

Quantum graphs: II. Some spectral properties of quantum and combinatorial graphs

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2005 J. Phys. A: Math. Gen. 38 4887

(<http://iopscience.iop.org/0305-4470/38/22/013>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.92

The article was downloaded on 03/06/2010 at 03:46

Please note that [terms and conditions apply](#).

Quantum graphs: II. Some spectral properties of quantum and combinatorial graphs

Peter Kuchment

Department of Mathematics, Texas A&M University, College Station, TX, USA

E-mail: kuchment@math.tamu.edu

Received 31 October 2004, in final form 30 December 2004

Published 18 May 2005

Online at stacks.iop.org/JPhysA/38/4887

Abstract

The paper deals with some spectral properties of (mostly infinite) quantum and combinatorial graphs. Quantum graphs have been intensively studied lately due to their numerous applications to mesoscopic physics, nanotechnology, optics and other areas. A Schnol-type theorem is proven that allows one to detect that a point λ belongs to the spectrum when a generalized eigenfunction with a sub-exponential growth integral estimate is available. A theorem on spectral gap opening for ‘decorated’ quantum graphs is established (its analogue is known for the combinatorial case). It is also shown that if a periodic combinatorial or quantum graph has a point spectrum, it is generated by compactly supported eigenfunctions (‘scars’).

PACS numbers: 02.10.Ab, 02.30.Jr, 05.45.Mt

Mathematics Subject Classification: 35Q, 35P, 05C

1. Introduction

We will use the name ‘quantum graph’ for a graph considered as a one-dimensional singular variety and equipped with a self-adjoint differential ‘Hamiltonian’, e.g. [10, 19, 26, 37]. Such objects naturally arise as simplified models in mathematics, physics, chemistry and engineering, in particular when one needs to consider wave propagation through a ‘mesoscopic’ quasi-one-dimensional system that looks like a thin neighbourhood of a graph. One can mention among the variety of areas of applications of quantum graphs the free-electron theory of conjugated molecules, quantum chaos, mesoscopic physics (circuits of quantum wires), waveguide theory, nanotechnology, dynamical systems and photonic crystals. We will not discuss any details of these origins of quantum graphs, referring the reader instead to [10, 12, 19, 20, 23, 25–29, 32–34, 37] for further information, recent surveys and literature.

In this paper, which is a continuation of [26], we present some results concerning spectra of quantum graphs, as well as of their combinatorial counterparts. While the (combinatorial)

spectral graph theory has been around for quite some time [4–6], the spectral theory of quantum graphs has not yet been developed well enough (see the collection [37] for recent developments and literature).

Let us describe the contents of the paper. The next section introduces the necessary notions concerning quantum graphs. Section 3 contains a Schnol–Bloch-type theorem. Such theorems show how the existence of a generalized eigenfunction with some control on its growth (e.g., bounded) allows one to claim that the corresponding point of the real axis is in fact in the spectrum (or to estimate its distance from the spectrum). Section 4 deals with opening gaps in the spectrum of a quantum graph by ‘decorating’ the graph by an additional graph attached to each vertex. Section 5 discusses point spectra of periodic quantum graphs. It is shown that the corresponding eigenspaces are generated by compactly supported eigenfunctions. The results of all the sections have their counterparts in the combinatorial setting as well.

It is interesting to note relations of the presented results with their counterparts for PDEs. The Schnol-type theorem is parallel to the classical one known for PDEs [8, 15, 40], except for the integral formulation that we adopt, which extends its applicability. The resonant gap opening procedure works to some extent for PDEs as well [36], but it is less clear and less studied there. Finally, the discussion of the bound states for periodic problems does not make much sense for PDEs, since periodic second-order elliptic operators with ‘reasonable’ coefficients have absolutely continuous spectrum¹.

The reader should note that although all the essential ingredients of the proofs are presented, due to size limitations the proofs are condensed and in some cases provided under some additional restrictions that can be removed. A more detailed exposition will appear elsewhere.

2. Quantum graphs

A *graph* Γ (see figure 1) consists of a finite or countably infinite set of vertices $V = \{v_i\}$ and a set $E = \{e_j\}$ of edges connecting the vertices². Each edge e can be identified with a pair (v_i, v_k) of vertices. Loops and multiple edges between vertices are allowed. *The degree (valence) d_v of a vertex v* is the number of edges containing the vertex and is assumed to be finite and positive.

Definition 1. A *graph* Γ is said to be a *metric graph*, if its each edge e is assigned a positive length $l_e \in (0, \infty)$.³

Each edge e will be identified with the segment $[0, l_e]$ of the real line, which introduces a coordinate x_e along e . In most cases we will denote the coordinate by x , omitting the subscript. A metric graph Γ can be equipped with a natural metric $\rho(x, y)$ and thus considered as a metric space. The graph is not assumed to be embedded into a Euclidean space or a more general Riemannian manifold. In some applications (e.g., in modelling quantum wire circuits) such a natural embedding exists, and then the coordinate x is usually the arc length. In some other cases (e.g., in quantum chaos), no embedding is assumed. All graphs under the consideration are *connected*.

We will also assume that the following additional condition is satisfied:

¹ Although this statement is not yet proven in complete generality, in many cases it has been established (e.g., [3, 13] and references therein).

² In this text we will be mostly interested in infinite graphs.

³ Sometimes edges of infinite length are allowed in quantum graphs. This is for instance the case when one considers scattering problems.

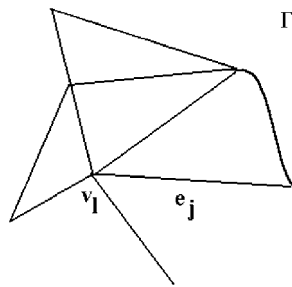


Figure 1. Graph Γ .

Condition A. The lengths of all the edges are bounded below and above by finite positive constants: $l_e \in [l_0, L]$ for some $l_0 > 0$, $L < \infty$.

Condition A obviously matters for graphs with infinitely many edges only. One can obtain some results without this condition as well, but we will not address this issue here.

Now one imagines a metric graph Γ as a one-dimensional variety, with each edge equipped with a smooth structure, and with singularities at the vertices:

The reader should note that the points of a metric graph are not only its vertices, as is normally assumed in the combinatorial setting, but all intermediate points x on the edges as well. So, while a function on a combinatorial graph is defined on the set V of its vertices, functions $f(x)$ on a quantum graph Γ are defined along the edges (including the vertices). One can naturally define the Lebesgue measure dx on the graph.

We will sometimes assume that a *root* vertex o is singled out (the results will not depend on the choice of the root). If this is done, one can define a ‘norm’ $\rho(x)$ of a point x as

$$\rho(x) = \rho(o, x).$$

This allows us to define for any $r \geq 0$ the *ball* B_r of *radius* r :

$$B_r = \{x \in \Gamma \mid \rho(x) \leq r\}.$$

The last step that is needed to finish the definition of a quantum graph is to introduce a differential Hamiltonian on Γ . The operators of interest in the simplest cases are the second arc length derivative

$$f(x) \rightarrow -\frac{d^2 f}{dx^2}, \quad (1)$$

or a more general Schrödinger operator

$$f(x) \rightarrow \left(\frac{1}{i} \frac{d}{dx} - A(x) \right)^2 f(x) + V(x)f(x). \quad (2)$$

Here x denotes the coordinate x_e along each edge e .⁴

Higher order differential and even pseudo-differential operators arise as well (see, e.g., the survey [25] and references therein). We, however, will concentrate here on second-order differential operators only.

In order for the definition of these self-adjoint Hamiltonians operators to be complete, one needs to describe their domains. For reasonable classes of potentials (e.g., measurable and bounded), the natural conditions require that f belongs to the Sobolev space $H^2(e)$ on each

⁴ Note that in order to introduce the magnetic operators, one needs the graph’s edges to be directed. This is not required in the absence of the magnetic potential.

edge e . One, however, clearly also needs to impose boundary value conditions at the vertices. These have been studied and described completely using both the standard extension theory of symmetric operators, as well as the symplectic geometry approach [11, 16, 19, 26, 32–34]. The simplest one is the so-called Neumann condition⁵

$$\begin{cases} f & \text{is continuous at each vertex } v \\ \sum_{v \in e} \frac{df}{dx_e}(v) = 0 & \text{at each vertex } v. \end{cases} \quad (3)$$

3. Schnol–Bloch theorems

Schnol-type theorems in PDEs ([40], see also [8, 15, 22, 41]) treat the following question. If there exists a nonzero L_2 -solution of the equation $Hu = \lambda u$, then clearly λ is a point of the point spectrum of H . Is there a similar test for detecting that λ belongs to the whole spectrum? Imagine that one has a solution (a generalized eigenfunction) of a self-adjoint equation $Hu = \lambda u$, and that one has some control of the growth of this solution (e.g., it is bounded). When can one guarantee that λ is a point of the spectrum of H ? For the Schrödinger equation in \mathbb{R}^n with a potential bounded from below, the standard Schnol theorem [8, 15, 40] says that existence of a sub-exponentially growing solution implies that $\lambda \in \sigma(H)$. A version of this theorem is known in solid-state physics as the Bloch theorem [1, 22, 38]: if H is a periodic Schrödinger operator, then existence of a bounded eigenfunction corresponding to a point λ guarantees that $\lambda \in \sigma(H)$. On the other hand, for the hyperbolic plane Laplace–Beltrami operator Δ_H , there is an infinite-dimensional space of bounded solutions of $\Delta_H u = 0$. Indeed, using the Poincaré unit disk model of the hyperbolic plane, one has $\Delta_H = (1 - |z|^2)^2 \Delta$, where Δ is the Euclidean Laplacian (see, e.g., section 4 of the introduction in [17], or any other book on hyperbolic geometry). Thus, all bounded harmonic functions u on the unit disk (which form an infinite-dimensional space) satisfy the equation $\Delta_H u = 0$. However, the point 0 is still not in the spectrum of Δ_H (e.g., [31]). This happens due to the exponential growth of the volume of the hyperbolic ball of radius r . A similar Schnol-type theorem here would need to request some decay of the generalized eigenfunction. The purpose of this section is to establish a Schnol–Bloch-type theorem for graphs.

Let Γ be a rooted connected infinite quantum graph satisfying the condition A and equipped with the Hamiltonian $-\frac{d^2}{dx^2}$ and any self-adjoint vertex conditions⁶.

Theorem 2 (a Schnol-type theorem). *Let the graph Γ satisfy the above conditions and $\lambda \in \mathbb{R}$. If there exists a function $\phi(x)$ on Γ that belongs to the Sobolev space H^2 on each edge, satisfies all vertex conditions, the equation*

$$-\frac{d^2\phi}{dx^2} = \lambda\phi \quad \text{for a.e. } x \in \Gamma, \quad (4)$$

and the sub-exponential growth condition

$$\int_{B_r} |\phi(x)|^2 dx \leq C_\epsilon e^{\epsilon r} \quad (5)$$

for any $\epsilon > 0$, then $\lambda \in \sigma(H)$.

This theorem implies in particular the following:

⁵ This name seems to be more appropriate than the often used name Kirchhoff condition; in particular for vertices of degree 1 one obtains the standard Neumann condition. Such conditions mean that the quantum probability currents at each vertex add up to zero.

⁶ More general Schrödinger operators can be treated similarly; see the remark after the theorem.

Corollary 3 (a Bloch-type theorem). *Let the graph Γ satisfy conditions of the theorem and be of a sub-exponential growth (i.e., the volume of B_r grows sub-exponentially). If there exists a bounded solution of the equation (4), then $\lambda \in \sigma(H)$.*

Simple examples show that existence of a bounded solution does not guarantee that $\lambda \in \sigma(H)$, if the graph is of exponential growth (i.e., a regular tree of degree 3 or higher).

Proof of theorem 2. Let us define for any $r > 0$ the following compact subset Γ_r of the graph: it consists of all points of the edges with both ends in B_r . The following inclusions hold:

$$\Gamma_{r-L} \subset B_r \subset \Gamma_{r+L}. \tag{6}$$

We hence conclude that the integral sub-exponential growth condition (5) holds if one replaces B_r by Γ_r . Let us introduce the function

$$J(r) := \int_{\Gamma_r} |\phi(x)|^2 dx. \tag{7}$$

Given an $\epsilon > 0$, one can find a sequence $r_k \rightarrow \infty$ such that

$$J(r_k + L) \leq e^\epsilon J(r_k),$$

otherwise one gets a contradiction with the sub-exponential growth condition. We remind the reader that each set Γ_r consists of complete edges only.

Let $\theta(x)$ be any smooth function on $[0, l_0/4]$ such that it is identically equal to 1 in a neighbourhood of 0 and identically equal to zero close to $l_0/4$. Here l_0 is the lower bound for the lengths of all edges of Γ , which was assumed to be strictly positive. We define a cut-off function θ_k on Γ . It is equal to 1 on Γ_{r_k} and to 0 on all edges which do not have vertices in Γ_{r_k} . We only need to define it along the edges that have exactly one vertex in Γ_{r_k} . Let e be an edge whose one vertex v is contained in Γ_{r_k} . The function θ_k is defined to be equal to 1 along e starting from v till the middle of the edge, then it is continued by an appropriately shifted copy of $\theta(x)$ (which by construction will become zero at least at the distance $l_e/4$ from the end of the edge), and stays zero after that. Note that due to the construction, any derivative of the functions $\theta_k(x)$ is uniformly bounded with respect to k and $x \in \Gamma$. Besides, these functions are identically equal to 1 or 0 around any vertex.

We can now construct a sequence of approximate eigenfunctions $\phi_k(x)$ of the operator H as follows:

$$\phi_k(x) = \theta_k(x)\phi(x).$$

One can note that the functions $\phi_k(x)$ satisfy the same boundary conditions that ϕ did, since the factors θ_k are identically equal to 1 or 0 around the vertices. This implies that $\phi_k(x)$ belongs to the domain of H in $L^2(\Gamma)$. Besides, we clearly have

$$\|\phi_k\|^2 \geq J(r_k). \tag{8}$$

One also notes that the functions ϕ_k are supported in Γ_{r_k+L} .

Let us now apply $H - \lambda$ to these test functions:

$$(H - \lambda)\phi_k = \theta_k(-\phi'' - \lambda\phi) - 2\theta'_k\phi' - \theta''_k\phi = -2\theta'_k\phi' - \theta''_k\phi. \tag{9}$$

We have used here that ϕ satisfies (4).

Using the properties of the cut-off functions θ_k , one gets

$$\|(H - \lambda)\phi_k\|^2 \leq C \int_{x \in \text{supp } \theta'_k} (|\phi(x)|^2 + |\phi'(x)|^2) dx. \tag{10}$$

Since the supports of the derivatives θ'_k belong to the interiors of the edges and are at a qualified distance from the vertices, we have standard Schauder estimates for

$$\int_{x \in \text{supp } \theta'_k} |\phi'(x)|^2 dx$$

by for instance the integral

$$\int_{\rho(x) \in [r_k + \frac{l_0}{4}, r_k + L - \frac{l_0}{4}]} |\phi(x)|^2 dx.$$

This leads to the estimate

$$\begin{aligned} \|(H - \lambda)\phi_k\|^2 &\leq C \int_{\rho(x) \in [r_k + \frac{l_0}{4}, r_k + L - \frac{l_0}{4}]} |\phi(x)|^2 dx \\ &\leq C(J(r_k + L) - J(r_k)) \leq C(e^\epsilon - 1)J(r_k) \leq C(e^\epsilon - 1)\|\phi_k\|^2, \end{aligned} \quad (11)$$

where the constant C does not depend on k, ϵ . Since $\epsilon > 0$ was arbitrary, we conclude that $\lambda \in \sigma(H)$. \square

Remark 4.

1. If one has a generalized eigenfunction that satisfies (5) for some fixed ϵ , rather than an arbitrary one as in the theorem, one cannot conclude that $\lambda \in \sigma(H)$. However, it is easy to modify the proof to estimate from above its distance $\text{dist}(\lambda, \sigma(H))$ to the spectrum, which when $\epsilon \rightarrow 0$ will reproduce the statement of the theorem.
2. The same result holds for more general Hamiltonians, e.g. for Schrödinger operators $-\frac{d^2}{dx^2} + q(x)$ with bounded from below potentials $q(x) \geq q_0 > -\infty$ and any self-adjoint vertex conditions.
3. Analogous results, with essentially the same (a little bit simpler) proofs hold for discrete operators on infinite combinatorial graphs as well. One can note then the relation of the Schnol-type theorems to the amenability properties of discrete groups and graphs (e.g., the Følner condition) and to the notion of infinite Ramanujan graphs.

The author will provide details concerning these remarks elsewhere.

4. Spectral gaps created by graph decorations

Existence of spectral gaps is known to be one of the spectral features of high interest in the various fields ranging from solid-state physics to photonic crystal theory, to waveguides, to theory of discrete groups and graphs. A standard way of trying to create spectral gaps is to make a medium periodic (e.g., [1, 22, 23, 38]). This is why most photonic crystal structures that are being created are periodic. However, periodicity neither guarantees existence of gaps (except in the 1D case), nor does it allow any easy control of gap locations or sizes, nor is it a unique way to achieve spectral gaps. It has been noted by several researchers (the first such references known to the author are [35, 36]) that spreading small geometric scatterers throughout the medium (not necessarily in a periodic fashion) might lead to spectral gaps as well. This has been confirmed on quantum graph models in [2, 9], and finally made very clear and precise in the case of combinatorial graphs in [39]. It was proposed in [39] that a simple procedure of ‘decorating’ a graph leads to a very controllable gap structure. We will show here that up to some caveat, the same procedure works in the case of quantum graphs. Let us describe the decoration procedure of [39] adopted to the quantum graph situation.

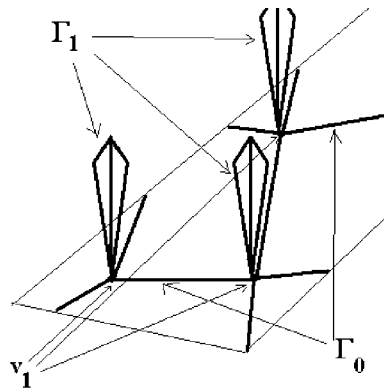


Figure 2. Decoration of a quantum graph Γ_0 by Γ_1 .

Let Γ_0 be a quantum graph satisfying the condition A and such that the corresponding Hamiltonian is the negative second derivative along the edges with the Neumann conditions (3) at the vertices⁷. Let also Γ_1 be a *finite* connected quantum graph with the same type of the Hamiltonian, with any self-adjoint vertex conditions. The graph Γ_1 will be our ‘decoration.’ We assume that a root vertex v_1 is singled out in Γ_1 . The decoration procedure works as follows: the new graph Γ is obtained by attaching a copy of Γ_1 to each vertex v of Γ_0 and identifying v_1 with v (see figure 2). Note that there is a natural embedding $\Gamma_0 \subset \Gamma$. We will denote by V, V_0 and V_1 the vertices sets of Γ, Γ_0 and Γ_1 correspondingly. The Hamiltonian H on Γ is defined as the negative second derivative on each edge, with the Neumann conditions at each vertex of Γ_0 (including the former v_1 vertices of the decorations) and the initially assumed conditions on $V_1 \setminus v_1$, repeated on each attached copy of the decoration.

Dirichlet eigenvalues of each edge (which are clearly directly related to the edge length spectrum) often play an exceptional role in quantum graph considerations (see the discussions below). Let $\{l_j\}$ be the lengths of the edges of the original graph Γ_0 . Then we define the *Dirichlet spectrum* σ_D of Γ_0 as the closure of the set

$$\bigcup_{n \in (\mathbb{Z} \setminus \{0\}, j)} \{ \pi^2 n^2 / l_j^2 \} \subset \mathbb{R}.$$

If the graph Γ_0 is finite, no closure is required.

Let us also define the operator H_1 on the decoration graph Γ_1 that acts as the negative second derivative on each edge and satisfies the self-adjoint conditions assumed before on $V_1 \setminus v_1$ and zero Dirichlet condition at v_1 .

We can now state the result of this section, which was previously announced in [24, 27]. The conditions of the theorem can be weakened, but we consider for brevity the simplest case here, which seems already rather useful.

Theorem 5. *Let $\lambda_0 \in \mathbb{R} \setminus \sigma_D$ be a simple eigenvalue of H_1 with the eigenfunction ψ such that the sum of the derivatives of ψ at v_1 along all outgoing edges is not zero. Then there is a punctured neighbourhood of λ_0 that does not belong to the spectrum $\sigma(H)$ of Γ .*

Proof. We will prove here the theorem for the case of a finite graph Γ_0 only. The case of an infinite graph is a little bit more technical and will be considered elsewhere. The proof consists of removing the decorations and replacing them by altered vertex conditions. This is

⁷ More general conditions can also be considered.

done simultaneously and in the same way at each vertex $v \in V_0 \subset V$, so we will describe it for one vertex v , which will be identified with $v_1 \in \Gamma_1$.

Let us define a function that we will call Dirichlet-to-Neumann function $\Lambda(\lambda)$ for Γ_1 .⁸ It is defined in a punctured neighbourhood of λ_0 not intersecting σ_D as follows. If $\lambda \neq \lambda_0$ is a regular point of H_1 , one can uniquely solve the problem

$$\begin{cases} -u'' = \lambda u & \text{on each edge of } \Gamma_1 \\ u & \text{satisfies the prescribed boundary conditions on } V_1 \setminus v_1 \\ u(v_1) = 1. \end{cases} \quad (12)$$

We denote by $\Lambda(\lambda)$ the sum of the outgoing derivatives of the solution $u(x)$ at the vertex v_1 . □

Lemma 6. *Under the conditions of the theorem, the Dirichlet-to-Neumann function $\Lambda(\lambda)$ is analytic in a punctured neighbourhood of λ_0 , with a first-order pole (with nonzero residue) at λ_0 .*

Proof of the lemma. Let ψ be the eigenfunction of H_1 assumed in the statement of the theorem. We denote by $\Psi \neq 0$ the sum of outgoing derivatives of ψ at v_1 . Let also f be a function on Γ_1 defined as follows: it is supported in a small neighbourhood of the vertex v_1 (so small that it does not contain other vertices of Γ_1), is equal to 1 near v_1 , and is smooth inside the edges. We also denote by $R_{H_1}(\lambda) = (H_1 - \lambda)^{-1}$ the resolvent of H_1 . Then we can represent the solution u of (12) as $\tilde{u} + f$, where

$$\begin{aligned} \tilde{u} &= -R_{H_1}(\lambda)(-f'' - \lambda f) \\ &= -(\lambda - \lambda_0)^{-1} \langle -f'' - \lambda f, \psi \rangle_{L_2(\Gamma)} \psi(x) + A(\lambda) \\ &= -(\lambda - \lambda_0)^{-1} \Psi \psi(x) + A(\lambda). \end{aligned}$$

Here $A(\lambda)$ is analytic in a neighbourhood of λ_0 . Noting that the sums of the outgoing derivatives at v_1 of both functions u and \tilde{u} on Γ_1 are the same, we see that $\Lambda(\lambda)$ has a first-order pole at λ_0 with a nonzero residue. This proves the lemma.

Let now λ_0 be as in the theorem. Suppose that $u(x)$ is an eigenfunction of H corresponding to an eigenvalue λ close to λ_0 . For any vertex $v \in V_0$, we can solve the equation $Hu = \lambda u$ on the decoration attached to v , using $u(v)$ as the Dirichlet data. Then the sum of outgoing derivatives of u at v along the edges of the decoration is equal to $\Lambda(\lambda)u(v)$. Hence, the eigenfunction equation for u on Γ can be rewritten on Γ_0 solely as follows:

$$\begin{cases} -u'' = \lambda u & \text{on each edge of } \Gamma_0 \\ u & \text{is continuous at all vertices } v \in V_0 \\ \sum_{v \in e} \frac{du}{dx_e}(v) = -\Lambda(\lambda)u(v). \end{cases} \quad (13)$$

We will show now that (13) is impossible for a nonzero function u , if λ is close to λ_0 . Indeed, with λ being at a positive distance from the Dirichlet spectrum σ_D of all edges, standard estimates give

$$\sum_{e \in \Gamma_0} \|u\|_{H^2(e)}^2 \leq C \sum_{v \in V_0} |u(v)|^2. \quad (14)$$

Now the Sobolev trace theorem implies

$$\sum_{\{e \in \Gamma_0, v \in V_0 | v \in e\}} \left| \frac{du}{dx_e}(v) \right|^2 \leq C \sum_{v \in V_0} |u(v)|^2. \quad (15)$$

⁸ This is in fact the Dirichlet-to-Neumann map for Γ_1 , if v_1 is considered as this graph's boundary.

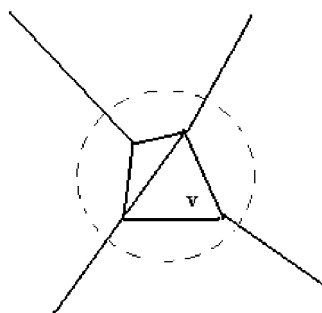


Figure 3. A 'spider' decoration.

Since $\Lambda(\lambda)$ has a pole at λ_0 , for λ and λ_0 sufficiently close, we get a contradiction between (15) and the last equality of (13). \square

Remark 7.

1. As was mentioned above, the proofs for the infinite case will be provided elsewhere.
2. The proof shows that the decorations attached to each vertex do not have to be the same in order to achieve spectral gaps. One only needs to guarantee a uniform blow-up of all the Dirichlet-to-Neumann functions at each vertex when $\lambda \rightarrow \lambda_0$. One can also provide some estimates of the size of the gap.
3. This theorem claims that spectral gaps are guaranteed to arise around the spectrum of the decoration (with the Dirichlet condition at the attachment point v_1), unless one deals with the Dirichlet spectrum of Γ_0 . Simple examples show that on the Dirichlet spectrum one cannot guarantee a gap. For instance, if Γ_0 contains a cycle consisting of edges of equal (or commensurate) lengths, then the decoration procedure cannot remove the eigenvalues that correspond to the sinusoidal waves running around this loop (see figure 4). However, a modification of the decoration procedure works even in the presence of Dirichlet spectrum. One just needs to introduce some 'fake' vertices along the edges at appropriate locations and attach the decorations at these new vertices as well. This will be described in detail elsewhere.
4. One can create gaps by a different decoration procedure rather than that of [39] described above. Namely, instead of attaching sideways the little 'flowers' (or 'kites,' as they were called in [39]) as in figure 2, one could incorporate an internal structure into each vertex, putting a little 'spider' there as shown in figure 3. This graph decoration procedure was probably used explicitly for the first time in [2] (see also [9]) for the same purpose of gap creation. It will be shown elsewhere how gaps can be created using this construction (the Dirichlet spectrum plays a distinguished role there as well).

5. Bound states on periodic graphs

It is 'well known' (albeit still not proven for the most general case) that elliptic periodic second-order operators in \mathbb{R}^n have no point spectrum⁹. In fact, their spectra are absolutely continuous. In the case of Schrödinger operators with periodic electric potentials, this constituted the celebrated Thomas' theorem [44] (see also [22, 38]). There has been a significant progress in

⁹ This is not true for higher order operators [22].

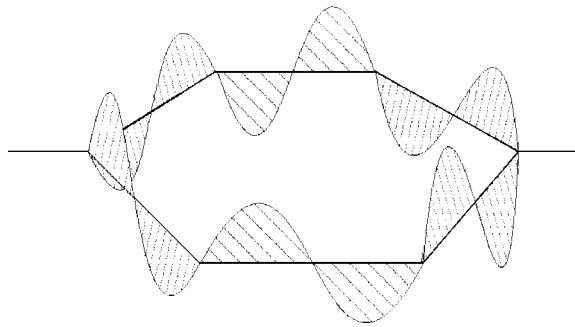


Figure 4. A loop bound state.

the last decade towards proving this for the general case. One can find the description of the status of this statement for the general elliptic periodic operators in [3, 13, 23, 30]. The validity of this theorem is intimately related to the uniqueness of continuation property (that is why it fails for higher order operators), which does not hold on graphs. It is well known that bound states, and even compactly supported eigenfunctions can easily be found in combinatorial and quantum graphs, whether periodic or not. If, for instance, the quantum graph has a cycle with commensurate lengths of the edges, one can easily create a sinusoidal wave supported on this loop only (see figure 4). The question arises whether any other causes exist besides compactly supported eigenfunctions, for appearance of the pure point spectrum on periodic graphs. It has been shown previously by the author [21] that in the case of combinatorial periodic graphs, existence of bound states implies existence of the compactly supported ones. In fact, the eigenfunctions with compact support generate the whole eigenspace. We will show here that the same holds true for periodic quantum graphs as well.

One should note that a point spectrum can arise for different reasons on graphs that are not periodic, e.g. on trees. For instance, one can have bound states on infinite trees with sufficiently fast-growing branching number [43].

We will consider an infinite combinatorial or quantum graph Γ with a faithful co-compact action of the free abelian group $G = \mathbb{Z}^n$ (i.e., the space of G -orbits is a compact graph).

Let us treat the combinatorial case first, so let Γ be a combinatorial graph and A a G -periodic finite difference (not necessarily self-adjoint) operator of a finite order acting on $l_2(V)$. Here, as before, V is the set of vertices of Γ . The first half of the following result is proven in [21]:

Theorem 8. *If the equation $Au = 0$ has a nonzero $l_2(V)$ solution, then it has a nonzero compactly supported solution. Moreover, the compactly supported solutions form a complete set in the space of all l_2 -solutions.*

Since this formulation is more complete than that in [21], we provide its brief proof here.

Proof. We will need to use the basic transform of Floquet theory (e.g., [22, 38]). Namely, for any compactly supported (or sufficiently fast decaying) function $u(v)$ on V , we define its Floquet transform

$$u(v) \mapsto \hat{u}(v, z) = \sum_{g \in \mathbb{Z}^n} u(gv)z^g, \quad (16)$$

where gv denotes the action of $g \in \mathbb{Z}^n$ on the point $v \in V$, $z = (z_1, \dots, z_n) \in (\mathbb{C} \setminus 0)^n$, and $z^g = z_1^{g_1} \times \dots \times z_n^{g_n}$. We will also denote $\hat{u}(v, z)$ by $\hat{u}(z)$, where the latter expression is a

function on W depending on the parameter z . Here W is a (finite) fundamental domain of the action of the group $G = \mathbb{Z}^n$ on V . Note that images of the compactly supported functions are exactly all finite Laurent series in z with coefficients in $\mathbb{C}^{|W|}$.

We will also need the unit torus

$$\mathbb{T}^n = \{z \in \mathbb{C}^n \mid |z_j| = 1, j = 1, \dots, n\} \subset \mathbb{C}^n.$$

It is well known and easy to establish [21, 22, 38] that the transform (16) extends to an isometry (up to a possible constant normalization factor) between $l_2(V)$ and $L_2(\mathbb{T}^n, \mathbb{C}^{|W|})$.

After this transform, A becomes the operator of multiplication in $L_2(\mathbb{T}^n, \mathbb{C}^{|W|})$ by a rational $|W| \times |W|$ matrix function $A(z)$. This means that nonzero l_2 -solutions of $Au = 0$ are in one-to-one correspondence with $\mathbb{C}^{|W|}$ -valued L_2 -functions \hat{u} on \mathbb{T}^n such that $A(z)\hat{u}(z) = 0$ a.e. on \mathbb{T}^n . Since we assumed that u , and hence \hat{u} is not a zero element of l_2 , we can conclude that the set of points of the torus \mathbb{T}^n over which the matrix $A(z)$ has a non-trivial kernel, has a positive measure. On the other hand, this set in \mathbb{C}^n is given by the algebraic equation $\det A(z) = 0$ and thus is algebraic. The only way it can intersect the torus over a subset of a positive measure is that it coincides with the whole space \mathbb{C}^n . Hence, $A(z)$ has a nonzero kernel at any point z . Thus, its determinant is identically equal to zero. Considering this matrix over the field \mathcal{Q} of rational functions, one can apply the standard linear algebra statement that claims existence of a nonzero rational solution $\phi(z)$ of $A(z)\phi(z) = 0$. As indicated before, such functions before the Floquet transform were compactly supported solutions of $Au = 0$. This proves the first statement of the theorem, about the existence of compactly supported eigenfunctions.

To prove completeness, we need to do a little bit more work. Let us denote by $Q_1(z), \dots, Q_r(z)$ a finite set of the generators of all nonzero polynomial (vector-valued) solutions of $A(z)Q(z) = 0$ (it is known to exist, e.g. [18 lemma 7.6.3, chapter VII]). Floquet transform reduces the completeness statement we need to prove to the following: \square

Lemma 9. Combinations

$$y(z) = \sum_{j=1, \dots, r} a_j(z) Q_j(z), \tag{17}$$

where $a_j(z)$ are finite Laurent sums, are L_2 -dense in the space of all $\mathbb{C}^{|W|}$ -valued L_2 -solutions of the equation

$$A(z)y(z) = 0. \tag{18}$$

Proof of the lemma. First of all, any $L_2(\mathbb{T}^n)$ -function a_j can be approximated by a finite Laurent sum. Indeed, this is done by taking finite partial sums of the Fourier series of a_j on the torus \mathbb{T}^n . So, it is sufficient to approximate any L_2 -solution $y(z)$ of (18) by sums (17) with L_2 coefficients a_j . Let $k > 0$ be the minimal (over $z \in \mathbb{C}^n$ or $z \in \mathbb{T}^n$, which is the same) dimension of $\text{Ker } A(z)$. The set $B \subset \mathbb{T}^n$ of points z where $\dim \text{Ker } A(z) > k$ is an algebraic variety of codimension at least 2, and hence has zero measure on \mathbb{T}^n . Hence, it is sufficient to do L_2 approximation outside of small neighbourhoods of B . Let $z_0 \in \mathbb{T}^n \setminus B$ and U be a sufficiently small neighbourhood of z_0 not intersecting B . Then over (a complex neighbourhood of) U the kernels $\text{Ker } A(z)$ form a trivial holomorphic vector bundle. Let $f_i(z)$ be a basis of holomorphic sections of this bundle. Then the portion of y over U can be represented as $\sum b_l(z) f_l(z)$ with L_2 -functions b_l . Now, one uses (18 lemma 7.6.3, chapter VII) again to see that sums (17) with analytic a_j approximate the sections f_i . This proves the lemma and hence the theorem. \square

The following observation is standard:

Proposition 10. *If the periodic operator A is self-adjoint, then its spectrum has no singular continuous part.*

Indeed, the singular continuous part is excluded for such periodic operators by the standard well-known argument (e.g., [14, 44], or the proof of theorem 4.5.9 in [22]).

Now the case of quantum graphs can be reduced to the combinatorial one, similarly to the way described in [26].

Theorem 11. *Let Γ be a $G = \mathbb{Z}^n$ -periodic (in the meaning already specified) quantum graph equipped with the second derivative Hamiltonian and arbitrary vertex conditions at the vertices. Then, existence of a nonzero L_2 -eigenfunction corresponding to an eigenvalue λ implies existence of a compactly supported eigenfunction, and the set of compactly supported eigenfunctions is complete in the eigenspace. If the vertex conditions are self-adjoint, the spectrum of the Hamiltonian has no singular continuous part.*

Proof. The first step is to make sure that λ stays away from the Dirichlet spectrum σ_D , which in the case we consider is discrete. If by any chance $\lambda \in \sigma_D$, one can introduce ‘fake’ additional vertices of degree 2 on the edges of the fundamental domain of the graph and then repeat them periodically in such a way that the Dirichlet eigenvalues of the new shorter edges will avoid λ . If one imposes Neumann conditions at these new vertices, their introduction does not influence the operator at all. So, we can assume from the start that λ is not in σ_D . Let now F be an L_2 -eigenfunction. Since we are away from the Dirichlet spectrum σ_D , resolvent and trace estimates analogous to those in the proof of the previous theorem show that the vector $f = \{F(v)\}$ of the vertex values belongs to $l_2(V)$ if and only if $F \in L_2(\Gamma)$. Since λ is not in σ_D , by solving the boundary value problem for the eigenfunction equation $HF = \lambda F$ on each edge separately in terms of the boundary values of F , we can express the derivatives of F at each vertex in terms of its vertex values f solely. Thus, boundary conditions (which involve the values of F and of its vertex derivatives) lead to a periodic finite-order difference equation $Af = 0$ on the combinatorial counterpart of the quantum graph. Theorem 8 claims existence and completeness of combinatorial compactly supported solutions. Reversing the procedure (which is possible since we are not on the Dirichlet spectrum), we conclude existence and completeness of compactly supported eigenfunctions of the quantum graph.

The part about the absence of singular continuous spectrum is standard (as for the combinatorial graphs). \square

Remark 12. Compactly supported eigenfunctions on graphs are sometimes called ‘scars.’

Acknowledgments

The author thanks M Aizenman, R Carlson, P Exner, R Grigorchuk, S Novikov, H Schenck, J Schenker and R Schrader for relevant information and M Solomyak and the reviewers for useful comments about the manuscript. This research was partly sponsored by the NSF through the Grants DMS 9610444, 0072248, 0296150, and 0406022. The author expresses his gratitude to NSF for this support. The content of this paper does not necessarily reflect the position or the policy of the federal government and no official endorsement should be inferred.

References

- [1] Ashcroft N W and Mermin N D 1976 *Solid State Physics* (New York: Holt, Rinehart and Winston)
- [2] Avron J, Exner P and Last Y 1994 Periodic Schrödinger operators with large gaps and Wannier–Stark ladders *Phys. Rev. Lett.* **72** 869–99
- [3] Sh Birman M and Suslina T A 2000 A periodic magnetic Hamiltonian with a variable metric. The problem of absolute continuity *Algebra i Analiz* **11** no. 2 pp 1–40
Sh Birman M and Suslina T A 2000 *St. Petersburg Math. J.* **11** 203–32 (Engl. Transl.)
- [4] Chung F 1997 *Spectral Graph Theory* (Providence, RI: American Mathematical Society)
- [5] Colin de Verdière Y 1998 *Spectres De Graphes* (Paris: Societe Mathematique De France)
- [6] Cvetkovic D, Doob M and Sachs H 1979 *Spectra of Graphs* (New York: Academic)
- [7] Cvetkovic D, Doob M, Gutman I and Targasev A 1988 *Recent Results in the Theory of Graph Spectra* (*Ann. Disc. Math.* vol 36) (Amsterdam: North-Holland)
- [8] Cycon H L, Froese R G, Kirsch W and Simon B 1987 *Schrödinger Operators with Applications to Quantum Mechanics and Global Geometry* (*Texts and Monographs in Physics*) (Berlin: Springer)
- [9] Exner P 1995 Lattice Kronig–Penney models *Phys. Rev. Lett.* **74** 3503–6
- [10] Exner P and Šeba P 1989 Electrons in semiconductor microstructures: a challenge to operator theorists *Schrödinger Operators, Standard and Nonstandard* (*Dubna 1988*) (Singapore: World Scientific) pp 79–100
- [11] Exner P and Šeba P 1989 Free quantum motion on a branching graph *Rep. Math. Phys.* **28** 7–26
- [12] Figotin A and Kuchment P 1998 Spectral properties of classical waves in high contrast periodic media *SIAM J. Appl. Math.* **58** 683–702
- [13] Friedlander L 1990 On the spectrum of a class of second order periodic elliptic differential operators *Commun. Partial Differ. Eq.* **15** 1631–47
- [14] Gerard C and Nier F 1998 The Mourre theory for analytically fibered operators *J. Funct. Anal.* **152** 202–19
- [15] Glazman I M 1965 *Direct Methods of Qualitative Spectral Analysis of Singular Differential Operators* (*Jerusalem: Isr. Progr. Sci. Transl.*)
- [16] Harmer M 2000 Hermitian symplectic geometry and extension theory *J. Phys. A: Math. Gen.* **33** 9193–203
- [17] Helgason S 1984 *Groups and Geometric Analysis* (New York: Academic)
- [18] Hörmander L 1966 *An Introduction to Complex Analysis in Several Variables* (Princeton, NJ: Van Nostrand)
- [19] Kostykin V and Schrader R 1999 Kirchhoff’s rule for quantum wires *J. Phys. A: Math. Gen.* **32** 595–630
- [20] Kottos T and Smilansky U 1997 Quantum chaos on graphs *Phys. Rev. Lett.* **79** 4794–97
- [21] Kuchment P 1991 To the Floquet theory of periodic difference equations *Geometrical and Algebraical Aspects in Several EditEl Complex Variables, (Cetraro, Italy, June 1989)* ed C Berenstein and D Struppa 203–9
- [22] Kuchment P 1993 *Floquet Theory for Partial Differential Equations* (Basle: Birkhäuser)
- [23] Kuchment P 2001 The mathematics of photonics crystals *Mathematical Modeling in Optical Science* ed G Bao, L Cowsar and W Masters (Philadelphia, PA: SIAM) pp 207–72
- [24] Kuchment P 2003 Differential and pseudo-differential operators on graphs as models of mesoscopic systems *Analysis and Applications* ed H Begehr, R Gilbert and M W Wang (Dordrecht: Kluwer) pp 7–30
- [25] Kuchment P 2002 Graph models of wave propagation in thin structures *Waves Random Media* **12** R1–R24
- [26] Kuchment P 2004 Quantum graphs: I. Some basic structures *Waves Random Media* **14** S107–S128
- [27] Kuchment P 2004 On some spectral problems of mathematical physics *Partial Differential Equations and Inverse Problems* (*Contemp. Math.* vol 362) ed C Conca, R Manasevich, G Uhlmann and M S Vogelius (Providence, RI: American Mathematical Society) pp 241–76
- [28] Kuchment P and Kunyansky L 1999 Spectral properties of high contrast band-gap materials and operators on graphs *Exp. Math.* **8** 1–28
- [29] Kuchment P and Kunyansky L 2002 Differential operators on graphs and photonic crystals *Adv. Comput. Math.* **16** 263–90
- [30] Kuchment P and Levendorskii S 2002 On the structure of spectra of periodic elliptic operators *Trans. AMS* **354** 537–69
- [31] Lang S 1985 $SL_2(\mathbb{R})$ (New York: Springer)
- [32] Novikov S 1997 Schrödinger operators on graphs and topology *Russ. Math. Surv.* **52** 177–8
- [33] Novikov S 1999 Discrete Schrödinger operators and topology *Asian Math. J.* **2** 841–53
- [34] Novikov S 1999 *Schrödinger Operators on Graphs and Symplectic Geometry* (*Fields Inst. Commun.* vol 24) *The Arnoldfest (Toronto, ON, 1997)* (Providence, RI: American Mathematical Society) pp 397–413
- [35] Pavlov B S 1984 A model of zero-radius potential with internal structure *Theor. Math. Phys.* **59** 544–80
- [36] Pavlov B S 1987 The theory of extensions and explicitly solvable models *Russ. Math. Surv.* **42** 127–68
- [37] Kuchment P (ed) 2004 Quantum graphs and their applications, *Waves Random Media* **14** (1) S1–185
- [38] Reed M and Simon B 1978 *Methods of Modern Mathematical Physics* vol 4 (New York: Academic)
- [39] Schenker J and Aizenman M 2000 The creation of spectral gaps by graph decoration *Lett. Math. Phys.* **53** 253

-
- [40] Schnol E 1957 On the behavior of eigenfunctions of the Schrödinger equation *Mat. Sbornik* **42** 273–86
 - [41] Shubin M A 1992 Spectral theory of elliptic operators on non-compact manifolds, methodes semi-classiques, vol I (Nantes, 1990) *Asterisque* **207** 35–108
 - [42] Shubin M A 1999 Spectral theory of elliptic operators on non-compact manifolds: qualitative results *Spectral Theory and Geometry (Edinburgh, 1998) (London Math. Soc. Lect. Ser. vol 273)* (Cambridge: Cambridge University Press) pp 226–83
 - [43] Solomyak M 2004 On the spectrum of the Laplacian on regular metric trees *Waves Random Media* **14** S155–S171
 - [44] Thomas L E 1973 Time dependent approach to scattering from impurities in a crystal *Commun. Math. Phys.* **33** 335–43