Topologically induced spectral behavior: 
the example of quantum graphs

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I am going to speak here about *spectral properties* of operators and the *topology* of the underlying space; I believe that there is no need to convince you that the two are related.

Moreover, one might expect that a nontrivial topology can give rise to a broader family of spectral types. My aim here is to illustrate this claim using the example of quantum graphs – I will explain in a minute what they are like.

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Periodic Schrödinger operators

A typical example of such an operator is

$$H = (-i\nabla - A(x))^* g(x) (-i\nabla - A(x)) + V(x)$$

on $L^2(\mathbb{R}^d)$, $d \geq 2$, where $g$ is a positive $d \times d$-matrix valued function and $A$ is a vector-valued magnetic potential.
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If the coefficients \( g, A, V \) are periodic the spectrum of \( H \) is found using Floquet method: we write

\[ H = \int_{Q^*} H(\theta) \, d\theta \]

where the fiber operator \( H(\theta) \) acts 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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If the coefficients \(g, A, V\) are *periodic* the spectrum of \(H\) is found using the *Floquet method*: we write

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where the fiber operator \(H(\theta)\) acts on \(L^2(Q)\), where \(Q \subset \mathbb{R}^d\) is *period cell* and \(Q^*\) is the *dual cell* (or *Brillouin zone*).

Using it one can prove, in particular, that the spectrum of \(H\)

- is *absolutely continuous*
- has a *band-and-gap structure*
The proof idea belongs to L. Thomas, in the case \( A = 0 \) and \( g = I \)


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- in the one-dimensional case the *number of open gaps is infinite* except for a particular class of potentials
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My message here is that if the system in question is a quantum graph, nothing of that needs to be true!
So, what are the quantum graphs?

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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

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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.
Vertex coupling

Denoting $\psi(v_k) = \{\psi_j(v_k)\}$ and $\psi'(v_k) = \{\psi'_j(v_k)\}$ the boundary values of functions and (outward) derivatives at the vertex $v_k$, respectively
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$$(U - I)\psi(v_k) + i(U + I)\psi'(v_k) = 0,$$

where $U$ is any $\text{deg}(v_k) \times \text{deg}(v_k)$ unitary matrix.
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It is easy to see: an elementary calculation gives

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\|\psi(v_k) + i\psi'(v_k)\|^2 - \|\psi(v_k) - i\psi'(v_k)\|^2 = 2 \sum_j (\bar{\psi}_j\psi'_j - \bar{\psi}'_j\psi_j)(v_k)
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and the right-hand side is a multiple of the boundary form which has to vanish to make the operator self-adjoint. Hence the two vectors $\psi(v_k) \pm i\psi'(v_k) \in \mathbb{C}^{\text{deg}(v_k)}$ have the same length being thus related by a unitary matrix.
An example: the $\delta$ coupling

In general the vertex coupling depends on the number of parameters, specifically $n^2$ for a vertex of degree $n$. 

The number is reduced if we require continuity at the vertex, then we are left with

$$\psi_j(0) = \psi_k(0) =: \psi(0),$$

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, $\alpha = 0$ is often called Kirchhoff coupling. It is an unfortunate name – free or standard or natural would be better – but it stuck.

The name $\delta$ coupling is natural because one can approximate it by scaled regular potentials similarly as a $\delta$ potential on the line; the parameter $\alpha$ is interpreted as the coupling strength.
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Why are quantum graphs interesting?

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- graphs offer a useful playground to study *quantum chaos*
- and a lot more as one can find, e.g., in the monograph


We focus, however, on a single aspect, namely how the topology can enrich spectral properties of quantum graphs.
No unique continuation principle

To describe how the quantum graphs differ from the standard PDE mentioned in the opening, we note first that the *unique continuation principle* may not hold in quantum graphs.

In particular, this means that the spectrum of a periodic quantum graph with the said property is not purely absolutely continuous.

The other claims made above are much less trivial, nevertheless, they can be demonstrated using relatively simple examples.
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This is elementary: a graph with a $\delta$ coupling which contains a *loop* with *rationally related edges* has the so-called *Dirichlet eigenvalues*.

![Diagram of a quantum graph](image)

Courtesy: Peter Kuchment
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Spectrum may not be absolutely continuous at all.

To demonstrate this claim, consider the graph in the form of a loop array exposed to a magnetic field as sketched below.

The Hamiltonian is the magnetic Laplacian, \( \psi_j \mapsto -D^2 \psi_j \) on each graph link, where \( D := -i \nabla - A \), and for definiteness we assume \( \delta \)-coupling in the vertices, i.e. the domain consists of functions from \( H^2_{\text{loc}}(\Gamma) \) satisfying

\[
\psi_i(0) = \psi_j(0) =: \psi(0), \quad i, j = 1, \ldots, n
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\sum_{i=1}^n D \psi_i(0) = \alpha \psi(0),
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If $A_j = A$, $j \in \mathbb{Z}$, we write $\psi_L(x) = e^{-iAx}(C_L^+ e^{ikx} + C_L^- e^{-ikx})$ for $x \in [-\pi/2, 0]$ and energy $E := k^2 \neq 0$, and similarly for the other three components.
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The functions have to be matched through (a) the $\delta$-coupling and (b) Floquet conditions. This yields equation for the phase factor $e^{i\theta}$,

$$
\sin k \pi \cos A \pi (e^{2i\theta} - 2\xi(k)e^{i\theta} + 1) = 0
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with the discriminant $D = 4(\xi(k)^2 - 1)$, where $\xi(k) := 4 \cos A \pi$ and $\eta(k) := 4 \cos k \pi + \alpha k \sin k \pi$ for any $k \in \mathbb{R} \cup i\mathbb{R} \{0\}$ and $A - \frac{1}{2} \not\in \mathbb{Z}$. Apart from $A - \frac{1}{2} \in \mathbb{Z}$ and $k \in \mathbb{N}$ we have thus $k^2 \in \sigma(-\Delta \alpha)$ iff the condition $|\eta(k)| \leq 4 |\cos A \pi|$ is satisfied.
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In picture: determining the spectral bands

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In the latter case, spectrum consists of infinitely degenerate eigenvalues (or flat bands as physicists would say) and elementary eigenfunctions are supported by pairs of adjacent loops.
Making it a little more complicated

Suppose now that the magnetic field is nonconstant and varies \textit{linearly} along the chain, \( A_j = \mu j + \theta \) for some \( \mu, \theta \in \mathbb{R} \) and every \( j \in \mathbb{Z} \).
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... while the experimentalist might collect all his data between breakfast and lunch in a small cluttered laboratory, his theoretical colleagues interpret those results in term of isolated systems moving eternally in an infinitely extended space.
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Making it a little more complicated

Suppose now that the magnetic field is nonconstant and varies \textit{linearly} along the chain, $A_j = \mu j + \theta$ for some $\mu, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$.

You may say, that in nature one never meets a (globally) linear magnetic field. As a possible excuse, let me quote Bratelli and Robinson:

... while the experimentalist might collect all his data between breakfast and lunch in a small cluttered laboratory, his theoretical colleagues interpret those results in term of isolated systems moving eternally in an infinitely extended space. The validity of such idealizations is the heart and soul of theoretical physics and has the same fundamental significance as the reproducibility of experimental data.

And I add: it is also a \textit{bridge at which mathematics and physics meet}, at least since Newton times.
A more practical point of view

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This simplifies the analysis in the case when the \textit{slope} \( \mu \) \textit{is rational}. Indeed, is such a situation we can assume without loss of generality that the sequence \( \{ A_j \} \) is \textit{periodic} and solve the problem using the Floquet method similarly as we did that for a constant \( A \).
Results of Floquet analysis

**Theorem**

Let $A_j = \mu j + \theta$ for some $\mu, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. Then for the spectrum $\sigma(-\Delta_{\alpha, A})$ the following holds:

(a) If $\mu, \theta \in \mathbb{Z}$ and $\alpha = 0$, then $\sigma_{ac}(-\Delta_{\alpha, A}) = [0, \infty)$ and $\sigma_{pp}(-\Delta_{\alpha, A}) = \{n^2 | n \in \mathbb{N}\}$

(b) If $\alpha \neq 0$ and $\mu = \frac{p}{q}$ with $p, q$ relatively prime, $\mu_j + \theta + \frac{1}{2} \in \mathbb{Z}$ for all $j = 0, \ldots, q-1$, then $-\Delta_{\alpha, A}$ has infinitely degenerate ev's $\{n^2 | n \in \mathbb{N}\}$ interlaced with an $ac$ part consisting of $q$-tuples of closed intervals.

(c) If the situation is as in (b) but $\mu_j + \theta + \frac{1}{2} \in \mathbb{Z}$ holds for some $j = 0, \ldots, q-1$, then the spectrum $\sigma(-\Delta_{\alpha, A})$ consists of infinitely degenerate eigenvalues only, the Dirichlet ones plus $q$ distinct others in each interval $(-\infty, 1)$ and $(n^2, (n+1)^2)$.
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Duality

The case of an irrational $\mu$ requires a different approach.

The idea is to rephrase our differential operator problem of the metric graph in terms of a difference equation, as proposed in the 1980's by physicists, Alexander and de Gennes, followed by mathematicians. It is particularly simple if the graph in question is equilateral like in our example. We consider

$$K := \{ k : \text{Im} k \geq 0 \land k \in \mathbb{Z} \}$$

to exclude Dirichlet ev's and seek the spectrum through solution of

$$(-\Delta_\alpha, A - k^2) \psi(x, k) \phi(x, k) = 0$$

This leads to the difference equation

$$2 \cos(A j \pi) \psi_{j+1}(k) + 2 \cos(A j - 1 \pi) \psi_{j-1}(k) = \eta(k) \psi_j(k), \quad k \in K,$$

where $\psi_j(k) := \psi(j \pi, k)$ and $\eta(k) := 4 \cos k \pi + \alpha k \sin k \pi$ as above, amended by $\eta(k) = 4 + \alpha \pi$ for $k = 0$. What is important, this is a two-way correspondence; we can reconstruct the solution of the original problem from that of the difference one.
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Duality, continued

Specifically, we have

\[
\begin{pmatrix}
\psi(x, k) \\
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\end{pmatrix}
= e^{\pm iA_j(x-j\pi)} \left[ \psi_j(k) \cos k(x-j\pi) \\
\psi_j(k) \cos k\pi \right] + \left[ (\psi_{j+1}(k)e^{\pm iA_j\pi} - \psi_j(k) \cos k\pi) \frac{\sin k(x-j\pi)}{\sin k\pi} \right],
\]

\[x \in (j\pi, (j+1)\pi),\]

and in addition, it belongs to $L^p(\Gamma)$ iff \{\psi_j(k)\}_{j \in \mathbb{Z}} \in \ell^p(\mathbb{Z})$, $p \in \{2, \infty\}$. 

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This relates weak solutions of the two problems but we can do better:


**Theorem**

For any interval \( J \subset \mathbb{R} \setminus \sigma_D \), the operator \((-\Delta_{\alpha,A})_J\) is unitarily equivalent to the pre-image \( \eta^{(-1)}((L_A)_{\eta(J)}) \), where \( L_A \) is the operator on \( \ell^2(\mathbb{Z}) \) acting as \((L_A \varphi)_j = 2 \cos(A_j\pi)\varphi_{j+1} + 2 \cos(A_{j-1}\pi)\varphi_{j-1}\).
Another way to rephrase the problem

Let me recall the *almost Mathieu equation*

\[ u_{n+1} + u_{n-1} + \lambda \cos(2\pi \mu n + \theta))u_n = \epsilon u_n \]

in the *critical case*, \( \lambda = 2 \), also called *Harper equation*

The spectrum of the corresponding difference operator \( H_{\mu,2,\theta} \), independent of \( \theta \), as a function of \( \mu \) is the well-known *Hofstadter butterfly*

Source: Fermat's Library
The Ten Martini Problem

If $\mu \in \mathbb{Q}$, the spectrum of $H_{\mu,2,\theta}$ is easily seen to be absolutely continuous and of the band-gap type.

Theorem

For any $\mu \not\in \mathbb{Q}$, the spectrum of $H_{\mu,2,\theta}$ does not depend on $\theta$ and it is a Cantor set of Lebesgue measure zero.


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For $\mu \notin \mathbb{Q}$ the problem is much harder. Its Cantor structure was conjectured – under the name proposed by B. Simon – but it took two decades to achieve the solution:


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N.B.: Such a behavior was anticipated in physics half a century ago,


and recently confirmed by several groups observing graphene lattices in a homogeneous magnetic field.
How is this related to our problem?

We employ the trick originally proposed in


and consider a rotation algebra $A_\mu$ generated by elements $u, v$ such that $uv = e^{2\pi i\mu} vu$. It is simple for $\mu \notin \mathbb{Q}$, thus having faithful representations.
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We construct two representations of $A_\mu$ which map a single element $u + v + u^{-1} + v^{-1} \in A_\mu$ to $L_A$ and $H_{\mu,2,\theta}$, respectively, which implies that their spectra coincide, $\sigma(L_A) = \sigma(H_{\mu,2,\theta})$. 
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Thus we get a nontrivial result \textit{in a cheap way}: using the duality and the fact that the function $\eta$ is \textit{locally analytic} we can complete the result from


\textbf{Theorem}

\( (d) \) \textit{If $\alpha \neq 0$ and $\mu \notin \mathbb{Q}$, then $\sigma(-\Delta_{\alpha,A})$ does not depend on $\theta$ and it is a disjoint union of the isolated-point family $\{n^2| n \in \mathbb{N}\}$ and \textit{Cantor sets}, one inside each interval $(-\infty, 1)$ and $(n^2, (n+1)^2)$, $n \in \mathbb{N}$. Moreover, the overall Lebesgue measure of $\sigma(-\Delta_{\alpha,A})$ is zero.}
Hausdorff dimension

The almost Mathieu operator is one of the most intensely studied, and there are other results which have implications for our magnetic chain model.


\[ A_j = \mu_j + \theta \]
for some \( \mu, \theta \in \mathbb{R} \) and every \( j \in \mathbb{Z} \). There exists a dense \( G_\delta \) set of the slopes \( \mu \) for which, and all \( \theta \), the Hausdorff dimension \( \dim H_\sigma(-\Delta \alpha, A) = 0 \).


There is another dense set of the slopes \( \mu \), with positive Hausdorff measure, for which, on the contrary, \( \dim H_\sigma(-\Delta \alpha, A) > 0 \).
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Corollary

Let $A_j = \mu j + \theta$ for some $\mu, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. There exists a dense $G_\delta$ set of the slopes $\mu$ for which, and all $\theta$, the Hausdorff dimension

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Changing topic: graphs with a few gaps only

The graphs in the previous example had ‘many’ gaps indeed. Let us now ask whether periodic graphs can have ‘just a few’ gaps.

As I have mentioned for ‘ordinary’ Schrödinger operators, the dimension is known to be decisive: systems which are $\mathbb{Z}$-periodic have generically an infinite number of open gaps, while $\mathbb{Z}_\nu$-periodic systems with $\nu \geq 2$ have only finitely many open gaps. This is the celebrated Bethe–Sommerfeld conjecture, rather plausible but mathematically quite hard, to which we have nowadays an affirmative answer in a large number of cases.


Question: How the situation looks for quantum graphs which can ‘mix’ different dimensionalities?


The literature says that – while the situation is similar – the finiteness of the gap number is not a strict law, and topology is the reason.
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Courtesy: Peter Kuchment
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\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{decorated_graph}
\caption{Decorated graph}
\end{figure}


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Thus, instead of ‘not a strict law’, the question rather is whether \textit{it is a ‘law’ at all}: do infinite periodic graphs having a \textit{finite nonzero} number of open gaps exist? From obvious reasons we would call them \textit{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

An infinite periodic quantum graph does not belong to the Bethe-Sommerfeld class if the couplings at its vertices are scale-invariant.

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

Nevertheless, the answer to our question is affirmative:

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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

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

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we neglect the Kirchhoff case, $\alpha = 0$, where $\sigma(H) = [0, \infty)$. 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 $\sigma(H) = [0, \infty)$.
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On the other hand, $\theta \in \mathbb{R}$ is badly approximable if there is a $c > 0$ such that

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(we note that \( \mu(\theta) = \mu(\theta^{-1}) \)) and its ‘one-sided analogues’.
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![Graph showing the golden mean situation](image-url)
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where the points approach the limit values *from above*. Note also that higher series open at \( \frac{\pi^2}{\sqrt{5ab}} \theta^{\pm1/2} |n^2 - m^2 - nm|, \ n, m \in \mathbb{N} \).

But a closer look shows a more complex picture


**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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-\frac{2\pi}{a} \tan \left( \frac{3 - \sqrt{5}}{4} \pi \right) \leq \alpha \leq \frac{\pi^2}{\sqrt{5}a},
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there are **no gaps in the positive spectrum**.

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The above theorem about the existence of BS graphs is valid.
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The window in which the golden-mean lattice has the BS property is narrow, it is roughly $4.298 \lesssim -\alpha a \lesssim 4.414$. 
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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

$$-\frac{2\pi \left( \theta^{2(N+1)} - \theta^{-2(N+1)} \right)}{\sqrt{5}a} \tan \left( \frac{\pi}{2} \theta^{-2(N+1)} \right) \leq \alpha < -\frac{2\pi \left( \theta^{2N} - \theta^{-2N} \right)}{\sqrt{5}a} \tan \left( \frac{\pi}{2} \theta^{-2N} \right).$$
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Note that the numbers $A_j := \frac{2\pi}{\sqrt{5}} \tan \left( \frac{\pi}{2} \theta^{-2j} \right)$ form an increasing sequence the first element of which is $A_1 = 2\pi \tan \left( \frac{3 - \sqrt{5}}{4} \pi \right)$ and

$$A_j < \frac{\pi^2}{\sqrt{5}}$$
holds for all $j \in \mathbb{N}$. 
More general result

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Let \( \theta = \frac{a}{b} \) and define

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then there is a nonzero and finite number of gaps in the positive spectrum.

This allows us to construct further examples, in particular, to show that also lattices with repulsive \( \delta \) coupling, \( \alpha > 0 \), may exhibit the BS property.
The third main topic: topology again

Now we want to show one more example where a topological characteristics – in this case the vertex degree, or rather its parity – has a substantial influence on the spectrum.
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There are different approaches to this question. The straightforward one starts from the observation that are models of *thin networks*; one can thus ask how spectral properties of the Laplacian behaves in the *limit of zero tube width*.

It is known that for *Neumann* Laplacian on a network such a limit yields the *Kirchhoff* coupling.

Squeezed network approximations

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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 $\beta < \frac{1}{3}$, one can approximate any vertex coupling in the norm-resolvent sense as $\varepsilon \to 0$.
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N.B.: The Dirichlet case is more difficult and I will not discuss it here.
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**Hall effect**


In which magnetic field induces a voltage perpendicular to the current. In the quantum regime the corresponding conductivity is quantized with a great precision – this fact lead already to two Nobel Prizes. However, in ferromagnetic material one can observe a similar behavior also in the absence of external magnetic field – being labeled anomalous.
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![Image of Hall effect](https://en.wikipedia.org/wiki/Hall_effect)

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Recently a quantum-graph model of the AHE was proposed by physicists in which the material structure of the sample is described by lattice of δ-coupled rings (topologically equivalent to a rectangular lattice)

Breaking the time-reversal invariance

Looking at the picture we recognize a *flaw in the model*. To mimic the rotational motion of atomic orbitals responsible for the magnetization, the authors had to impose 'by hand' the requirement that the electrons move only one way on the loops of the lattice. Naturally, such an assumption cannot be justified from the first principles. On the other hand, it is possible to break the time-reversal invariance, not at graph edges but in its vertices. Consider an example: note that 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 - 1},
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in particular, we have $U = S(1)$. The 'maximum rotation' at $k = 1$ is thus achieved with $U = \begin{pmatrix}
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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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which is non-trivial for \( N \geq 3 \) and obviously non-invariant w.r.t. the reverse in the edge numbering order, or equivalently, w.r.t. the complex conjugation representing the *time reversal*.

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 \( 1, \ldots, \lfloor N/2 \rfloor \) for \( N \) odd and \( 1, \ldots, \lfloor (N-1)/2 \rfloor \) for \( N \) even.

Thus \( \sigma_{\text{disc}}(H) \) is always nonempty, in particular, \( H \) has a single negative eigenvalue for \( N = 3, 4 \) which is equal to \(-1\) and \(-3\), respectively.
Spectrum for such a coupling

Consider first a *star graph*, i.e. $N$ semi-infinite edges meeting in a single vertex. Writing the coupling conditions componentwise, we have

$$(\psi_{j+1} - \psi_j) + i(\psi'_{j+1} + \psi'_j) = 0, \quad j \in \mathbb{Z} \text{ (mod } N) ,$$

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The on-shell S-matrix

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 \( +1 \) or \( -1 \) 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 \( \eta = 1 - \frac{k}{1+k} \) we have

\[
S_{ij}(k) = 1 - \eta^2 \begin{cases} 
-\eta & \text{if } j = i - 1 \pmod{N} \\
\eta & \text{otherwise}
\end{cases} + (1 - \delta_{ij}) \eta (j - i - 1) \pmod{N}.
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$$S_{ij}(k) = 1-\eta \frac{1}{1-\eta \eta^N} \left\{ -\eta \delta_{ij} + (1-\delta_{ij}) \eta (j-i-1) \mod N \right\}$$
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The role of vertex degree parity

This suggests, in particular, that the high-energy behavior, $\eta \rightarrow -1$, could be determined by the parity of the vertex degree $N$. In the cases with the lowest $N$ we get

$$S(k) = 1 + \frac{\eta}{1 + \eta} + \frac{\eta}{1 + \eta} \left( -\frac{1}{1 + \eta} \right)$$

and

$$S(k) = 1 + \frac{1}{1 + \eta} \left( -\frac{1}{1 + \eta} \right)$$

for $N = 3, 4$, respectively. 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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Comparison of two lattices

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

and respectively

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

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

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is the quasimomentum. They are tedious to solve except the flat band cases, however, we can present the band solution in a graphical form.
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Spectral condition for the two cases are easy to derive, i.e. \[(\theta_1 + \theta_2) k \sin k \ell \left[ (k^2 - 1)(\cos \theta_1 + \cos \theta_2) + 2(k^2 + 1) \cos k \ell \right] = 0\]
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\[-i(\theta_1 + \theta_2) k^2 \sin k \ell \left( 3 + 6k^2 - k^4 + 4d \theta \right) - \left( k^2 + 3 \right) 2 \cos 2k \ell \right] = 0\],

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

And one more topic: band edges positions

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The second one shows that this may be true even for *graphs periodic in one direction*.

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The number of connecting edges had to be \( N \geq 2 \). An example:
Band edges, continued

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  ___  ___  ___
 /   /   /   /
|   |   |   |
```

Its analysis shows:
- two-sided comb is *transport-friendly*, bands dominate
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\begin{center}
\begin{tikzpicture}
\foreach \i in {0,1,2,3,4,5,6,7}
\filldraw[blue, circle, radius=0.1cm] (2*\i,0) circle (0.2cm);
\end{tikzpicture}
\end{center}

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- and what about the dispersion curves?
Two-sided comb: dispersion curves

P.E., Daniel Vašata: Spectral properties of \( \mathbb{Z} \) periodic quantum chains without time reversal invariance, *in preparation*
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- for *finite graphs* one can ask about the dependence of *spectral asymptotics* or *nodal properties* on the graph topology and the vertex coupling.
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- for finite graphs one can ask about the dependence of spectral asymptotics or nodal properties on the graph topology and the vertex coupling
- spectral optimization w.r.t. to graph properties is also of interest
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