Spectral gaps of periodic quantum graphs

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In memoriam Hagen Neidhardt

A talk at the conference Operator Theory and Krein Spaces
Vienna, December 20, 2019
We knew each other for quite a long time
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This drawing comes from the QMath2 conference proceedings, about 31 years ago
And we enjoyed doing mathematics together
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I rush to add that sometimes even more involved than indicated here
Quantum graphs

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![Diagram of a metric graph]

We associate with the graph the Hilbert space $\mathcal{H} = \bigoplus_j L^2(e_j)$ and consider the operator $H$ acting on $\psi = \{\psi_j\}$ that are locally $H^2$ as

$$H\psi = \{-\psi''\} \quad \text{or more generally} \quad H\psi = \{(-i\psi' - A\psi)^2 + V\psi\}$$
Vertex coupling

To make such an $H$ a self-adjoint operator we have to match the functions $\psi_j$ properly at each graph vertex.
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To make such an $H$ a *self-adjoint operator* we have to match the functions $\psi_j$ properly at each graph vertex. Denoting $\psi = \{\psi_j\}$ and $\psi' = \{\psi'_j\}$ the boundary values of functions and (outward) derivatives at a given vertex of degree $n$, respectively:

$$
(U - I)\psi(v_k) + i(U + I)\psi'(v_k) = 0,
$$

where $U$ is any $n \times n$ unitary matrix.

Such a coupling depends on $n^2$ real parameters; the number is reduced if we require continuity at the vertex, then we are left with $\psi_j(0) = \psi_k(0) =: \psi(0)$, $j, k = 1, \ldots, n$, and

$$
\sum_{j=1}^n \psi'_j(0) = \alpha \psi(0),
$$

depending on a single parameter $\alpha \in \mathbb{R}$ which we call the $\delta$ coupling; the corresponding unitary matrix is $U = 2n + i\alpha J - I$, where $J$ is the $n \times n$ matrix whose all entries are equal to one.

In particular, the case with $\alpha = 0$ is often called Kirchhoff coupling.
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As consequence, the spectrum of a *periodic* quantum graph with the said commensurability property is *not* purely absolutely continuous.
Quantum graphs spectra, continued

In fact, spectrum of a periodic graph *may not be ac at all*. An example is provided as sketched below:

\[
\begin{align*}
\psi_j \mapsto &-D^2 \psi_j \\
D := &-i \nabla - A,
\end{align*}
\]

with a \(\delta\)-coupling at the vertices. If \(A_j = m + \frac{1}{2}\) for all \(j \in \mathbb{Z}\) and some \(m \in \mathbb{Z}\), the spectrum consists of infinitely degenerate eigenvalues only.


P.E.: Spectral gaps of periodic graphs

OTKR Vienna

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with the fiber operator \( H(\theta) \) acting on \( L^2(Q) \), where \( Q \subset \mathbb{R}^d \) is *period cell* and \( Q^* \) is the *dual cell* (or *Brillouin zone*).
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How many gaps are open?

Concerning the first question, recall first that for the ‘usual’ Schrödinger operators the dimension is known to be decisive:
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Question: How the situation looks for quantum graphs which can ‘mix’ different dimensionalities? The standard reference, [Berkolaiko-Kuchment'13, loc.cit.], says that Bethe-Sommerfeld heuristic reasoning is applicable again, however, the finiteness of the gap number is not a strict law.
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![Graph decoration diagram](https://via.placeholder.com/150)

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![Graph decoration diagram](image)

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Thus, instead of ‘not a strict law’, the question rather is whether *it is a ‘law’ at all*: do infinite periodic graphs having a *finite nonzero* number of open gaps exist?
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Thus, instead of ‘not a strict law’, the question rather is whether *it is a ‘law’ at all*: do infinite periodic graphs having a *finite nonzero* number of open gaps exist? From obvious reasons we would call them *Bethe-Sommerfeld graphs*
The answer depends on the vertex coupling

Recall that self-adjointness requires the matching conditions $(U - I)\psi + i(U + I)\psi' = 0$, where $\psi, \psi'$ are vectors of values and derivatives at the vertex of degree $n$ and $U$ is an $n \times n$ unitary matrix.
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The condition can be decomposed into Dirichlet, Neumann, and Robin parts corresponding to eigenspaces of \(U\) with eigenvalues \(-1, 1,\) and the rest, respectively; if the latter is absent we call such a coupling scale-invariant.
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Theorem

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Worse than that, there is a heuristic argument showing in a ‘typical’ periodic graph the probability of being in a band or gap is $\neq 0, 1$.


The existence

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It is sufficient, of course, to demonstrate an example. With this aim we are going to revisit the model of a *rectangular lattice graph* with a $\delta$ *coupling* in the vertices introduced in

Spectral condition

A number $k^2 > 0$ belongs to a gap iff $k > 0$ satisfies the gap condition which is easily derived; it reads

$$2k \left[ \tan \left( \frac{ka}{2} - \frac{\pi}{2} \left\lfloor \frac{ka}{\pi} \right\rfloor \right) + \tan \left( \frac{kb}{2} - \frac{\pi}{2} \left\lfloor \frac{kb}{\pi} \right\rfloor \right) \right] < \alpha \quad \text{for } \alpha > 0$$

and

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Note that for $\alpha < 0$ the spectrum extends to the negative part of the real axis and may have a gap there, which is not important here because there is not more than a single negative gap, and this gap always extends to positive values.
What is known about this model

The spectrum depends on the ratio $\theta = \frac{a}{b}$. If $\theta$ is rational, $\sigma(H)$ has clearly infinitely many gaps unless $\alpha = 0$ in which case $\sigma(H) = [0, \infty)$.

The same is true if $\theta$ is an irrational well approximable by rationals, which means equivalently that in the continued fraction representation $\theta = [a_0; a_1, a_2, ...]$ the sequence $\{a_j\}$ is unbounded.

On the other hand, $\theta \in \mathbb{R}$ is badly approximable if there is a $c > 0$ such that $|\theta - \frac{p}{q}| > \frac{c}{q^2}$ for all $p, q \in \mathbb{Z}$ with $q \neq 0$.

Let us turn now to the question about the gaps number. We can answer it for any $\theta$ but for the purpose of this talk we limit ourselves with the example of the 'worst' irrational, $\theta = \frac{\sqrt{5+1}}{2} = [1; 1, 1, ...]$. 
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The golden mean situation

Theorem

Let \( \frac{a}{b} = \theta = \frac{\sqrt{5} + 1}{2} \), then the following claims are valid:

(i) If \( \alpha > \frac{\pi^2}{\sqrt{5}a} \) or \( \alpha \leq -\frac{\pi^2}{\sqrt{5}a} \), there are infinitely many spectral gaps.

(ii) If

\[
-\frac{2\pi}{a} \tan\left(\frac{3 - \sqrt{5}}{4} \pi \right) \leq \alpha \leq \frac{\pi^2}{\sqrt{5}a},
\]

there are no gaps in the positive spectrum.

Corollary

The above theorem about the existence of BS graphs is valid.

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The golden mean situation

Theorem

Let \( \frac{a}{b} = \theta = \frac{\sqrt{5}+1}{2} \), then the following claims are valid:

(i) If \( \alpha > \frac{\pi^2}{\sqrt{5}a} \) or \( \alpha \leq -\frac{\pi^2}{\sqrt{5}a} \), there are infinitely many spectral gaps.

(ii) If
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(iii) If
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-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a} \tan \left( \frac{3 - \sqrt{5}}{4} \pi \right),
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The above theorem about the existence of BS graphs is valid.

More about this example

The window in which the golden-mean lattice has the BS property is narrow, it is roughly $4.298 \lesssim -\alpha a \lesssim 4.414$. 

We are also able to control the number of gaps in the BS regime; in the same paper the following result was proved:

Theorem

For a given $N \in \mathbb{N}$, there are exactly $N$ gaps in the positive spectrum if and only if $\alpha$ is chosen within the bounds

$-\frac{2}{\pi} \left( \theta^2(N+1) - \theta - 2(N+1) \right) \sqrt{5} \tan \left( \frac{\pi}{2} \theta - 2(N+1) \right) \leq \alpha < -\frac{2}{\pi} \left( \theta^2 N - \theta - 2N \right) \sqrt{5} \tan \left( \frac{\pi}{2} \theta - 2N \right)$.

Note that the numbers $A_j = 2 \pi \left( \theta^2 j - \theta - 2j \right) \sqrt{5} \tan \left( \frac{\pi}{2} \theta - 2j \right)$ form an increasing sequence the first element of which is $A_1 = 2 \pi \tan \left( 3 - \frac{\sqrt{5}}{4} \pi \right)$ and $A_j < \pi \sqrt{5}$ holds for all $j \in \mathbb{N}$. 

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Meaning of the vertex coupling

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Consider a magnetic Schrödinger operator in the sketched network with *Neumann boundary*. Choosing properly the scalar and vector potentials as functions of $\varepsilon$ and $\beta < \frac{1}{13}$, one can approximate any vertex coupling in the *norm-resolvent sense* as $\varepsilon \to 0$.

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An alternative is to take a *pragmatic approach* and to look which particular coupling would suit a given physical model
Modeling anomalous Hall effect

The *Hall effect*, classical and quantum, is nowadays well understood. This is not the case for the anomalous Hall effect which occurs without the presence of a magnetic field. Recently a quantum-graph model of the AHE was proposed in which the material structure of the sample is described by a lattice of $\delta$-coupled rings (topologically equivalent to a rectangular lattice).


There is a flaw in the model: to mimic the rotational motion of atomic orbitals responsible for the magnetization, the requirement was imposed 'by hand' that the electrons move only one way on the loops of the lattice. Naturally, this cannot be justified from the first principles.
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On the other hand, it *is* possible to break the time-reversal invariance, not at graph edges but in its *vertices*.

For a vertex coupling $U$, the on-shell $S$-matrix at the momentum $k$ is

$$S(k) = k - 1 + (k+1)U_k + 1 + (k-1)U_k,$$

in particular, we have $U = S(1)$. The 'maximum rotation' at $k = 1$ is thus achieved with

$$U = \begin{pmatrix}
0 & 1 & 0 & 0 & \cdots \\
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$$(\psi_{j+1} - \psi_j) + i(\psi'_{j+1} + \psi'_j) = 0, \quad j \in \mathbb{Z} \pmod{N},$$

which is non-trivial for $N \geq 3$ and obviously non-invariant w.r.t. the reverse in the edge numbering order.
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For such a star-graph Hamiltonian we obviously have $\sigma_{\text{ess}}(H) = \mathbb{R}_+$. It is also easy to check that $H$ has eigenvalues $-\kappa^2$, where

$$\kappa = \tan \frac{\pi m}{N}$$

with $m$ running through $1, \ldots, \left[\frac{N}{2}\right]$ for $N$ odd and $1, \ldots, \left[\frac{N-1}{2}\right]$ for $N$ even. Thus $\sigma_{\text{disc}}(H)$ is *always nonempty*.
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The on-shell $S$-matrix

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We have mentioned already that $S(k) = \frac{k-1+(k+1)U}{k+1+(k-1)U}$. It might seem that transport becomes trivial at small and high energies, since $\lim_{k \to 0} S(k) = -I$ and $\lim_{k \to \infty} S(k) = I$. However, caution is needed; the formal limits lead to a false result if $\pm 1$ or $\pm 1$ are eigenvalues of $U$. A counterexample is the (scale invariant) Kirchhoff coupling where $U$ has only $\pm 1$ as its eigenvalues; the on-shell $S$-matrix is then independent of $k$ and it is not a multiple of the identity. A straightforward computation yields the explicit form of $S(k)$: denoting for simplicity $\eta := \frac{1-k}{1+k}$ we have

$$S_{ij}(k) = 1 - \eta^2 1 \leq \eta^N \{ -\eta 1 \leq -\eta^N - 2 1 \leq -\eta \delta_{ij} + (1 - \delta_{ij}) \eta (j - i - 1) \mod N \}.$$
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The role of vertex degree parity

This suggests, in particular, that the high-energy behavior, $\eta \to -1$, could be determined by the *parity* of the vertex degree $N$. We see that $\lim_{k \to \infty} S(k) = I$ holds for $N = 3$ and more generally for all odd $N$, while for the even ones the limit is not a multiple of identity. This is related to the fact that in the latter case $U$ has both $\pm 1$ as its eigenvalues, while for $N$ odd $-1$ is missing. Let us look how this fact influences spectra of periodic quantum graphs.
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This suggests, in particular, that the high-energy behavior, $\eta \to -1-$, could be determined by the parity of the vertex degree $N$.

In the cases with the lowest $N$ we get

$$S(k) = \frac{1 + \eta}{1 + \eta + \eta^2} \begin{pmatrix}
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Let us look how this fact influences spectra of periodic quantum graphs.
Comparison of two lattices

Spectral condition for the two cases are easy to derive, 

\[
\left(\theta_1 + \theta_2\right)k \sin k \ell \left[\left(k^2 - 1\right)\cos \theta_1 + \cos \theta_2\right) + 2\left(k^2 + 1\right)\cos k \ell \right] = 0
\]

and respectively

\[
-i\left(\theta_1 + \theta_2\right)k^2 \sin k \ell \left(3 + 6k^2 - k^4 + 4d\theta\left(k^2 - 1\right) + \left(k^2 + 3\right)\right)^2\cos 2k \ell \right] = 0
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where 

\[d\theta := \cos \theta_1 + \cos(\theta_1 - \theta_2) + \cos \theta_2\]

and 

\[\ell(\theta_1, \theta_2) \in [-\pi \ell, \pi \ell]\]

is the quasimomentum. They are tedious to solve except the flat band cases, 

\[\sin k \ell = 0\]

however, we can present the band solution in a graphical form.


P.E.: Spectral gaps of periodic graphs

OTKR Vienna

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\[ -i (\theta_1 + \theta_2) k_2 \sin k_\ell \left( 3 + 6 k_2^2 - k_4^2 + 4 \frac{d\theta}{k_2^2 - 1} + \left( k_2^2 + 3 \right)^2 \cos 2k_\ell \right) = 0, \]

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\[ 16i e^{i(\theta_1 + \theta_2)} k \sin k\ell \left[ (k^2 - 1)(\cos \theta_1 + \cos \theta_2) + 2(k^2 + 1) \cos k\ell \right] = 0 \]
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![diagram of two lattices]

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\[ 16i \, e^{-i(\theta_1 + \theta_2)} \, k^2 \, \sin k\ell \left( 3 + 6k^2 - k^4 + 4d_\theta(k^2 - 1) + (k^2 + 3)^2 \cos 2k\ell \right) = 0 , \]

where \( d_\theta := \cos \theta_1 + \cos(\theta_1 - \theta_2) + \cos \theta_2 \) and \( \frac{1}{\ell}(\theta_1, \theta_2) \in [-\frac{\pi}{\ell}, \frac{\pi}{\ell}]^2 \) is the quasimomentum. They are tedious to solve except the flat band cases, \( \sin k\ell = 0 \).
Comparison of two lattices

Spectral condition for the two cases are easy to derive,

\[ 16i e^{i(\theta_1+\theta_2)} k \sin k\ell \left[ (k^2 - 1)(\cos \theta_1 + \cos \theta_2) + 2(k^2 + 1) \cos k\ell \right] = 0 \]

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A picture is worth of thousand words

For the two lattices, respectively, we get (with $\ell = \frac{3}{2}$, dashed $\ell = \frac{1}{4}$)
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Comparison and further results

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P.E., P. Lokvenc: Rectangular lattice graphs with the coupling noninvariant with respect to time reversal, *in preparation*
Comparison and further results

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I just mention that the time-reversal noninvariance destroys the finite gap number effect discussed above.
One more model

Let us look what this coupling influences graphs *periodic in one direction*.
One more model

Let us look what this coupling influences graphs *periodic in one direction*. Consider again a *loop chain*, first *tightly connected*

\[
\begin{array}{c}
\psi_1 & \psi_2 & \psi_3 & \psi_4 \\
\end{array}
\]

The spectrum of the corresponding Hamiltonian looks as follows:

**Theorem**

The spectrum of \( H_0 \) consists of the absolutely continuous part which coincides with the interval \([0, \infty)\), and a family of infinitely degenerate eigenvalues, the isolated one equal to \(-1\), the threshold one at zero, and the embedded ones equal to the positive integers.

A loosely connected chain
Replace the direct coupling of adjacent rings by connecting segments of length \( \ell > 0 \), still with the same vertex coupling.
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Theorem

The spectrum of $H_\ell$ has for any fixed $\ell > 0$ the following properties:

- Any non-negative integer is an eigenvalue of infinite multiplicity.
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- The negative spectrum is contained in $(-\infty, -1)$ consisting of a single band if $\ell = \pi$, otherwise there is a pair of bands and $-3 \not\in \sigma(H_\ell)$. 

P.E.: Spectral gaps of periodic graphs

OTKR Vienna

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- The positive spectrum has infinitely many gaps.
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- The negative spectrum is contained in $(-\infty, -1)$ consisting of a single band if $\ell = \pi$, otherwise there is a pair of bands and $-3 \not\in \sigma(H_\ell)$.
- The positive spectrum has infinitely many gaps.
- $P_{\sigma}(H_\ell) := \lim_{K \to \infty} \frac{1}{K} |\sigma(H_\ell) \cap [0, K]| = 0$ holds for any $\ell > 0$. 

P.E.: Spectral gaps of periodic graphs
The limit $\ell \to 0^+$

Here $P_\sigma(H_\ell)$ is the *probability of being in the spectrum* introduced by

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We have, however, obviously $P_\sigma(H_0) = 1$, hence the said convergence is *rather nonuniform*!
Back to the main theme of the conference

Hagen was an exceptional mathematician with a gift to look at a complicated argument and identify its weaknesses.
Hagen and QMath

He not only participated in these conferences from the beginning but he was the one who gave it the new life after the first four issues.
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Hagen and QMath

He not only participated in these conference from the beginning but he was the one who gave it the new life after the first four issues.

Apart from the QMath5 (Blossin 1993) and QMath12 (Berlin 2013) proceedings we coedited, here is a picture from QMath7 (Prague 1998)
His other service to the community

2008
His other service to the community
How we saw him
The above shows he was *highly practical* and *efficient* when doing his work.
How we saw him

The above shows he was *highly practical* and *efficient* when doing his work, and at the same time *rather impractical* as seen in many situations.
How we saw him

The above shows he was *highly practical* and *efficient* when doing his work, and at the same time *rather impractical* as seen in many situations.

In view of all that, you could not overlook him in the community.
And we enjoyed his company
And we enjoyed his company
And we enjoyed his company
And we enjoyed his company
One thing is clear

We miss him!
One thing is clear

We miss him!