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Graph models for waves in thin structures

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Abstract

A brief survey on graph models for wave propagation in thin structures is presented. Such models arise in many areas of mathematics, physics, chemistry, and engineering (dynamical systems, nanotechnology, mesoscopic systems, photonic crystals, etc.). Considerations are limited to spectral problems, although references to works with other studies are provided.

Keywords: Spectral theory, mesoscopic physics, waveguide, graph **AMS subject classification**: Primary 35P, Secondary 05C90, 78A50, 81U99, 81V99

Introduction

This article¹ aims to survey some parts of a field that has been emerging in the last couple of decades, namely modeling propagation of waves in thin, graphlike structures by differential or pseudo-differential equations on graphs. We will be in particular concerned with the spectral behavior of the corresponding operators. Although spectral problems are far from being the only ones

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¹A short version of this text was presented as an invited address at the 3rd Congress of ISAAC [119].

studied, it is probably unrealistic to try to cover the whole range of problems discussed in this area of research. We present the references to the literature where the interested reader can learn about other facets of the existing studies.

The motivation for studying wave propagation in thin structures comes from various areas of mathematics and sciences, some of which will be discussed in more detail elsewhere in this article. Here we only mention briefly some of these topics. Historically, probably the first graph model of the type discussed above was developed in chemistry [98, 99, 142, 162]. We address it in more detail below in Section 2.1. One can also refer to the mesoscopic physics and nanotechnology. Mesoscopic systems (e.g., [3, 9, 42, 67, 95, 102, 105, 134, 178) are those that have some dimensions too small to be treated using purely classical physics, while too large to be conveniently considered on the quantum level only. More precisely, these are physical systems whose one, two, or all three dimensions are reduced to a few nanometers. They hence look as surfaces, wires, or dots and are called correspondingly quantum walls, quantum wires, and quantum dots. While quantum dots are probably most familiar to general scientific public, in this article we will be concerned with circuits of quantum wires only. Such circuits, due to recent progress of microelectronics, are subjects of intensive studies. We will also consider thin graph-like acoustic or optical structures [16, 80, 81, 84, 117, 120, 121]. Interest in such systems comes from the thriving area of photonic crystals (see | 106, 117, 146, 165 | for surveys of this topic). In this case the word mesoscopic would be abused, since the characteristic dimensions of such systems are normally much larger than nanometers.

One can expect that transport of electronic, electromagnetic, or acoustic waves in thin graph-like media could be studied using some approximate models on graphs (when the "thin" dimensions are ignored). This is exactly the direction that we choose in this paper. Besides the ones mentioned above, there are quite a few other cases when one wants to use a graph model. One can think, for instance, of thin acoustic, electromagnetic, or quantum waveguides (see e.g., [50, 67, 70, 30, 31, 131, 182]). Another option is to use graph models as test grounds for studying the features that depend upon or are influenced by multiple connectedness of the material, for instance Aharonov-Bohm effect [3, 13, 15], quantum chaos [17, 23, 112, 176], Anderson localization [11], and scattering [1, 5, 12, 54, 93, 94, 109, 110, 111, 126, 130, 140, 145]. Yet another source of such models is averaging in dynamical systems in the presence of a slow motion in graph directions and a fast one

across the graph. Then averaging naturally leads to the models of the kind described above. One can find a very interesting discussion of the origins of and results on such problems in [86, 87]. There is a large variety of other topics that also lead to differential operators on graphs (e.g., [2, 12, 29], [32]–[36], [43], [45]–[79], [97, 127, 128, 135, 136, 137, 147, 148, 149, 166, 171, 175, 179, 180]). One should also mention books [115, 129], where important techniques for PDE problems in thin domains are developed.

It is practically impossible to provide even a brief survey of all existing studies of the kind described above, so according to the author's own interests, we will concentrate on some spectral problems only, while providing references to other topics.

We would like to mention that in this article graphs are considered as onedimensional singular (due to presence of vertices) varieties, rather than purely combinatorial objects, as is customary in standard graph theory. Correspondingly, our graphs will be equipped with differential rather than difference operators. In order to emphasize this difference, such graphs are sometimes called in physics literature quantum graphs. In the mathematics literature sometimes the name metric graphs is used. The reader should be aware, however, that there is no commonly accepted name for such objects, and in most cases researchers use neither of the above notions. At the same time, spectral theory of difference operators on (combinatorial) graphs is well developed (e.g., [37, 40, 41, 132]) and has been used in a variety of applications from random walks theory to solid state physics, to spectral geometry, to scattering (see for instance [25, 26, 27, 38, 39, 91, 92, 132, 138, 139, 140, 152, 181], albeit this list is rather arbitrary and a complete list would be huge).

The article is structured as follows. We introduce the pertinent mathematical objects in Section 1. Then we present in Section 2 in a little bit more detailed fashion than in this introduction some of the motivations for studying such systems. In the next Section 3, results are described that concern approximations of the spectra of the original problems by spectra of certain graph models. Finally, some token examples are presented in Section 4 of effects one can discover using such models (these examples are far from exhausting all known cases). We also supply a bibliography on the subject, which in spite of being rather extensive, is probably still incomplete.

1 Main mathematical objects

As was mentioned in the introduction, we will be dealing with *quantum* graphs, i.e. with graphs considered as one-dimensional singular varieties, and correspondingly equipped with differential (or sometimes "pseudo-differential") operators.

1.1 Quantum (or metric) graphs

The graphs will be interpreted as one-dimensional varieties with singularities at the vertices, rather than purely combinatorial objects. In other words, a graph Γ with finite valences of all its vertices v_i will be assumed to be embedded into \mathbb{R}^2 (albeit higher dimensional analogs also exist) in such a way that all edges e_j are sufficiently smooth (usually C^2 suffices) finite length curves with transversal intersections at vertices. We also assume that every compact domain contains only a finite number of edges and vertices. In most cases our graphs of interest will be finite or periodic with respect to a lattice in \mathbb{R}^2 .

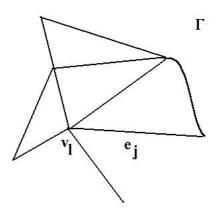


Figure 1: Graph Γ .

Each edge e_j is equipped with the arc length coordinate x_j that will often be denoted by x, which should not lead to any confusion. The functions f(x)on Γ are defined along the edges (rather than at the vertices as in discrete models). One can define in a natural way the space $L_2(\Gamma)$ of square integrable measurable functions on Γ . Our spectral problems will be introduced for some operators in this space.

1.2 Operators

The operators of interest in the simplest cases are: the second arc length derivative

$$f(x) \to -\frac{d^2 f}{dx_i^2},\tag{1}$$

a more general Schrödinger operator

$$f(x) \to -\frac{d^2 f}{dx_j^2} + V(x)f(x), \tag{2}$$

or a magnetic Schrödinger operator

$$f(x) \to \left(\frac{1}{i}\frac{d}{dx_i} - A(x)\right)^2 + V(x)f(x).$$
 (3)

The (vector and scalar) real potentials A and V will be assumed sufficiently smooth and in the case of infinite periodic graphs also periodic. Precise conditions can be found in the cited literature and partly below. In order for the definition of the operators to be complete, one needs to describe their domains. The natural conditions require that f belongs to the Sobolev space H^2 on each edge e_j , however one also needs to impose boundary value conditions at the vertices. It is possible to describe all the vertex conditions that make these operators self-adjoint (see [67] and references therein and also [109, 110]). This is done either by using the standard theory of extensions of symmetric operators, or by a more recent version of it that amounts to finding Lagrangian planes with respect to the symplectic boundary form that corresponds to the maximal operator (see for instance [5, 100, 126, 140, 144] for the accounts of this approach). Self-adjointness guarantees that the quantum probability current is conserved at the graph vertices. One standard type of such "Kirchhoff" boundary conditions is

$$\begin{cases} f(x) \text{ is continuous on } \Gamma \\ \text{at each vertex } v_l \text{ one has } \sum_{\{j \mid v_l \in e_j\}} \frac{df}{dx_j}(v_l) = \alpha_l f(v_l) \end{cases} , \tag{4}$$

where the sum is taken over all edges e_j containing the vertex v_l , and derivatives are taken in the directions away from the vertex. Here α_l are some fixed real numbers. The most common case is when $\alpha_l = 0$, i.e.

$$\begin{cases} f(x) \text{ is continuous on } \Gamma \\ \text{at each vertex } v_l \text{ one has } \sum_{\{j \mid v_l \in e_j\}} \frac{df}{dx_j}(v_l) = 0 \end{cases}$$
 (5)

There are many other plausible vertex conditions, and one of the questions to consider is which of these conditions (if any) arise in the asymptotic limit of a problem of interest in a thin domain.

We will also have to face more general operators, including those of higher order, the ones with more general boundary conditions, and also "pseudo-differential" operators (whatever such an operator on a graph could mean).

1.3 Spectral problem

We consider wave propagation through a system that looks like a narrow neighborhood of a graph Γ . Such propagation can be governed by different types of operators: Laplace (or more general Schrödinger), Maxwell, acoustic, etc. As it has already been indicated, we will be particularly interested in the spectra of these operators. For instance, the presence of spectral gaps is of interest. Existence of such a gap means that waves of certain frequencies (electrons of certain energies) cannot propagate through the system. This is known to be one of the major considerations in the solid state theory [8] and in the theory of photonic crystals [106, 117, 165]. It is clear that studying these spectra in the domains of such a complex nature most probably will turn out to be very complicated. The main thrust of this paper is to discuss the possibility of approximating the spectra of such operators by the spectra of appropriate operators on Γ , which should be much easier to study, due to reduced dimensionality of the problem.

2 The origins of the problem

There are manifold reasons for studying the operators on graphs of the type described in the previous section. They naturally arise as simplified (due to reduced dimension) models in chemistry, physics, engineering (nanotechnology) and mathematics. We have already mentioned in particular the

free-electron theory of conjugated molecules in chemistry, quantum chaos, quantum wires, dynamical systems, photonic crystals, scattering theory, and a variety of other applications. We will address at some length only a few of them, leaving it to the audience to look up the rest in the literature (the reader can refer to the introduction for the pertinent references).

2.1 A free-electron theory of conjugated molecules

Although the origins of this approach go probably back to [142] (see the references on p. 1566 in [162]), we will follow the formulation of the graph model given in probably the most complete form in [162] (see also [98, 99, 142]). Some organic molecules like the one of naphthalene shown in Fig. 2, contain systems of conjugated (i.e. alternating single and double) bonds.

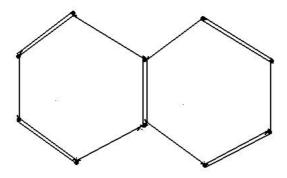


Figure 2: Naphtalene molecule.

Every atom contributes three electrons for chemical binding. In the first approximation one thinks that two of those (so called σ -electrons) form bonds that maintain the "skeleton," or the frame of the molecule, i.e. the graph obtained by eliminating the doubling of bonds (Fig. 3).

This "skeleton" creates a potential in which the remaining so called π -electrons (one per each atom) move through the entire structure. So, the π -electrons can be thought of as confined to the "skeleton" graph by the

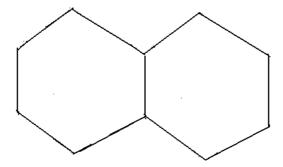


Figure 3: The "skeleton" of the naphtalen molecule.

potential. It was suggested in [162] that one can obtain a simplified approximate model for studying the motion (in particular, the spectra) of π -electrons using a second order (ordinary) differential Hamiltonian on the skeleton Γ . In order to obtain such a model the authors of [162] assumed first that the single particle Hamiltonian for a π -electron is the Laplace operator (an electric potential can also be added) in a narrow tube around Γ with zero Dirichlet condition on its boundary. The Dirichlet conditions are responsible for confinement of the π electrons to a vicinity of Γ . Then the width of the tube was allowed to tend to zero. In this case, because of the presence of transversal modes in the narrow tube, the ground energy increases to infinity, so one needs to subtract it to shift the spectrum back to zero. An heuristic argument was provided in [162] in order to support the claim that after the shift the asymptotic limit of the spectrum is given by the spectrum of the second arc length derivative on Γ (1) with the boundary conditions (5). The boundary conditions were interpreted as conservation of the quantum-mechanical current density. Then this much simpler model was used for studying the orbitals of π -electrons.

Let us briefly address the heuristic derivation of the boundary conditions presented in [162]. Consider a small neighborhood Ω of a junction that looks as shown in Fig. 4 below.

Let Φ be an eigenfunction of the Dirichlet Laplacian in the branching tube

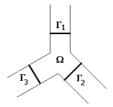


Figure 4: A junction neighborhood.

and λ be the corresponding eigenvalue. Then the Green's theorem applied to Ω together with the Dirichlet conditions on the tube's boundary give:

$$\int_{\Omega} |\nabla \Phi|^2 dx - \sum_{i=1}^{3} \int_{\Gamma_i} \overline{\Phi} \frac{\partial \Phi}{\partial x_j} ds = \lambda \int_{\Omega} |\Phi|^2 dx.$$

Here x_j is the axial coordinate along the jth tube. When one simultaneously shrinks the width of the tube and diameter of Ω to zero, it was argued in [162] that now the volume integrals tend to zero faster than the surface one, and so in the limit one gets the condition

$$\overline{\Phi} \sum_{i=1}^{3} \frac{\partial \Phi}{\partial x_{j}} = 0$$

and hence

$$\sum_{i=1}^{3} \frac{\partial \Phi}{\partial x_j} = 0$$

at the vertex. It is clear that some assumptions are implicitly applied here, for instance that the eigenfunction does not concentrate around the vertex. In particular, one has to exclude the possibility of existence of bound states confined to the vertex. This is however the effect that actually does take place (see further discussions in Section 3.2). The final conclusion of [162] about validity of the boundary conditions (5) is incorrect, and the matter is essentially still open.

2.2 Circuits of quantum wires

As it has been mentioned already, quantum wires (or quantum waveguides) are quasi-one-dimensional semi-conductor or metallic objects whose other two dimensions are reduced to a few nanometers. So one can envision a graph Γ with a "fattened graph" domain Ω_d around Γ of thickness $d \ll 1$ (see the figure below).

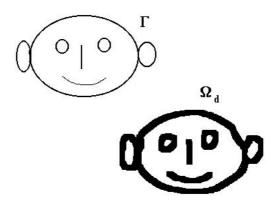


Figure 5: A 'fattened' graph.

Wave propagation in Ω_d is assumed to be governed by the Laplace operator $-\Delta u = -\sum \frac{\partial^2 u}{dx_j^2}$ (or more general Schrödinger operators) with either Dirichlet or Neumann conditions on $\partial\Omega_d$ (i.e., either the function or its normal derivative vanishes at the boundary). Such models arise while studying quantum and also electromagnetic and acoustic waveguides and thin superconducting structures (e.g., [6, 20, 30, 31, 44], [46]–[50], [67, 73, 131], [156]–[161]).

So, now the problem is: How do the spectra of the Neumann $-\Delta_N$ and Dirichlet $-\Delta_D$ Laplacians in Ω_d behave when $d \to 0$ (i.e. in the thin domain limit)? In particular, do they converge to the spectrum of a differential operator on the graph? Some answers and open questions are given in Sections 3.1 and 3.2.

2.3 Photonic crystals

Here the domain Ω_d of the previous section is assumed to be filled with an optically dense dielectric, while the rest is filled with air. One is interested in the behavior when $d \to 0$ of the frequency spectra of electromagnetic waves in such a medium, in particular whether this behavior is governed by an operator on Γ . It is rather clear that in general this is not the case, since the waves do penetrate the air, but for some "dielectric" modes that stay mostly inside the narrow dielectric tubes, a pseudodifferential operator on Γ arises (see details in Section 3.3 below and in [16], [80]–[85], [117, 120, 121]).

2.4 Other applications

Besides the already mentioned quantum wires, waveguide theory, superconductivity, and photonic crystal theory, there are quite a few other cases when one wants to use a quantum graph model. We refer the reader again to the already mentioned in the introduction studies of the adiabatic quantum transport [13, 15], quantum chaos [17, 23, 112, 176], Anderson localization [11], direct and inverse scattering problems [1, 5, 12, 54, 93, 94, 109, 110, 111, 114, 126, 130, 140, 145], averaging in dynamical systems [86, 87], and a large variety of other topics that also lead to differential operators on graphs (e.g., [2, 12, 29], [32]–[36], [43], [45]–[79], [97, 127, 128, 135, 136, 137, 147, 148, 149, 166, 171, 175, 179, 180]).

3 Convergence results

We present here the results that guarantee convergence of the spectrum of a problem in a thin domain to the spectrum of a problem on the graph. The importance of such theorems lies not only in providing rigorous justification for asymptotics, but also in finding the correct asymptotic models, since the choice (or even existence) of such a model is sometimes far from obvious.

3.1 Neumann Laplacian

The case of the Neumann Laplacian is probably the simplest. We assume that a finite graph Γ is C^2 embedded into \mathbb{R}^2 (natural multidimensional generalizations also hold). The "fattened graph" domain Ω_d consists of narrow tubes along the edges joined by some neighborhoods of vertices. The tubes

have width $d \times p(x)$, where p(x) > 0 is a C^1 function on the edge and x is the arc length coordinate. Notice that the width function p is allowed to be discontinuous at the vertices. Each vertex neighborhood is contained in a ball of radius of order $\sim d$ and starshaped with respect to a smaller ball of a radius of the same order of smallness.

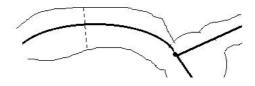


Figure 6: Local structure of Ω_d .

Consider the Schrödinger operator H_d in Ω_d

$$H_d(\mathbf{A}, q) = (\frac{1}{i}\nabla - \mathbf{A}(x))^2 + q(x),$$

where the scalar electric q(x) and vector magnetic $\mathbf{A}(x)$ potentials are defined in a fixed neighborhood of Γ , q is of the Lipschitz class, and \mathbf{A} belongs to C^1 . We impose Neumann conditions on $\partial\Omega_d$.

We also consider the following operator $H(\mathbf{A}, q)$ on Γ (we skip the exact definition):

$$H(\mathbf{A}, q)f(x_j) = -\frac{1}{p} (\frac{d}{dx_j} - iA_j^{\tau}(x))p(\frac{d}{dx_j} - iA_j^{\tau}(x))f + qf,$$

where we use q(x) to denote the restriction of the potential q to Γ and A_j^{τ} is the tangential component of the field \mathbf{A} to the edge e_j of Γ . In order to complete the description of the operator we need to impose some boundary conditions at vertices. These are:

- 1. f is continuous through each vertex.
- 2. at each vertex v

$$\sum_{\{j\mid v\in e_i\}} p_j\left(v\right) \left(\frac{df_j}{dx_j} - iA_j^{\tau} f_j\right) (v) = 0.$$

Here p_j denotes the function that provides the width of the tube along e_j (see the description of the domain above). So, the values $p_j(v)$ at the same vertex can be different for different edges e_j adjacent to v.

The next theorem summarizes some of the results of [123, 124], [156]-[159], [167]:

Theorem 1 For any n = 1, 2, ...

$$\lim_{d\to 0} \lambda_n(H_d(\mathbf{A}, q)) = \lambda_n(H(\mathbf{A}, q)),$$

where λ_n is the n-th eigenvalue counted in increasing order (taking into account multiplicities).

This result shows that the asymptotic behavior of the spectrum of $H_d(\mathbf{A}, q)$ when $d \to 0$ is dictated by the spectrum of the graph operator $H(\mathbf{A}, q)$. A certain kind of resolvent convergence in the case of trees was shown in [163, 164]. Convergence of solutions of the corresponding heat equations in absence of potentials was shown in [86, 87].

3.1.1 Large protrusions at the vertices

We address here the case when the vertex neighborhoods are of radii decaying slower than the width d of the tubes. One can expect that for sufficiently large protrusions at vertices the coupling of different edges might decay and an additional "life at vertices" can arise. The result (and the proof provided in [123]) of Theorem 1 still holds while the exterior and interior sizes of the vertex neighborhoods decay as d^{α} , where $\alpha \in (0.5, 1]$. The situation changes however, when $\alpha < 0.5$. One can understand the threshold value $\alpha = 0.5$ as follows: when $\alpha \in (0.5, 1]$ the area of the tube around an edge behaves as d and hence dominates the area of the vertex neighborhood, which decays as $d^{2\alpha}$. For $\alpha = 0.5$ the two areas have the same order, and when $\alpha < 0.5$ the vertex neighborhood area dominates. In the case when $\alpha < 0.5$ the limit operator does not act in the space $L_2(\Gamma)$ anymore, but rather in some finitedimensional extension of this space that corresponds to vertex states. Let us formulate the corresponding results of [124, 185]. We assume ² that the potentials are equal to zero, the edges are straight, the tubes have thickness 2d, and the vertex neighborhoods are balls of radii d^{α} .

We denote by m the number of vertices and by H_d the negative Neumann Laplacian $-\Delta_{N,d}$ in Ω_d . Consider the space $\mathcal{H} = L_2(\Gamma) \oplus \mathbb{C}^m$ and the operator

²There is little doubt that the results hold in the more general situations considered before in Section 3.1.

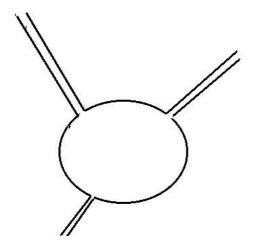


Figure 7: A large protrusion at a vertex.

H on this space that can be described as follows: it acts on $L_2(\Gamma) \oplus \{0\}$ as the negative second derivative along each edge with zero Dirichlet conditions at each vertex, and the whole space $\{0\} \oplus \mathbb{C}^m$ is in the kernel of H.

Theorem 2 ([124, 185]) Let $0 < \alpha < 0.5$, then when $d \to 0$, the spectrum of the operator H_d converges to the spectrum of H.

This theorem shows in particular that in the limit the edges completely decouple, while some additional vertex states arise. This is not that surprising, since in the situation when the protrusions are much larger than the tubes, a particle entering a protrusion from a tube has almost no chance to get back, which in the limit enforces Dirichlet conditions. Besides, states arise that are localized at protrusions, among which only the ground states survive in the limit.

In order to tackle the borderline case $\alpha = 0.5$ one needs to introduce a slightly different operator in the same extended space $\mathcal{H} = L_2(\Gamma) \oplus \mathbb{C}^m$. We will avoid giving the precise description of the operator, since the corresponding spectral problem can be rewritten onto Γ itself, which results in a problem that involves the spectral parameter in the boundary conditions (see the theorem below).

Theorem 3 ([124, 185]) Let $\alpha = 0.5$, then when $d \to 0$ the spectrum of the operator H_d converges to the spectrum of the following problem on the graph:

$$\begin{cases} -\frac{d^2f}{dx_j^2} & = \lambda f & on \ each \ edge \ e_j \\ f & is \ continuous \ through \ each \ vertex \ v_l \\ \sum_{\{j|v_l \in e_j\}} \frac{df}{dx_j}(v_l) & = \frac{\lambda\pi}{2} f(v_l) & at \ each \ vertex \ v_l \end{cases}.$$

3.2 Dirichlet Laplacian

The more difficult problem of convergence of spectra of Dirichlet Laplacians arises in mesoscopic physics (see surveys in [47, 67]). Consider the domain Ω_d which is the parallel strip of width d along a smooth curve Γ (see the picture below).

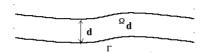


Figure 8: A strip of width d.

One is interested in the behavior of the spectrum of the (negative) Dirichlet Laplacian $-\Delta_{D,d}$ in Ω_d when $d \to 0$. It is easy to see (for instance, on the example of a linear strip) that due to the transversal modes, the spectrum of $-\Delta_{D,d}$ blows up (i.e., its bottom goes to infinity) when $d \to 0$. It is natural hence to shift the spectrum down by the first transversal eigenvalue $\lambda_1 = \left(\frac{\pi}{d}\right)^2$. Changing the coordinates appropriately in order to flatten the strip, one can derive then the following result, which we state in a very general way (the reader should see precise formulation and a survey in [47]):

Theorem 4 [47] The spectrum of $-\Delta_{D,d} - \lambda_1$ converges to the spectrum of the operator

$$-\frac{d^2}{dx^2} - \frac{\gamma(x)^2}{4},\tag{6}$$

where x is the arc length coordinate on Γ and $\gamma(x)$ is the curvature of Γ .

This result is one of the reasons for studying Schrödinger operators with potentials involving curvature (e.g., [63]). It, however, does not translate to the case of a graph Γ easily. Indeed, let us assume for simplicity that the edges are straight. Then one expects to obtain the second arc length derivative along the edges. The question remains whether one can impose some boundary conditions at vertices such that the spectrum of the resulting operator on Γ provides the asymptotics of the (appropriately shifted) spectrum of the Dirichlet Laplacian in a thin neighborhood. As the reader might remember, we have quoted chemistry studies [162] where it was suggested that the right boundary conditions are (5). This conclusion, however, does not seem correct. The first indication that one can expect trouble comes from (6). Indeed, trying to force a smooth curve Γ to turn sharply in order to approximate an angle formed by two rays, one observes that the square of curvature term would lead to the "square of the δ -function" at the corner. Here is another argument: the results of [10, 72, 169] show that if Γ is an angle with straight sides, then the Dirichlet Laplacian has a bound ground state, whose energy and simultaneously its distance from the rest of the spectrum grow to infinity when d tends to zero. This immediately shows that no choice of boundary conditions at vertices can ever make convergence results analogous to Theorems 1 or 4 possible. A close look at heuristic arguments of [162] shows that they implicitly assumed the absence of states confined to vertices, which is exactly what does occur. One can imagine, however, that the limit operator could live on an extension of the space $L_2(\Gamma)$ rather than on Γ itself, the additional components being responsible for the vertex states. In this case, though, the convergence must probably have different meaning for different components of the extension. This program has not yet been implemented.

Besides imposing Dirichlet conditions on the boundary of a narrow strip, one can think of other ways of confining motion to a curve (a graph) Γ . One can add to the governing Hamiltonian a potential cV(x) that grows with the distance from the curve and study the large coupling constant limit $c \to \infty$. Alternatively, one can consider the large coupling constant limit with a deep potential well potential $-c\delta_{\Gamma}(x)$, where δ_{Γ} is the delta function supported on Γ . In the case of a smooth curve (or even a higher dimensional manifold) Γ this was done respectively in [90] and [64, 65, 78, 79]. The graph case (i.e., in presence of vertices) has not been explored.

3.3 Photonic crystals

We will survey here some results of the theory of photonic crystals that are of the nature addressed in this survey. A photonic crystal, first suggested in [107, 183] (see also [106, 117, 146, 165] for surveys of this topic), is a periodic dielectric medium, whose properties with regard to light resemble properties of semi-conductors with respect to electron propagation. governing equation is the Maxwell system in a periodic medium, which serves here as an analog of the Schrödinger operator with periodic potential in the solid state theory. One of the issues of particular interest is the structure of the spectrum of the stationary Maxwell operator in a periodic medium, in particular existence of spectral gaps (which means existence of frequency regions in which electromagnetic waves are not allowed to propagate in the medium). We will concentrate here on the case of 2D photonic crystals, i.e. the ones that are periodic with respect to two variables and homogeneous with respect to the third one. The figure below shows an example of the cross-section of such a medium. Here the dark areas are assumed to be filled with an optically dense dielectric, while the rest is filled with the air (or another dielectric of low optical density).



Figure 9: The crossection of a 2D photonic crystal.

The dielectric constant is assumed to be $\varepsilon(x) = \varepsilon_0 > 1$ in the dark domains of thickness d and $\varepsilon = 1$ (air) in the white ones. The material is assumed to have no magnetic properties, so the magnetic permeability μ equals 1. We will be interested in this paper in the thin high contrast structures, i.e., those where d is small and ε_0 is large. Neither of these two conditions can be easily satisfied in practice with existing optical materials (although the situation might change, for instance in presence of metallic components).

However, acoustic analogs of photonic crystals, which enjoy many similar properties, allow for very high contrast materials. Besides, it has been discovered that in some instances the thin high contrast approximation gives interesting hints to the properties of more realistic media [16, 120, 121].

It is well known [104, 106] that in the 2D case there are two polarizations of the electromagnetic waves: the one where the magnetic field is orthogonal to the plane of periodicity (i.e., the plane of the picture above), and the one where the electric field is directed this way. For monochromatic waves of frequency ω the Maxwell equation for these two polarizations boils down correspondingly to the following spectral problems:

$$-\nabla \cdot \frac{1}{\varepsilon} \nabla H = \lambda H \tag{7}$$

and

$$-\Delta E = \lambda \varepsilon E,\tag{8}$$

where $\lambda = (\omega/c)^2$ and c is the speed of light.

High contrast and thin structure asymptotics $d \to 0$, $\varepsilon_0 d \to \infty$ were considered in [16], [86]-[86], [117, 120, 121, 172] (the more realistic cases of the finite limit of $\varepsilon_0 d$ were treated in [86, 87, 120, 18]). It was discovered that for the H-mode (7) the waves become increasingly "air waves," i.e. tend to concentrate overwhelmingly in the air, and correspondingly the spectrum of (7) asymptotically concentrates in a small vicinity of the spectrum of the Neumann Laplacian on one "air bubble," thus opening large gaps in between. However, the E-mode (8) leads to two distinct types of waves: air waves that behave in a manner essentially similar to the one just described, and dielectric waves that prefer to stay inside the narrow dielectric tubes (due to the total internal reflection) and are evanescent in the air. The latter provide a much more complicated spectrum with a very narrow bands separated by narrow gaps of approximately the same size. One can suspect that the dielectric waves could be governed by an operator living on the graph Γ obtained when the dielectric tubes shrink. This happens to be true.

Theorem 5 [86] After rescaling by multiplying the spectral parameter λ by $\varepsilon_0 d$ (zooming in in order to make the small bands and gaps observable), the spectrum of dielectric modes converges to the spectrum of the problem

$$-\Delta u = \lambda \delta_{\Gamma} u,\tag{9}$$

where δ_{Γ} is the Dirac's delta-function of the graph Γ (i.e. $<\delta_{\Gamma}, \phi>=\int\limits_{\Gamma}\phi dx$).

Although the problem (9) seems to involve the whole plane, its spectrum in fact can be described as the spectrum of the Dirichlet-to-Neumann operator Λ_{Γ} on the graph Γ . Let us remind the reader the construction of this operator. Starting with a function $\phi(x)$ on Γ one uses it as the Dirichlet boundary value to find a harmonic function u on each face of the planar graph Γ (see Fig. 10).

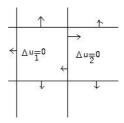


Figure 10: Dirichlet – to – Neuman map.

When such a function u is found, it is automatically continuous through Γ , while its normal derivatives do not have to be continuous. Now one takes the jump across Γ of the normal derivatives of u to get a function $\psi(x)$ on Γ . The "jump" here means the sum of outward normal derivatives of u from the two faces adjacent to a given edge. Now the Dirichlet-to-Neumann operator Λ_{Γ} is the operator transforming ϕ into ψ :

$$\Lambda_{\Gamma}\phi = \psi. \tag{10}$$

In the case when Γ is smooth (i.e., when no vertices are present), Λ_{Γ} coincides up to a smoothing operator with $2\sqrt{-\Delta_{\Gamma}}$ (the full symbols of both operators are the same), where $-\Delta_{\Gamma}$ is the Laplace-Beltrami operator on Γ (i.e., just the second arc length derivative). In particular, the spectra $\sigma(\Lambda_{\Gamma})$ and $\sigma(2\sqrt{-\Delta_{\Gamma}})$ asymptotically coincide for high energies. This also holds in higher dimensions [120]. In sufficiently smooth cases the spectra converge very rapidly (see [120] for this and other related discussions). Since the spectrum of $2\sqrt{-\Delta_{\Gamma}}$ can be immediately calculated, this gives a fast method of approximating the spectrum of $\sigma(\Lambda_{\Gamma})$ and hence the frequency spectrum of the dielectric modes.

The question arises: is there any analog of this approximation in the more realistic case of presence of vertices, i.e. of a non-smooth graph Γ ? Analogously to the smooth case, can one think of Λ_{Γ} as a "pseudo-differential" operator of first order on Γ (whatever this could mean)? Rephrasing the question, one can ask whether there exists a differential spectral problem A of order 2m on the graph such that the 2mth power of Λ_{Γ} is in some sense close to A, and hence $\sigma(\Lambda_{\Gamma}) \approx \sigma(\sqrt[2m]{A})$. There are not that many indications that this should be true, besides that it would be helpful to have such a relation. This study was attempted in [121] with some heuristic analysis. It was discovered that in the case of symmetric junctions at vertices one can sometimes write some reasonable differential operators as candidates for A. Although no theorem about comparison of spectra was proven, the numerical experiments conducted showed strong agreement of spectra. Take for example the case of symmetric triple junctions at the vertices (e.g., honeycomb lattice). Then the analysis of [121] shows that the spectrum of the following problem is a good candidate for the approximation to the spectrum of Λ_{Γ} :

$$\begin{cases}
-\frac{d^2 u_j}{dx_j^2} = \lambda^2 u & \text{on each edge } e_j \\
u \text{ is continuous} & \text{at each vertex } v \\
\sum_{j \in J(v)} \frac{du}{dx_j}(v) = -\left(\frac{3\lambda}{2}\right) \cot \frac{\pi}{3} u(v) & \text{at each vertex } v
\end{cases}$$
(11)

In the case of the honeycomb lattice, this problem can be solved explicitly [121]. The numerics show amazing agreement between the spectra of the two problems. This is especially interesting since the nature of the two spectra can be significantly different: the spectrum of the problem (11) has a pure point part of infinite multiplicity (see [120, 121] and Section 4.4), while the spectrum of Λ_{Γ} was conjectured [117, 120], and then proven [22] to be absolutely continuous.

Another observation of [121] was that in the case of a symmetric quadruple junction at each vertex (square lattice) one needs to employ a fourth order differential problem on the graph Γ , which is also responsible for some observed differences between the spectral behavior of the square and honeycomb Dirichlet-to-Neuman operators [120].

It is not clear at the moment how to make the analysis of [121] rigorous and whether there exists any analog of it for asymmetric vertex junctions.

4 Studies of graph models and some applications

Spectra of the graph models described above have been studied analytically and numerically (see, for instance [12, 14, 16, 22], [32]–[35], [57]–[60], [62, 66, 69], [109]–[111], [120, 121, 125, 135, 166, 175]). These studies have been used in several different ways in order to understand the properties of systems that they approximate. For instance, in [43, 23] for some quantum graphs exact trace formulas were obtained for energy density in terms of periodic classical orbits, results of [112, 113] show that the spectral statistics on complete graphs is well reproduced by random matrix theory, etc. Without trying to survey these applications, we will just provide a few nuggets of such nature.

4.1 Curved wires can bind electrons

Looking at (6) one understands that if the quantum wire Γ is essentially flat except for a bend, the operator (6) is the one-dimensional Schrödinger operator with a potential well $-\gamma^2/4$. This means that one expects bound states to arise. One can show (e.g., [67] and references therein) that a bound state survives also for small non-zero values of the width d of the wire. In fact, it has been shown that this is true for any width d [96]. In other words, bent quantum wires can bind electrons. This conclusion has been verified numerically and experimentally [30, 31]. Analogously, bent quantum walls can create currents confined to their edges [67] (see the figure below).



Figure 11: Electring current along a bent quantum wall.

Analogous observation has been also made for acoustic waveguides [50]. This has lead to a whole "industry" of proving existence and studying properties of bound states arising in domains of tubular type due to local

bends, protrusions, changed boundary conditions, etc. ([7, 28, 30, 31, 47, 48, 49], [54]–[56], [58, 61], [66]–[77], [96, 151]).

In the case of a periodic rather than singly bent curve one naturally expects that the bound states, due to tunneling, will spread into spectral bands, but for a sufficiently narrow tube one expects to preserve spectral gaps. This program was implemented in [184] using a variational approach.

4.2 Photonic band gaps

The main property that would make a photonic crystal useful is existence of a gap in the frequency spectrum of electromagnetic waves propagating in it. That is why the scientists working with photonic crystals have been involved from the start in the search for media with such gaps (e.g., [106, 107, 117, 146, 165, 183]). After some initial failures, firm experimental and numerical evidence of the existence of photonic band gaps in several such structures has been found (see the references above). Mathematically the problem amounts to determining parameters of a periodic dielectric medium such that the corresponding Maxwell operator has a spectral gap (e.g., [117]). The first (and probably still the only) analytic proof of possibility of opening spectral gaps in photonic crystalline materials was obtained in [82, 83] using asymptotic analysis of the type described in Section 3.3 above. See also [88, 101, 172] for similar considerations.

4.3 Opening spectral gaps by "decorating" the graph

Existence of spectral gaps is a favorite question in many areas, most prominently in solid state physics and photonic crystal theory (e.g., [8, 106, 117, 165]). The most common situation when the gaps might arise is in a periodic medium, since according to the Floquet theory (e.g., [116, 117, 150]) the spectrum of an elliptic periodic operator has a natural band-gap structure. There have been indications of a different mechanism that leads to spectral gaps, namely, proliferation in the medium of small scatterers with an internal structure. This has been noticed for systems modeled in \mathbb{R}^n [143, 144] as well as on graphs [14]. However, the simplest and clearest model was probably delivered in the recent paper [168]. It deals with a discrete problem, i.e. graphs are considered as combinatorial objects, functions on graphs take their values at vertices, and the operators of interest are discrete Laplacians or some generalizations thereof. Let us have a graph Γ (considered as a set of

vertices) and a bounded (although the boundedness condition can be relaxed) self-adjoint operator H_0 in $l^2(\Gamma)$, for instance the discrete Laplacian. Here we denote by $l^2(\Gamma)$ the space of square summable functions at the vertices of the graph. Consider an auxiliary **finite** graph Σ with a distinguished vertex v and a self-adjoint operator A in $l^2(\Sigma)$ (for instance a discrete Laplacian). Let us now attach a copy of Σ to each vertex of Γ identifying this vertex with the distinguished vertex v of Σ . In other words, we "decorate" the graph Γ with copies of Σ - "flowers" grown out of each and every vertex of Γ . In Fig. 12 below, the underlying graph Γ is drawn in the plane and the vertically attached pieces are copies of Σ .

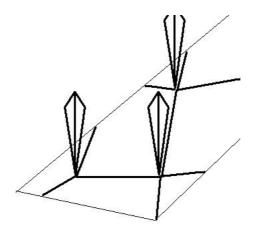


Figure 12: Graph decoration.

The authors of [168] denote the extended graph by $\Gamma \lhd \Sigma$. It is clear that $l^2(\Gamma \lhd \Sigma) = l^2(\Gamma) \otimes l^2(\Sigma)$ and that there is a natural embedding of Γ into $\Gamma \lhd \Sigma$ and hence a natural orthogonal projection P from $l^2(\Gamma \lhd \Sigma)$ onto $l^2(\Gamma)$. One can now define the extended operator

$$H = PH_0P + I \otimes A \tag{12}$$

on $l^2(\Gamma \lhd \Sigma)$. For instance, in the case when both H_0 and A are discrete Laplace operators, so is also H. In order to obtain the best result of [168], one also needs to assume that the delta-function at the distinguished vertex ν of Σ is a cyclic vector for A. We will also denote by Q the orthogonal projection operator in $l^2(\Sigma)$ onto the subspace of functions vanishing at ν .

Theorem 6 The following relation between the spectra of the operators H and H_0 holds:

$$\sigma(H) = \gamma^{-1}(\sigma(H_0)),$$

where γ is the rational function of the form

$$\gamma(\lambda) = \lambda + c + \sum_{j} w_{j} \frac{1}{\lambda - \lambda_{j}},$$

 $\{\lambda_j\}$ is the spectrum of the operator QAQ, and c and w_j are constants. In particular, decoration creates gaps in the spectrum of operator H at locations that depend on the decoration (Σ, ν, A) only.

One can find precise details and extensions of this result in [168]. Here is the main idea of the proof: Studying the spectral problem for H on the decorated graph, one can first solve it on each of the copies of Σ , provided that λ is not in the spectrum of the operator A with Dirichlet condition at ν (i.e., of the operator QAQ). Doing so one replaces the roles of the decoration by an energy-dependent "potential" at each vertex of Γ . This potential is a rational function of λ with poles at $\sigma(QAQ)$, and hence close to these poles it forces the operator to be invertible.

At the first glance the techniques of [168] do not apply to the case of differential (rather than difference) operators on graphs considered in this text, the reasons being for instance the lack of the tensor product structure, absence of formulas like (12), unboundedness of the operators involved, etc. It is possible, however, using an approach from [6] to show that an analog of Theorem 6 still holds for the differential operators on graphs of the sort considered in this survey [118].

It is interesting to mention that there has been at least one instance when without analysis similar to the one done in [168] the effect of decoration was effectively used in engineering, namely the ground plane for cellular phone antennas developed in the UCLA photonic crystals group headed by E. Yablonovitch [173]. Fig. 13 shows this ground plane, which is essentially a metallic plate with little metallic "mushrooms" grown on it.

Its main feature is that at certain frequencies of electromagnetic waves the plate turns into an insulator, i.e. a frequency gap arises. It seems that

³One can notice that this procedure involves the "Dirichlet to Neumann" operator on the decoration Σ with the distinguished point considered to be the boundary.

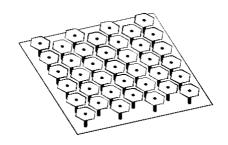


Figure 13: UCLA ground plane.

this effect is in direct relation with the decoration mechanism described in this section.

4.4 Confinement of waves in purely periodic media

There is a general understanding that probably came first from solid state physics (e.g., [8]) that one cannot confine a wave in a periodic medium, i.e. that the corresponding periodic operators of mathematical physics have no pure point spectrum. In physics terms this means absence of bound states. To be precise, one is talking here about elliptic operators with periodic coefficients, with one of the main examples being the Schrödinger operator with a periodic potential $-\Delta + V(x)$. Other periodic operators of interest include, for instance, Maxwell operator or divergence—type second order operators (it is known that bound states do occur for operators of higher orders [116]). Starting with [177], the problem of absence of bound states in periodic media has been attracting intense interest of researchers, with major advancements occurring in the last several years (see for instance [21, 89, 117, 122] for surveys, references, and recent advances).

One can also consider from this point of view differential and pseudodifferential operators of the type discussed above on periodic graphs and ask the same question: can a pure point spectrum (i.e., a bound state) arise? Let us look first at second order differential problems on graphs with conditions (4). It is easy to observe that there are resonant situations when one can have compactly supported eigenfunctions that look like sinusoidal waves running around a cycle in the graph [120] (see also [16, 117, 121]). This happens when the lengths of edges in the cycle are commensurable. Surprisingly enough, this had been overlooked in some previous physics studies of such systems. One should notice that this effect takes place essentially for any choice of boundary conditions at the vertices. What about the Dirichlet-to-Neumann operator (10) on a periodic graph that arises in the study of photonic crystals? Because of non-locality of the operator, it seemed unlikely that such states would exist. On the other hand, numerical analysis of certain geometries (for instance, of the honeycomb structure) suggested that "bound states" confined to cycles might exist [120]. Some analysis of this effect was done in [120] and it was conjectured [117, 120] that these are not actual bound states, but strong resonances, so that the spectrum of the Dirichlet-to-Neumann operator on a periodic graph is in fact absolutely continuous. This conjecture was proven in [22, 174]. We remind the reader that existence of bound states is crucial for applications like enhancement of spontaneous emission and lasing and that they are usually created by introducing impurities into an otherwise purely periodic medium. One can think that the resonance (slowly leaking) states mentioned above could be used for similar purposes. This is exactly what was done in experimental studies for spontaneous emission enhancement [24] and for lasing [103]. In both cases photonic crystals with no impurities were used and the leaky modes were employed in the ways impurity states usually are. It needs to be noted that this was done with no knowledge of the mathematical analysis of the problem indicated in this section.

4.5 Opening spectral gaps for long waves

The general rule of thumb (which is also the basis of homogenization theory, see [19]) is that long waves in a medium periodic with a small period "do not notice" the periodic variations and essentially behave as in a "homogenized" medium. In particular, no spectral gaps should open in the long wave (i.e., low frequency) region. Analysis done in [82, 83] of high contrast thin photonic crystal structures shows that one can open spectral gaps for arbitrarily long waves without increasing the characteristic sizes of the structure. In fact, similar observation was used in creating the UCLA ground plane mentioned above [173].

4.6 Scattering problems

Significant attention has been paid to direct and inverse scattering theory on graphs [1, 5, 12, 54, 93, 94, 109, 110, 111, 126, 130, 140, 145] (see also

[138]-[140] for scattering on combinatorial graphs). The reader can find the up to date survey of the available results in [126]. The situation in general terms looks as follows. Consider a Schrödinger operator on a finite (i.e. with a finite number of edges) metric graph. Assume that m of the graph's edges are of infinite length (i.e., one deals with a compact graph with a finite number of infinite leads attached). Then one can define in a natural way the $m \times m$ scattering matrix S(k). When the graph is a simple star structure of infinite edges attached at the vertex, then it has been shown that natural inverse problems can be resolved: recovery of the potentials from known scattering matrix and vertex conditions and recovery of the boundary conditions from known scattering matrix and potentials [93, 94, 109, 110, 111. In the general case one can also consider the problem of recovering the topological and the metric structure of the graph. It was shown, however, in [126] on examples of simplest topologically non-trivial graphs (a loop with two leads attached) that in general none of the inverse problems listed above has a unique solution. This means that either additional information for the unique solvability of the inverse problem needs to be introduced, or the class of graphs should be limited. For instance, it was conjectured in [126] that if one requires that the graph has no automorphisms that keep the infinite leads fixed, then the inverse scattering problem must have a unique solution (here one should understand automorphisms in a metric rather than purely combinatorial sense).

The inverse eigenvalue problem on compact graphs was considered in [33, 34].

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