \cos(\frac{n_0 \pi}{l}x) + b_e \sin(\frac{n_0 \pi}{l}x)$ on each edge. The Dirichlet-to-Neumann matrix is

$$\Lambda(\lambda) = \frac{\sqrt{\lambda}}{\sin(\sqrt{\lambda}l)} \begin{bmatrix} -2\cos(\sqrt{\lambda}l) & 1 & 1 \\ 1 & -2\cos(\sqrt{\lambda}l) & 1 \\ 1 & 1 & -2\cos(\sqrt{\lambda}l) \end{bmatrix}.$$

For $\phi = (1, \dots, 1)^T$ and $\lambda_0 = (n_0 \pi l^{-1})^2$,then

$$\Lambda(\lambda)\phi = 2\frac{\sqrt{\lambda}(1 - \cos(\sqrt{\lambda}l))}{\sin(\sqrt{\lambda}l)}\phi \overset{\lambda \to \lambda_0}{\longrightarrow} 0$$

□

Example 2: Let G be a graph with four vertices and four edges with each vertex having degree two. Assume that all four edges are of same length l. Thus the graph is a quadrilateral and

$$\Lambda(\lambda) = \frac{\sqrt{\lambda}}{\sin(\sqrt{\lambda}l)} \begin{bmatrix} -2\cos(\sqrt{\lambda}l) & 1 & 0 & 1 \\ 1 & -2\cos(\sqrt{\lambda}l) & 1 & 0 \\ 0 & 1 & -2\cos(\sqrt{\lambda}l) & 1 \\ 1 & 0 & 1 & -2\cos(\sqrt{\lambda}l) \end{bmatrix}.$$

Take $\phi = (1, -1, 1, -1)^T$ and $\lambda_0 = (n_0 \pi l^{-1})^2$ where n_0 is an odd positive integer. Then

$$\Lambda(\lambda)\phi = -\frac{2\sqrt{\lambda}(1+\cos(\sqrt{\lambda}l))}{\sin(\sqrt{\lambda}l)}\phi \overset{\lambda\to\lambda_0}{\longrightarrow} 0$$

□

Example 3: Let G be a graph on 4 vertices and looks like the picture below (see Fig. 10). The side of the equilateral triangle has length l.

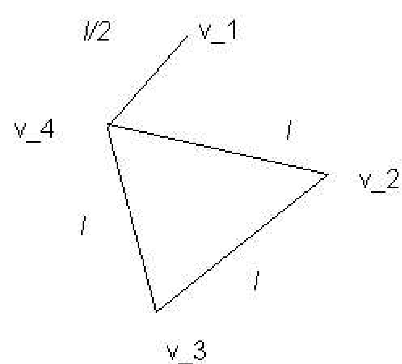

Fig. 10. Graph G for Example 3

Take $\lambda_0 = (\pi l^{-1})^2$ to be an odd Dirichlet eigenvalues, then (3.26) for $\lambda = \lambda_0$ has a solution for $\phi = (1,0,0,0)^T$. Indeed, the solution u which is zero on the triangle and has the form $\sin(\pi x/l)$ on the remaining edge.

$$\Lambda(\lambda) = \frac{\sqrt{\lambda}}{\sin(\sqrt{\lambda}l)} \begin{bmatrix} -p & 0 & 0 & q \\ 0 & -2\cos(\sqrt{\lambda}l) & 1 & 1 \\ 0 & 1 & -2\cos(\sqrt{\lambda}l) & 1 \\ q & 1 & 1 & -2\cos(\sqrt{\lambda}l) - p \end{bmatrix}.$$

where $p = \cot(\sqrt{\lambda}l/2)\sin(\sqrt{\lambda}l)$ and $q = \csc(\sqrt{\lambda}l/2)\sin(\sqrt{\lambda}l)$. Once again

$$\Lambda(\lambda)\phi \to 0$$

Example 4: Let G be a graph like in the above except all four edges have the same length l. Also take $\lambda_0 = (n_0\pi l^{-1})^2$ to be an odd Dirichlet eigenvalue. Then (3.26) for $\lambda = \lambda_0$ does not have a solution for any nonzero ϕ and $\Lambda(\lambda) = \dfrac{\sqrt{\lambda}}{\sin(\sqrt{\lambda}l)}A(\lambda)$ where

$$A := \begin{bmatrix} -\cos(\sqrt{\lambda}l) & 0 & 0 & 1 \\ 1 & -2\cos(\sqrt{\lambda}l) & 1 & 0 \\ 0 & 1 & -2\cos(\sqrt{\lambda}l) & 1 \\ 1 & 0 & 1 & -3\cos(\sqrt{\lambda}l) \end{bmatrix}.$$

Let $p_1 = -\cos(\sqrt{\lambda}l)$. Note that $\det(A(\lambda)) = 3p_1^2(4p_1^2 - 3)$. For $-\cos(\sqrt{\lambda_0}l) = 1$, $\det(A(\lambda_0)) = 3 \neq 0$. Hence

$$\lim_{\lambda \to \lambda_0} \parallel \Lambda(\lambda)\phi \parallel = \infty.$$

Remark 24. *Conditions of Theorem 22 are rather restrictive. It requires that for a graph on n vertices, at least n edges need to be of the same length corresponding to the Dirichlet eigenvalue λ_0. By perturbation theory, it is clear that spectral gaps are stable under small perturbation and hence such restrictive conditions are not necessary.*

CHAPTER IV

SUMMARY

In this dissertation, we described our results concerning two areas of applied spectral theory.

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 $2D$ photonic or any dimension acoustic guides) and the full $3D$ Maxwell cases. See **[43, 44]** .

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.

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. The limiting 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 spectra of 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 application and 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.

The results are published in one paper **[44]** , one more paper is accepted for publication **[49]** , and two more are in preparation **[43, 45]** .

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