Periodic quantum graphs with asymptotically predefined spectral gaps

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Published in Journal of Physics A: Mathematical and Theoretical, 48(25) (2015), 255201
Outline of the talk

- Preliminaries
  - Quantum graphs
  - Spectrum of periodic operators and spectral gaps
  - Previous results on spectral gaps

- Main results
Quantum graph is a pair $(\Gamma, \mathcal{H})$, where $\Gamma$ is a network-shaped structure of vertices connected by edges ("metric graph", see figure) and $\mathcal{H}$ is a second order self-adjoint differential operator on $\Gamma$ ("Hamiltonian").
Notations:
- $V_\Gamma$ – the set of vertices of $\Gamma$
- $\mathcal{E}_\Gamma$ – the set of edges of $\Gamma$
- $l_e$ – the length of $e \in \mathcal{E}_\Gamma$
- $x_e \in [0, l_e]$ – the local coordinate on $e \in \mathcal{E}_\Gamma$

Let $u : \Gamma \to \mathbb{C}$, $e \in \mathcal{E}_\Gamma$. We denote by $u_e$ the restriction of $u$ onto $e$. Using a coordinate $x_e$ we identify $u_e$ with a function on $(0, l_e)$. 
The Hamiltonian $\mathcal{H}$ is a second order self-adjoint differential operator, which is determined by differential operations on the edges and certain interface conditions at the vertices.
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**Examples of operations**

\[
\begin{align*}
u &\mapsto -\frac{d^2 u}{dx^2}, \\
f &\mapsto -\frac{d^2 u}{dx^2} + V(x)u, \\
u &\mapsto -\frac{1}{b(x)} \frac{d}{dx} \left( a(x) \frac{du}{dx} \right), \ldots
\end{align*}
\]
The **Hamiltonian** $\mathcal{H}$ is a second order self-adjoint differential operator, which is determined by differential operations on the edges and certain interface conditions at the vertices.

### Examples of operations

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- $f \mapsto -\frac{d^2 u}{dx^2} + V(x)u$,
- $u \mapsto -\frac{1}{b(x)} \frac{d}{dx} \left( a(x) \frac{du}{dx} \right)$, ...  

### Examples of interface conditions at $v \in \mathcal{V}_\Gamma$ (for $\mathcal{H} = -\frac{d^2}{dx^2}$)

- $u$ is continuous at $v$,  
  $\sum_{e \in \mathcal{E}_\Gamma(v)} \frac{du_e}{dx_e} = 0$  
  (Kirchhoff conditions)
- $u$ is continuous at $v$,  
  $\sum_{e \in \mathcal{E}_\Gamma(v)} \frac{du_e}{dx_e} = \alpha u$, $\alpha \in \mathbb{R}$  
  ($\delta$-coupling)
- $\sum_{e \in \mathcal{E}_\Gamma(v)} \frac{du_e}{dx_e} = 0$,  
  $\frac{du_e}{dx_e} - \frac{du_e'}{dx_e'} = \beta (u_e - u_e')$, $\beta \in \mathbb{R}$  
  ($\delta'$-coupling)

Here $\mathcal{E}_\Gamma(v)$ is a set of edges emanating from $v$, $x_e = 0$ at $v$ for $e \in \mathcal{E}_\Gamma(v)$. 
The metric graph $\Gamma \subset \mathbb{R}^d$ is periodic (or $\mathbb{Z}^n$-periodic) if it is invariant under translations through linearly independent vectors $e_1, \ldots, e_n$:

$$\Gamma = \Gamma + e_j, \quad j = 1, \ldots, n.$$ 

The Hamiltonian $\mathcal{H}$ on a periodic metric graph $\Gamma$ is said to be periodic if it commutes with the operators $T_j, \ j = 1, \ldots, n$,

$$(T_j u)(x) := u(x + e_j)$$
Let \((\Gamma, \mathcal{H})\) be a periodic quantum graph.

The Floque-Bloch theory says that the spectrum of \(\mathcal{H}\) has a band structure, i.e. the spectrum is a locally finite union of compact intervals called bands.

The open interval \((\alpha, \beta)\) is called a gap if \((\alpha, \beta) \cap \sigma(\mathcal{H}) = \emptyset\) and \(\alpha, \beta \in \sigma(\mathcal{H})\).
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In general the presence of gaps in the spectrum of periodic Hamiltonians is not guaranteed.

Example: If \(\Gamma\) is a rectangular lattice and \(\mathcal{H}\) is defined by the operation \(-d^2/dx^2\) on its edges and the Kirchhoff conditions at the vertices then \(\sigma(\mathcal{H}) = [0, \infty)\).
Decorated graphs

**Example**: given a graph $\Gamma_0$ we “decorate” it attaching to each vertex of $\Gamma_0$ a copy of certain graph $\Gamma_1$, the obtained graph we denote by $\Gamma$. The gaps open up in the spectrum of the operator $\mathcal{H}$ defined by the operation $-\frac{d^2}{dx^2}$ on the edges of $\Gamma$ and the Kirchhoff conditions at its vertices.

* B.-S. Ong, PhD thesis, Texas A&M University, 2006 (“spider” decorations)
Preliminaries
How to create periodic quantum graphs with spectral gaps?

Decorated graphs

**Example**: given a graph $\Gamma_0$ we “decorate” it attaching to each vertex of $\Gamma_0$ a copy of certain graph $\Gamma_1$, the obtained graph we denote by $\Gamma$. The gaps open up in the spectrum of the operator $\mathcal{H}$ defined by the operation $-\frac{d^2}{dx^2}$ on the edges of $\Gamma$ and the Kirchhoff conditions at its vertices.

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Change of Kirchhoff conditions by more “advanced” ones

**Example**: let $\Gamma$ be a rectangular lattice and $\mathcal{H}$ be defined by the operation $-\frac{d^2}{dx^2}$ on its edges and $\delta$ coupling at the vertices with $\alpha \neq 0$. Then the spectrum of $\mathcal{H}$ has infinitely many gaps provided $\alpha \neq 0$ and the lengths of edges satisfies some mild assumptions.

Main results

The graph $\Gamma$

$\Gamma$ is a $\mathbb{Z}^n$-periodic metric graph (with compact period cell)

$\{Y_{ij}, \ i \in \mathbb{Z}^n, \ j = 1, \ldots, m\}$ is a family of compact graphs satisfying $Y_{ij} \approx Y_{0j}, \ \forall j$

$\Gamma := \Gamma_0 \cup \left( \bigcup_{i,j} Y_{ij} \right)$

$\nu_{ij} := Y_{ij} \cap \Gamma_0$
Let $\varepsilon > 0$ be a small parameter.
Main results

Hamiltonian $H_\varepsilon$

Let $\varepsilon > 0$ be a small parameter. The operator $H_\varepsilon$ acts on edges as follows:

$$(H_\varepsilon u)_e = -\varepsilon^{-1} \frac{d^2 u_e}{dx_e^2}, \ e \in \mathcal{E}_\Gamma.$$ 

At vertices $v \in \mathcal{V}$ the functions from its domain satisfy

\begin{align*}
\forall v \notin \bigcup_{i,j} \{v_{ij}\} : \\
&\begin{align*}
&\text{• } u \text{ is continuous in } v, \\
&\text{• } \sum_{e \in \mathcal{E}_\Gamma(v)} \frac{du_e}{dx_e} = 0
\end{align*}
\end{align*}

\begin{align*}
\forall v = v_{ij} : \\
&\begin{align*}
&\text{• } \text{the limiting value of } u(x) \text{ as } x \to v_{ij} \text{ along } e \in \mathcal{E}_\Gamma(v_{ij}) \cap \Gamma_0 \text{ is independent of } e. \text{ We denote this value by } u_0(v_{ij}) \\
&\text{• } \text{the limiting value of } u(x) \text{ as } x \to v_{ij} \text{ along } e \in \mathcal{E}_\Gamma(v_{ij}) \cap Y_{ij} \text{ is independent of } e. \text{ We denote this value by } u_j(v_{ij}) \\
&\text{• } \sum_{e \in \mathcal{E}_\Gamma(v) \cap \Gamma_0} \frac{du_e}{dx_e} = - \sum_{e \in \mathcal{E}_\Gamma(v) \cap Y_{ij}} \frac{du_e}{dx_e} = q_j \varepsilon (u_0(v) - u_j(v)),
\end{align*}
\end{align*}

where $q_j$ are positive constants.
For \( j = 1, \ldots, m \) we set:

\[
l_j := \sum_{e \in \mathcal{E}_\Gamma \cap \mathcal{Y}_{0j}} l_e.
\]
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$$l_j := \sum_{e \in \mathcal{E} \cap \mathcal{Y}_{0j}} l_e.$$ 

For $j = 1, \ldots, m$ we set:

$$a_j := \frac{q_j}{l_j}.$$ 

It is assumed that the numbers $a_j$ are pairwise non-equivalent. We renumber them in the ascending order: $a_j < a_{j+1}, \forall j = 1, \ldots, m - 1$. 

We consider the following equation (with unknown $\lambda \in \mathbb{C}$):

$$1 + m \sum_{i=1}^{m} q_i l_i (\lambda l_i - q_i) = 0,$$

where $l_0$ is a total length of edges belonging to the period cell of $\mathcal{G}_0$. This equation has exactly $m$ roots $b_j$ satisfying (after appropriate renumbering) $a_j < b_j < a_j + 1, \forall j = 1, \ldots, m - 1, a_m < b_m < \infty$. 

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Periodic quantum graphs with asymptotically predefined spectral gap
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where $l_0$ is a total length of edges belonging to the period cell of $\Gamma_0$. This equation has exactly $m$ roots $b_j$ satisfying (after appropriate renumbering)

$$a_j < b_j < a_{j+1}, \quad j = 1, \ldots, m - 1, \quad a_m < b_m < \infty.$$
Main results
Convergence theorem

Theorem 1

Let $L > 0$ be an arbitrary number. Then the spectrum of the operator $H_\varepsilon$ in $[0, L]$ has the following structure for $\varepsilon$ small enough:

$$\sigma(H_\varepsilon) \cap [0, L] = [0, L] \setminus \bigcup_{j=1}^{m} (a_j(\varepsilon), b_j(\varepsilon)),$$

where the endpoints of the intervals $(a_j(\varepsilon), b_j(\varepsilon))$ satisfy the relations

$$\lim_{\varepsilon \to 0} a_j(\varepsilon) = a_j, \quad \lim_{\varepsilon \to 0} b_j(\varepsilon) = b_j, \quad j = 1, \ldots, m.$$
Above we have defined the map

\[ \mathcal{L} : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}^m \times \mathbb{R}^m, \quad (q_1, \ldots, q_m; l_1, \ldots, l_m) \mapsto (a_1, \ldots, a_m; b_1, \ldots, b_m), \]

\[ \text{dom}(\mathcal{L}) = \left\{ (q; l) \in \mathbb{R}^m \times \mathbb{R}^m : q_j > 0, \ l_j > 0, \ \frac{q_{j+1}}{l_{j+1}} > \frac{q_j}{l_j} \right\}. \]
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\[ \text{dom}(\mathcal{L}) = \left\{ (q; l) \in \mathbb{R}^m \times \mathbb{R}^m : q_j > 0, l_j > 0, \frac{q_{j+1}}{l_{j+1}} > \frac{q_j}{l_j} \right\}. \]

**Theorem 2**

The map \( \mathcal{L} \) maps \( \text{dom}(\mathcal{L}) \) onto the set

\[ \left\{ (a; b) \in \mathbb{R}^m \times \mathbb{R}^m : a_j < b_j < a_{j+1}, j = 1, \ldots, m - 1, a_m < b_m < \infty \right\}. \]

Moreover \( \mathcal{L} \) is one-to-one and the inverse map \( \mathcal{L}^{-1} \) is given by

\[ q_j = a_j l_0 \frac{b_j - a_j}{a_j} \prod_{i=1, m | i \neq j} \left( \frac{b_i - a_j}{a_i - a_j} \right), \]

\[ l_j = l_0 \frac{b_j - a_j}{a_j} \prod_{i=1, m | i \neq j} \left( \frac{b_i - a_j}{a_i - a_j} \right). \]
Main results
Proof ingredients

- Floque-Bloch theory and Neumann-Dirichlet bracketing
- Convergence theorems for monotonically increasing sequence of forms [B. Simon, J. Funct. Anal. 28 (1978)]
- Some algebra
Thank you for your attention!