Topologically induced spectral behavior: the example of quantum graphs

Pavel Exner

Doppler Institute
for Mathematical Physics and Applied Mathematics
Prague

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What is this talk about

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

To be specific, I am going to consider *elliptic second-order* operators with *periodic coefficients* commonly used in physics to describe crystals and other *periodically structured materials*

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.

If the coefficients g, A, V are *periodic* the spectrum of H is found using *Floquet method*: we write

$$H = \int_{Q^*} H(\theta)\, \mathrm{d}\theta$$

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*)

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

- is *absolutely continuous*
- has a *band-and-gap structure*

Periodic Schrödinger operators, continued

The proof idea belongs to L. Thomas, in the case $A = 0$ and $g = I$

L.E. Thomas: Time dependent approach to scattering from impurities in a crystal, *Commun. Math.Phys.* **33** (1973), 335–343.

For a review and a general result under weak regularity assumptions see

M.Sh. Birman, T.A. Suslina: A periodic magnetic Hamiltonian with a variable metric. The problem of absolute continuity, *St. Petersburg Math. J.* **11** (2000), 203–232.

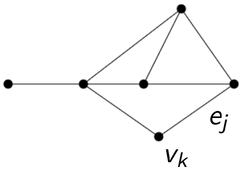
Moreover, the dimension of the configuration space is important:

- in the one-dimensional case the *number of open gaps is infinite* except for a a particular class of potentials
- on the contrary, in higher dimensions the *Bethe-Sommerfeld conjecture*, nowadays verified for a wide class of interactions, says that the number of open gaps is *finite*

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?

We consider a *metric graph* which is a collection of *vertices* and *edges* the each of which is homothetic to a (finite or semi-infinite) intervals



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

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

To make such an H a *self-adjoint operator* we have to match the functions ψ_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, the most general self-adjoint matching conditions read

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

where U is *any* $\deg(v_k) \times \deg(v_k)$ *unitary matrix*.

It is easy to see: an elementary calculation gives

$$\|\psi(v_k) + i\psi'(v_k)\|^2 - \|\psi(v_k) - i\psi'(v_k)\|^2 = 2\sum_j \left(\bar{\psi}_j\psi'_j - \bar{\psi}'_j\psi_j\right)(v_k)$$

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 $\psi(v_k) \pm i\psi'(v_k) \in \mathbb{C}^{\deg(v_k)}$ have the same length being thus related by a unitary matrix.

An example: the δ 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

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,,\; j,k = 1,\dots,n\,, \quad \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0)$$

depending on a single parameter $\alpha \in \mathbb{R}$ which we call the δ *coupling*; the corresponding unitary matrix is $U = \frac{2}{n+i\alpha}\mathcal{J} - I$, where $\mathcal{J}$ 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 δ *coupling* is natural because one can approximate it by *scaled regular potentials* similarly as a δ potential on the line; the parameter α is interpreted as the *coupling strength.*

Why are quantum graphs interesting?

There are numerous situations where one encounters quantum graphs:

- from the 'practical' physical point of view they model graphlike *nanostructures* made of semiconductors, carbon nanotubes, and other materials
- they offer a number of interesting *mathematical questions*, coming in the first place form the spectral and scattering theory, both *direct* and *inverse* (e.g., can on hear the shape of a graph?)
- they have *combinatorial graph* counterparts, as we will see, which may exhibit interesting *dynamical effects*, for instance

Yong Lin, Gábor Lippner, Shing-Tung Yau: Quantum tunneling on graphs, *Commun. Math. Phys.* **311** (2012), 113–132.

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

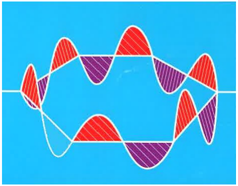
G. Berkolaiko, P. Kuchment: *Introduction to Quantum Graphs*, AMS, Providence, R.I., 2013.

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 other words, one can have *compactly supported eigenfunctions*

This is elementary: a graph with a δ coupling which contains a *loop* with *rationally related edges* has the so-called *Dirichlet eigenvalues*



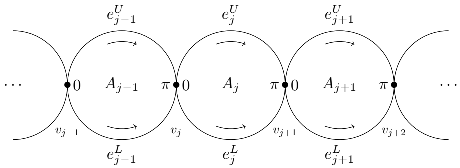
Courtesy: Peter Kuchment

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*

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



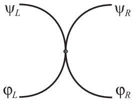
The Hamiltonian is *magnetic Laplacian*, $\psi_j \mapsto -\mathcal{D}^2\psi_j$ on each graph link, where $\mathcal{D} := -i\nabla - A$, and for definiteness we assume *δ-coupling* in the vertices, i.e. the domain consists of functions from $H^2_{\mathrm{loc}}(\Gamma)$ satisfying

$$\psi_i(0) = \psi_j(0) =: \psi(0)\,, \quad i,j = 1,\dots,n\,, \quad \sum_{i=1}^{n} \mathcal{D}\psi_i(0) = \alpha\,\psi(0)\,,$$

where $\alpha \in \mathbb{R}$ is the coupling constant and $n = 4$ holds in our case

V. Kostrykin, R. Schrader: Quantum wires with magnetic fluxes, *Commun. Math. Phys.* **237** (2003), 161–179.

Floquet analysis of the fully periodic case



If $A_j = A,\ j \in \mathbb{Z}$, we write $\psi_L(x) = \mathrm{e}^{-iAx}(C_L^+ \mathrm{e}^{ikx} + C_L^- \mathrm{e}^{-ikx})$ for $x \in [-\pi/2, 0]$ and energy $E := k^2 \neq 0$, and similarly for the other three components; for $E < 0$ we put instead $k = i\kappa$ with $\kappa > 0$.

The functions have to be matched through *(a) the δ-coupling* and *(b) Floquet conditions*. This yields equation for the phase factor $\mathrm{e}^{i\theta}$,

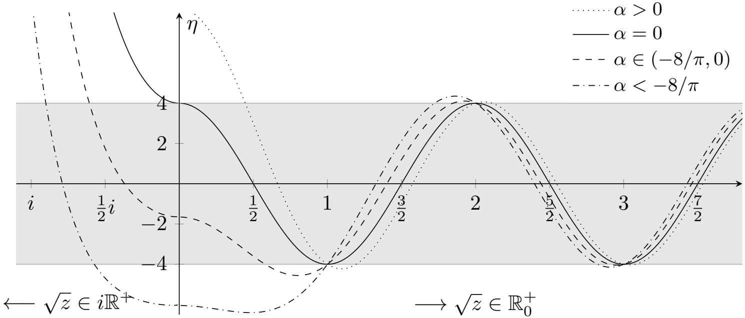
$$\sin k\pi \cos A\pi (\mathrm{e}^{2i\theta} - 2\xi(k)\mathrm{e}^{i\theta} + 1) = 0$$

with the discriminant $D = 4(\xi(k)^2 - 1)$, where $\xi(k) := \frac{\eta(k)}{4\cos A\pi}$ and

$$\eta(k) := 4\cos k\pi + \frac{\alpha}{k}\sin k\pi$$

for any $k \in \mathbb{R} \cup i\mathbb{R} \setminus \{0\}$ and $A - \frac{1}{2} \notin \mathbb{Z}$. 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.

In picture: determining the spectral bands



The picture refers to the non-magnetic case, $A = 0$.

For $A - \frac{1}{2} \notin \mathbb{Z}$ the situation is similar, just the strip width changes to $8|\cos A\pi|$, on the other hand, for $A - \frac{1}{2} \in \mathbb{Z}$ it *shrinks to a line*

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 *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 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 *bridge at which mathematics and physics meet*, at least since Newton times

A more practical point of view

In fact, the unbounded character of the sequence $\{A_j\}$ need not bother us as it is not essential. The point is that from the spectral point of view only the *fractional part of each A_j matters.*

The reason is that our operator – which we denote as $-\Delta_{\alpha,A}$ a given $\alpha \in \mathbb{R}$ and $A = \{A_j\} \subset \mathbb{R}$ – is *unitarily equivalent* to $-\Delta_{\alpha,A'}$ with $A'_j = A_j + n$ with $n \in \mathbb{Z}$ by the operator acting as $\psi_j(x) \mapsto \psi_j(x)\,\mathrm{e}^{-inx}$; a physicist would call it a *gauge transformation*.

This simplifies the analysis in the case when the *slope μ is rational*. Indeed, is such a situation we can assume without loss of generality that the sequence $\{A_j\}$ is *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 $\mu = p/q$ with p, q relatively prime, $\mu j + \theta + \frac{1}{2} \notin \mathbb{Z}$ for all $j = 0, \dots, q-1$, 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 $j = 0, \dots, q-1$, 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 $\big(n^2, (n+1)^2\big)$.*

P.E., D.Vašata: Cantor spectra of magnetic chain graphs, *J. Phys. A: Math. Theor. 50* (2017), 165201.

Duality

The case of an *irrational* μ requires a different approach.

The idea is to rephrase our *differential operator* problem of the metric graph in term 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 $\mathfrak{K} := \{k \colon \mathrm{Im}\, k \geq 0 \wedge k \notin \mathbb{Z}\}$ to exclude Dirichlet ev's and seek the spectrum through solution of $(-\Delta_{\alpha,A} - k^2)\begin{pmatrix} \psi(x,k) \\ \varphi(x,k) \end{pmatrix} = 0$

This leads to the difference equation

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

where $\psi_j(k) := \psi(j\pi, k)$ and $\eta(k) := 4\cos k\pi + \frac{\alpha}{k}\sin k\pi$ 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

Duality, continued

Specifically, we have

$$\begin{pmatrix} \psi(x,k) \\ \varphi(x,k) \end{pmatrix} = \mathrm{e}^{\mp iA_j(x-j\pi)}\Big[\psi_j(k)\cos k(x-j\pi)$$

$$+(\psi_{j+1}(k)\mathrm{e}^{\pm iA_j\pi}-\psi_j(k)\cos k\pi)\frac{\sin k(x-j\pi)}{\sin k\pi}\Big],\quad x\in\big(j\pi,(j+1)\pi\big),$$

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

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

K. Pankrashkin: Unitary dimension reduction for a class of self-adjoint extensions with applications to graph-like structures, *J. Math. Anal. Appl.* **396** (2012), 640–655.

Theorem

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

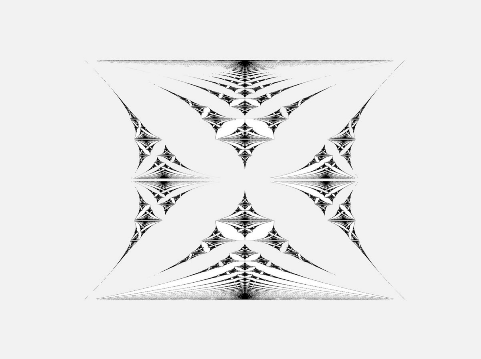
Another way to rephrase the problem

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 θ, as a function of μ 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.

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:

A. Avila, S. Jitomirskaya: The Ten Martini Problem, *Ann. Math.* **170** (2009), 303–342.

Theorem

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

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

M.Ya. Azbel: Energy spectrum of a conduction electron in a magnetic field, *J. Exp. Theor. Phys.* **19** (1964), 634–645.

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

M.A. Shubin: Discrete magnetic Laplacian, *Commun. Math. Phys. 164* (1994), 259–275.

and consider a rotation algebra A_μ generated by elements u, v such that $uv = \mathrm{e}^{2\pi i\mu} vu$. It is simple for $\mu \notin \mathbb{Q}$, thus having faithful representations.

We construct two representations of A_μ 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, $\sigma(L_A) = \sigma(H_{\mu,2,\theta})$.

Thus we get a nontrivial result *in a cheap way*: using the duality and the fact that the function η is *locally analytic* we can complete the result from

P.E., D.Vašata: Cantor spectra of magnetic chain graphs, *J. Phys. A: Math. Theor. 50* (2017), 165201.

Theorem

(d) *If $\alpha \neq 0$ and $\mu \notin \mathbb{Q}$, then $\sigma(-\Delta_{\alpha,A})$ does not depend on θ and it is a disjoint union of the isolated-point family $\{n^2 |\, n \in \mathbb{N}\}$ and Cantor sets, one inside each interval $(-\infty, 1)$ and $\left(n^2, (n+1)^2\right)$, $n \in \mathbb{N}$. 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. Let us mention two of them with their consequences:

Y. Last, M. Shamis: Zero Hausdorff dimension spectrum for the almost Mathieu operator, *Commun. Math. Phys.* **348** (2016), 729–750.

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_δ set of the slopes μ for which, and all θ, the Haussdorff dimension

$$\dim_H \sigma(-\Delta_{\alpha,A}) = 0$$

B. Helffer, Qinghui Liu, Yanhui Qu , Qi Zhou: Positive Hausdorff dimensional spectrum for the critical almost Mathieu operator, *Commun. Math. Phys.* (2019), to appear.

Corollary

There is another dense set of the slopes μ, with positive Hausdorff measure, for which, on the contrary, $\dim_H \sigma(-\Delta_{\alpha,A}) > 0$.

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

L. Parnovski: Bethe-Sommerfeld conjecture, *Ann. Henri Poincaré* **9** (2008), 457–450.

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

G. Berkolaiko, P. Kuchment: *Introduction to Quantum Graphs*, AMS, Providence, R.I., 2013.

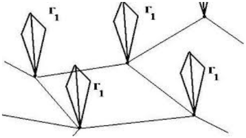
The literature says that – while the situation is similar – the finiteness of the gap number *is not a strict law*, and topology is the reason

Graph decoration

Once create an infinite number of gaps in the spectrum of a periodic graph by *decorating* its vertices by copies of a fixed compact graph. This fact was observed first in the *combinatorial graph context*,

J.H. Schenker, M. Aizenman: The creation of spectral gaps by graph decoration, *Lett. Math. Phys.* **53** (2000), 253–262.

and the argument extends easily to metric graphs we consider here



Courtesy: Peter Kuchment

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 ψ, ψ' are vectors of values and derivatives at the vertex of degree n and U is an $n \times n$ unitary matrix

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*. As an example, one can mention the *Kirchhoff coupling*.

P.E., O. Turek: Periodic quantum graphs from the Bethe- Sommerfeld perspective, *J. Phys. A: Math. Theor.* **50** (2017), 455201.

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 $\neq 0, 1$.

R. Band, G. Berkolaiko: Universality of the momentum band density of periodic networks, *Phys. Rev. Lett.* **113** (2013), 130404.

The existence

Nevertheless, the answer to our question is affirmative:

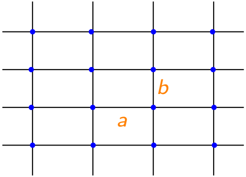
Theorem

Bethe–Sommerfeld graphs exist.

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 δ *coupling* in the vertices introduced in

P.E.: Contact interactions on graph superlattices, *J. Phys. A: Math. Gen.* **29** (1996), 87–102.

P.E., R. Gawlista: Band spectra of rectangular graph superlattices, *Phys. Rev.* **B53** (1996), 7275–7286.



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

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

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 θ is rational, $\sigma(H)$ has clearly infinitely many gaps unless $\alpha = 0$ in which case $\sigma(H) = [0, \infty)$

The same is true if θ is is *an irrational well approximable by rationals*, which means equivalently that in the continued fraction representation $\theta = [a_0; a_1, a_2, \dots]$ 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

$$\left|\theta - \frac{p}{q}\right| > \frac{c}{q^2}$$

for all $p, q \in \mathbb{Z}$ with $q \neq 0$. For such numbers we define the *Markov constant* by

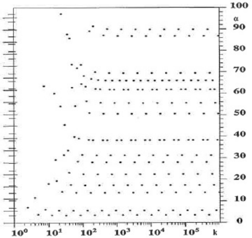
$$\mu(\theta) := \inf \left\{ c > 0 \,\middle|\, (\exists_\infty (p,q) \in \mathbb{N}^2) \left(\left|\theta - \frac{p}{q}\right| < \frac{c}{q^2} \right) \right\};$$

(we note that $\mu(\theta) = \mu(\theta^{-1})$) and its *'one-sided analogues'*

The golden mean situation

As an example, take the *golden mean*, $\theta = \frac{\sqrt{5}+1}{2} = [1; 1, 1, \dots]$, which can be regarded as the 'worst' irrational.

It may be *infinity or nothing*, e.g., plotting the minima of the function appearing in the first gap condition, $\alpha > 0$, the picture looks as follows



where the points approach the limit values *from above*. Note also that higher series open at $\frac{\pi^2}{\sqrt{5ab}}\theta^{\pm 1/2}|n^2 - m^2 - nm|,\ n, m \in \mathbb{N}$.

P.E., R. Gawlista: Band spectra of rectangular graph superlattices, *Phys. Rev.* **B53** (1996), 7275–7286.

But a closer look shows a more complex picture

P.E., O. Turek: Periodic quantum graphs from the Bethe-Sommerfeld point of view, *J. Phys. A: Math. Theor.* **50** (2017), 455201.

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 $\alpha \le -\frac{\pi^2}{\sqrt{5}a}$, there are infinitely many spectral gaps.*

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

(iii) *If*
$$-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right),$$
there is a nonzero and finite number of gaps in the positive spectrum.

Corollary

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 α is chosen within the bounds

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

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

$$A_j < \frac{\pi^2}{\sqrt{5}} \quad \text{holds for all } \; j \in \mathbb{N}\,.$$

More general result

Proofs of the above results are based on properties of Diophantine approximations. In a similar way one can prove

Theorem

Let $\theta = \frac{a}{b}$ and define

$$\gamma_+ := \min\left\{\inf_{m\in\mathbb{N}}\left\{\frac{2m\pi}{a}\tan\left(\frac{\pi}{2}(m\theta^{-1}-\lfloor m\theta^{-1}\rfloor)\right)\right\},\inf_{m\in\mathbb{N}}\left\{\frac{2m\pi}{b}\tan\left(\frac{\pi}{2}(m\theta-\lfloor m\theta\rfloor)\right)\right\}\right\}$$

and γ_- similarly with $\lfloor\cdot\rfloor$ replaced by $\lceil\cdot\rceil$. If the coupling constant α satisfies

$$\gamma_\pm < \pm\alpha < \frac{\pi^2}{\max\{a,b\}}\mu(\theta)\,,$$

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 δ coupling*, $\alpha > 0$, may exhibit the BS property.

P.E., O. Turek: Periodic quantum graphs from the Bethe-Sommerfeld point of view, *J. Phys. A: Math. Theor.* **50** (2017), 455201.

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.

Before doing that let us make a small detour and comment on the *meaning of the vertex coupling*, or the parametres that characterize it.

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.

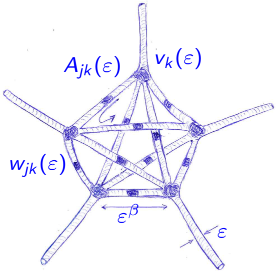
P.E., O. Post: Convergence of spectra of graph-like thin manifolds, *J. Geom. Phys.* **54** (2005), 77–115.

Squeezed network approximations

For other couplings one must amend the Laplacian. The *δ coupling* is easy: one has employs the Schrödinger operator with a family of *scaled potentials*, the integral of which yields the coupling constant.

In general, one has add more potentials as well as *magnetic fields*, and also to modify locally the *network topology:*

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



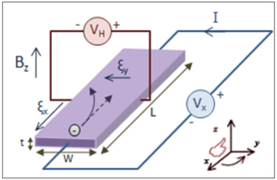
P.E., O. Post: A general approximation of quantum graph vertex couplings by scaled Schrödinger operators on thin branched manifolds, *Commun. Math. Phys.* **322** (2013), 207–227.

N.B.: The Dirichlet case is more difficult and I will not discuss it here.

Hall effect

An alternative approach is *pragmatic*: let us look whether a given vertex coupling could be useful to model a particular system.

Let me show one such example which could serve as a motivation for our further discussion. It concerns the well-known *Hall effect*



Source: Wikipedia

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.

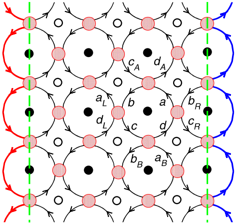
However, in ferromagnetic material one can observe a similar behavior also in the *absence of external magnetic field* – being labeled *anomalous*

Anomalous Hall effect

In contrast to the 'usual' Hall effect, the mechanism of the anomalous one is not well understood; it is conjectured that it comes from internal magnetization in combination with the spin-orbit interaction.

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*)

P. Středa, J. Kučera: Orbital momentum and topological phase transformation, *Phys. Rev.* **B92** (2015), 235152.



Source: the cited paper

Breaking the time-reversal invariance

Looking at the picture we recognize a *flaw in the model*: to mimick 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

$$S(k) = \frac{k-1+(k+1)U}{k+1+(k-1)U}\,,$$

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

$$U = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix},$$

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

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

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 $\sigma_{\rm ess}(H) = \mathbb{R}_+$. It is also easy to check that H has eigenvalues $-\kappa^2$, where

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

with m running through $1, \dots, [\frac{N}{2}]$ for N odd and $1, \dots, [\frac{N-1}{2}]$ for N even. Thus $\sigma_{\rm disc}(H)$ is *always nonempty*, in particular, H has a single negative eigenvalue for $N = 3, 4$ which is equal to -1 and -3, respectively.

P.E., M. Tater: Quantum graphs with vertices of a preferred orientation, *Phys. Lett.* **A382** (2018), 283–287.

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 ± 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

$$S_{ij}(k) = \frac{1-\eta^2}{1-\eta^N} \left\{ -\eta\, \frac{1-\eta^{N-2}}{1-\eta^2}\, \delta_{ij} + (1-\delta_{ij})\, \eta^{(j-i-1)(\mathrm{mod}\, N)} \right\}$$

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

In the cases with the lowest N we get

$$S(k) = \frac{1+\eta}{1+\eta+\eta^2} \begin{pmatrix} -\frac{\eta}{1+\eta} & 1 & \eta \\ \eta & -\frac{\eta}{1+\eta} & 1 \\ 1 & \eta & -\frac{\eta}{1+\eta} \end{pmatrix}$$

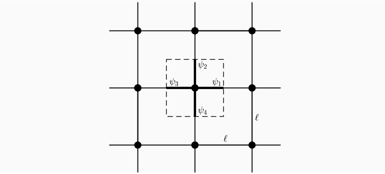
and

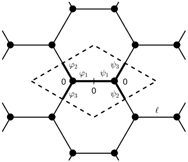
$$S(k) = \frac{1}{1+\eta^2} \begin{pmatrix} -\eta & 1 & \eta & \eta^2 \\ \eta^2 & -\eta & 1 & \eta \\ \eta & \eta^2 & -\eta & 1 \\ 1 & \eta & \eta^2 & -\eta \end{pmatrix}$$

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 is related to the fact that in the latter case U has both ± 1 as its eigenvalues, while for N odd -1 is missing.

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,

$$16i\,\mathrm{e}^{i(\theta_1+\theta_2)}\,k\,\sin k\ell\big[(k^2-1)(\cos\theta_1+\cos\theta_2)+2(k^2+1)\cos k\ell\big]=0$$

and respectively

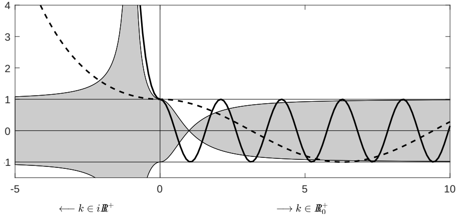
$$16i\,\mathrm{e}^{-i(\theta_1+\theta_2}\,k^2\sin k\ell\,\Big(3+6k^2-k^4+4d_\theta(k^2-1)+(k^2+3)^2\cos 2k\ell\Big)=0\,,$$

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*, $\sin k\ell=0$, however, we can present the band solution in a *graphical form*

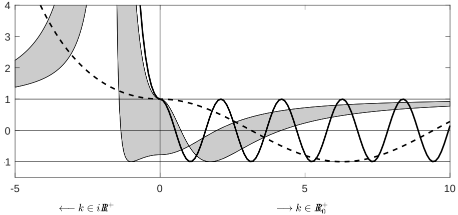
P.E., M. Tater: Quantum graphs with vertices of a preferred orientation, *Phys. Lett.* **A382** (2018), 283–287.

A picture is worth of thousand words

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



and



Comparison summary

Some features are common:

- the number of open gaps is *always infinite*
- the gaps are centered around the flat bands except the lowest one
- for some values of ℓ a band may *degenerate*
- the negative spectrum is *always nonempty*, the gaps become *exponentially narrow* around star graph eigenvalues as $\ell \to \infty$

But the *high energy behavior* of these lattices is *substantially different*:

- the spectrum is dominated by *bands* for square lattices
- it is dominated by *gaps* for hexagonal lattices

Other interesting results concern *interpolation* between the δ-coupling and the present one, but I am not going to speak about them here.

P.E., O. Turek, M. Tater: A family of quantum graph vertex couplings interpolating between different symmetries, *J. Phys. A: Math. Theor.* **51** (2018), 285301.

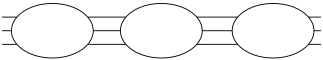
And one more topic: band edges positions

Looking for extrema of the dispersion functions, people usually seek them at the border of the respective Brillouin zone. Quantum graphs provide a warning: there are examples of a periodic graph in which (some) band edges correspond to *internal points* of the Brillouin zone

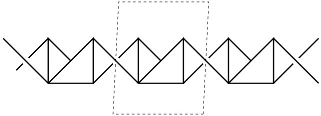
J.M. Harrison, P. Kuchment, A. Sobolev, B. Winn: On occurrence of spectral edges for periodic operators inside the Brillouin zone, *J. Phys. A: Math. Theor.* **40** (2007), 7597–7618.

P.E., P. Kuchment, B. Winn: On the location of spectral edges in $\mathbb{Z}$-periodic media, *J. Phys. A: Math. Theor.* **43** (2010), 474022.

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



The number of connecting edges had to be $N \geq 2$. An example:



Band edges, continued

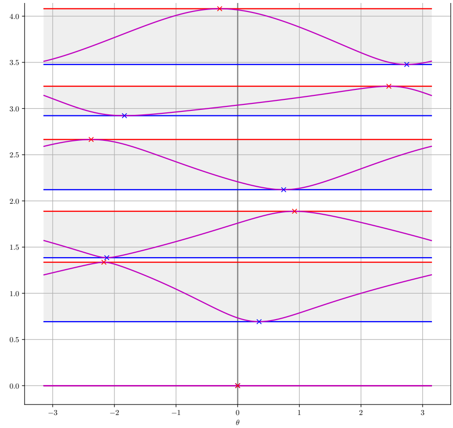
In the same paper we showed that if $N = 1$, the band edges correspond to *periodic* and *antiperiodic* solutions

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*. To show that this assumption was essential consider a *comb-shaped graph* with our non-invariant coupling at the vertices

Its analysis shows:

- *two-sided comb* is *transport-friendly*, bands dominate
- *one-sided comb* is *transport-unfriendly*, gaps dominate
- sending the one side edge lengths to zero in a two-sided comb *does not yield* one-sided comb transport
- 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*

This is not the end of the story

Other interesting questions related to quantum graphs arise, e.g.

- 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
- for graphs with *semi-infinite edges* the distribution of *resonances* is of interest; for some topologies in may *violate the Weyl formula*
- infinite graphs *without a positive lower edge length bound*, for instance *fractal*, one offer many types of spectral behavior
- other linear operators on graphs are of interest, *Dirac* as well as those coming from well *wave* or *elasticity* equations
- *nonlinear operators*, also beyond the NLSE
- quantum graphs with *random* parameters
- squeezing limit of Schrödinger operators on a *Dirichlet networks*
- and many, many more

It remains to say

感謝您的關注

Gǎnxiè nín de guãnzhù