Some unusual spectra of periodic quantum graphs

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A talk at the conference Chaos, and what it can reveal

Hradec Králové, May 10, 2017

Do you recognize these two guys?

This is to show that I know the man who brought us here for more than a half of his life – and little less of mine

What I am going to tell you

Do not be afraid, I am not going to tell old armiger stories of what we did when we were young

There is a connection, though. Three decades ago we started studying *quantum graphs*

It was not our invention, of course, the idea was put forward by Linus Pauling in 1936 but after the first serious application in 1953 it was happily forgotten for more than there decades

We were lucky to witness its revival in the second half of the eighties, but we did not suspect then how fruitful the topic will appear; it is enough to refer to the book [Berkolaiko-Kuchment'13]

Today I want to mention a few fresh results

Periodic quantum systems

I choose this topic, remembering a moment when it fascinated Petr.

Being a born experimentalist, he once in old days in Russia spent time at a corrugated iron hedge, hitting it with different objects, and trying to distinguish whether some tones propagate better along it

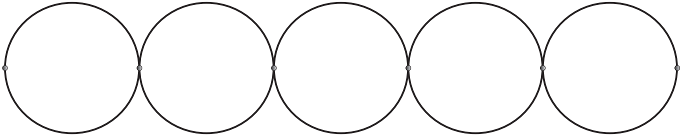
It is a standard part of the quantum lore that spectrum of periodic has familiar properties:

- it is *absolutely continuous*
- it bas a *band-and-gap structure*
- 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-Sommerfled conjecture*, nowadays verified for a wide class of interactions, says that the number of open gaps is *finite*

Our starting observation is that if the system is a quantum graph, nothing of that needs to be true!

First example: chain graphs

Consider a *chain graph*, an array of identical rings as sketched here

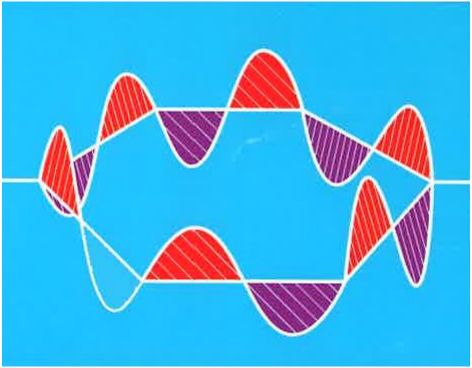


with the Hamiltonian acting as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ at each edge. We know that that to make it a self-adjoint operator, one has to impose *coupling conditions* at the vertices, and different conditions give rise to different Hamiltonians

Nevertheless, it is clear that n^2 with $n \in \mathbb{N}$ will (infinitely degenerate) eigenvalues irrespective of the coupling conidition choice; one usually speak of *Dirichlet eigenvalues*

Hence the spectrum is not purely *ac* and this trivial conclusion remains valid even if the chain loses it s mirror symmetry but the 'upper' and 'lower' edge lengths are *rationally related*

Dirichlet eigenvalues are easy to understand

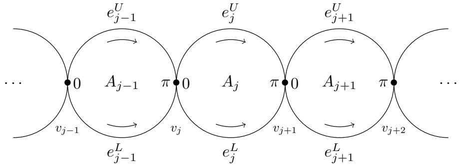


Courtesy: Peter Kuchment

It is also clear that quantum graphs can have compactly supported eigenfunctions

Spectrum may not be absolutely continuous at all

To illustrate this less trivial claim, consider the same graph 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 $H^2_{\rm loc}(\Gamma)$ satisfying

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

where $\mathfrak{n} = \{1, 2, \dots, n\}$ is the index set numbering the edges – in our case $n = 4$ – and $\alpha \in \mathbb{R}$ is the coupling constant

This is a particular case of the general conditions that make the operator self-adjoint [Kostrykin-Schrader'03]

Remarks

- The detailed shape of the magnetic field is not important, what matters is the flux through each ring. Without loss of generality we may suppose that A is constant on each ring

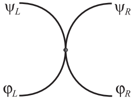
- In general, the field and the coupling constants may change from ring to ring. We denote the operator of interest as $-\Delta_{\alpha,A}$, where $\alpha = \{\alpha_j\}_{j\in\mathbb{Z}}$ and $A = \{A_j\}_{j\in\mathbb{Z}}$ are sequences of real numbers; in any of them is constant we replace it simply by that number

- At the moment we are interested in the *fully periodic case* when both α and A are constant; later we will consider perturbations of such a system

- We exclude the case when some $\alpha_j = \infty$ which corresponds to Dirichlet decoupling of the chain in the particular vertex

- Without loss of generality we may suppose that the circumference of each ring is 2π, and as usual we employ units in which we have $\hbar = 2m = e = c = 1$, where e is electron charge (forget $\frac{e^2}{\hbar c} = \frac{1}{137}$)

Floquet-Bloch analysis of the fully periodic case



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 negative we put instead $k = i\kappa$ with $\kappa > 0$.

The functions have to be matched through *(a) the δ-coupling* and *(b) Floquet-Bloch conditions*. This 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

$$\xi(k) := \frac{1}{\cos A\pi}\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right),$$

for any $k \in \mathbb{R} \cup i\mathbb{R} \setminus \{0\}$ and the discriminant equal to $D = 4(\xi(k)^2 - 1)$

Apart from the cases $A - \frac{1}{2} \in \mathbb{Z}$ and $k \in \mathbb{N}$ we have $k^2 \in \sigma(-\Delta_\alpha)$ *iff* the condition $|\xi(k)| \leq 1$ is satisfied.

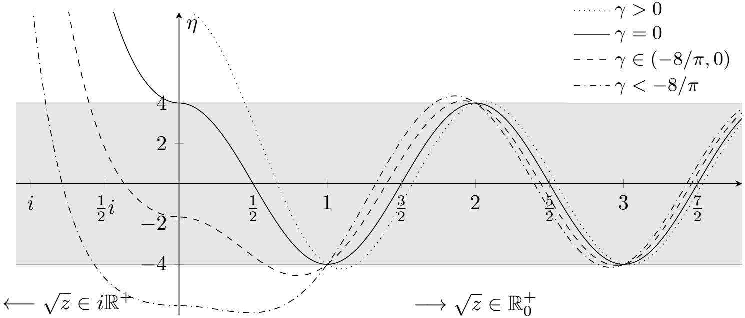
The fully periodic case, continued

Theorem (E-Manko'15)

Let $A \notin \mathbb{Z}$. If $A - \frac{1}{2} \in \mathbb{Z}$, then the spectrum of $-\Delta_\alpha$ consists of two series of infinitely degenerate ev's $\{k^2 \in \mathbb{R} \colon \xi(k) = 0\}$ and $\{k^2 \in \mathbb{R} \colon k \in \mathbb{N}\}$. On the other hand, if $A - \frac{1}{2} \notin \mathbb{Z}$, the spectrum of $-\Delta_\alpha$ consists of infinitely degenerate eigenvalues k^2 with $k \in \mathbb{N}$, and absolutely continuous spectral bands. Each of these bands except the first one is contained in an interval $(n^2, (n+1)^2)$ with $n \in \mathbb{N}$. The first band is included in $(0,1)$ if $\alpha > 4(|\cos A\pi| - 1)/\pi$, or it is negative if $\alpha < -4(|\cos A\pi| + 1)/\pi$, otherwise it contains the point $k^2 = 0$.

Remarks: (a) We ignore the case $A \in \mathbb{Z}$ which is by a simple gauge transformation equivalent to the non-magnetic case, $A = 0$
(b) In contrast to 'Dirichlet' eigenfunctions with one ring as an 'elementary cell', the 'other' eigenvalues arising for $A - \frac{1}{2} \in \mathbb{Z}$ are supported by *two adjacent rings*

In picture: determining the spectral bands



The picture refers to $A = 0$ with $\eta(z) := 4\xi(\sqrt{z})$ and $\gamma = \alpha$

For $A - \frac{1}{2} \notin \mathbb{Z}$ the situation is similar, just the width of the band changes to $4\cos A\pi$, on the other hand, for $A - \frac{1}{2} \in \mathbb{Z}$ it *shrinks to a line*

Local perturbations

Let me spend a minute on *local perturbations* of such chain graphs. A common wisdom is that they give rise to *eigenvalues in the gaps*

Again the usual intuition should be treated with caution when graphs are involved – it *may* or *may not* be so

Local perturbations may be of many different sorts:

- geometric: changing edge lengths or vertex positions
- coupling constant changes
- local variations of the magnetic field

A useful tool to treat them is to rephrase the problem as a system of *difference equation*

Duality

The idea was put forward by physicists – *Alexander* and *de Gennes* – and later treated rigorously in [Cattaneo'97] [E'97], and [Pankrashkin'13]

We exclude possible Dirichlet eigenvalues from our considerations assuming $k \in \mathfrak{K} := \{z\colon \operatorname{Im} z \geq 0 \wedge z \notin \mathbb{Z}\}$. On the one hand, we have the differential equation

$$(-\Delta_{\alpha,A} - k^2) \begin{pmatrix} \psi(x,k) \\ \varphi(x,k) \end{pmatrix} = 0$$

with the components referring to the upper and lower part of Γ, on the other hand the difference one

$$\psi_{j+1}(k) + \psi_{j-1}(k) = \xi_j(k)\psi_j(k)\,, \quad k \in \mathfrak{K}\,,$$

where $\psi_j(k) := \psi(j\pi, k)$ and $\xi(k)$ was introduced above, ξ_j corresponding the coupling α_j. The two equations are intimately related.

Duality, continued

Theorem

Let $\alpha_j \in \mathbb{R}$, then any solution $\begin{pmatrix} \psi(\cdot,k) \\ \varphi(\cdot,k) \end{pmatrix}$ with $k^2 \in \mathbb{R}$ and $k \in \mathfrak{K}$ satisfies the difference equation, and conversely, the latter defines via

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

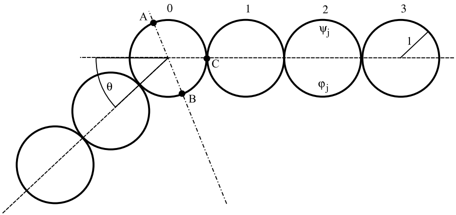
$$+ (\psi_{j+1}(k)\mathrm{e}^{\pm iA\pi} - \psi_j(k) \cos k\pi) \frac{\sin k(x-j\pi)}{\sin k\pi} \Big], \quad x \in (j\pi, (j+1)\pi),$$

solutions to the former satisfying the δ-coupling conditions. In addition, the former belongs to $L^p(\Gamma)$ if and only if $\{\psi_j(k)\}_{j\in\mathbb{Z}} \in \ell^p(\mathbb{Z})$, the claim being true for both $p \in \{2, \infty\}$.

Local perturbation examples

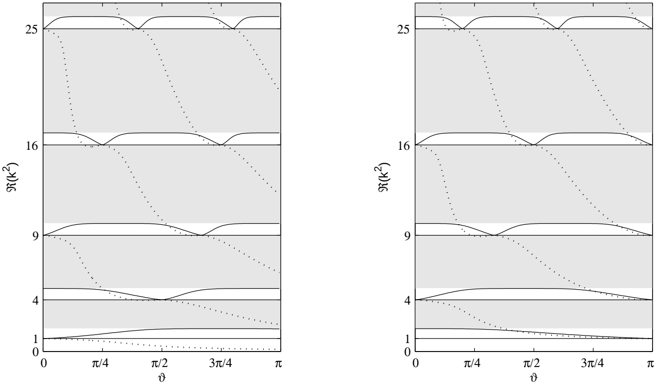
Consider first non-magnetic perturbations. We skip the theory referring to [Duclos-E-Turek'08, E-Manko'15] and show just examples of the results

Bending the chain: we move one vertex as sketched here



and ask how the spectrum depends on the angle ϑ. In this example we suppose that the magnetic field is absent

In picture: bent-chain spectrum for $\alpha = 3$



for the even and odd part of the problem, respectively [Duclos-E-Turek'08]

Similar pictures we get for other values of α, the dotted lines in the figures mark (real values) of resonance positions

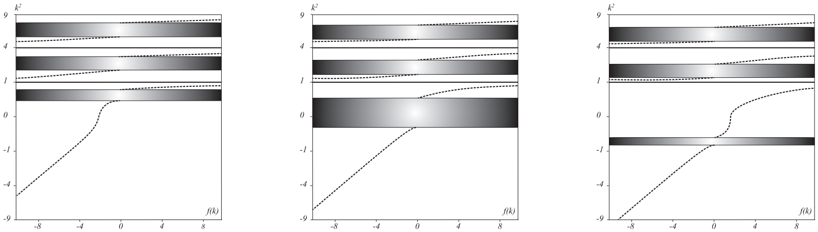
We see that the eigenvalues in gaps may be absent but only at rational values of ϑ and never simultaneously

Example: a single coupling constant changed

Let the couplings be $\{\dots, \alpha, \alpha+\gamma_1, \alpha, \dots\}$ and $A \notin \mathbb{Z}$, then we have

Proposition ([E-Manko'15])

Let $A \notin \mathbb{Z}$. The essential spectrum of $-\Delta_{\alpha+\gamma,A}$ coincides with that of $-\Delta_\alpha$. If $\gamma_1 < 0$ there is precisely one simple impurity state in every odd gap, on the other hand, for $\gamma_1 > 0$ there is precisely one simple impurity state in every even gap.



The energy k^2 *vs.* $\gamma_1 = f(k)$ for $\cos A\pi = 0.6$ and the coupling strength (i) $\alpha = 1$, (ii) $\alpha = -1$, (iii) $\alpha = -3$

More general duality

We may consider more general chain graphs, for instance, the magnetic field may vary, $A = \{A_j\}_{j\in\mathbb{Z}}$, the same may be true for the ring (half-)perimeters, $\ell = \{\ell_j\}_{j\in\mathbb{Z}}$, etc.

What is important, the above *duality holds again*, with the difference relation being

$$\sin(k\ell_{j-1})\cos(A_j\ell_j)\psi_{j+1}(k) + \sin(k\ell_j)\cos(A_{j-1}\ell_{j-1})\psi_{j-1}(k) \\ = \Big(\frac{\alpha}{2k}\sin(k\ell_{j-1})\sin(k\ell_j) + \sin k(\ell_{j-1}+\ell_j)\Big)\psi_j(k)\,, \quad k\in\mathfrak{K}\,,$$

where $\psi_j(k) := \psi(x_j,k)$, and the reconstruction formula becomes

$$\begin{pmatrix} \psi(x,k) \\ \varphi(x,k) \end{pmatrix} = \mathrm{e}^{\mp iA_j(x-x_j)}\Big[\psi_j(k)\cos k(x-x_j) \\ +(\psi_{j+1}(k)\mathrm{e}^{\pm iA_j\ell_j} - \psi_j(k)\cos k\ell_j)\frac{\sin k(x-x_j)}{\sin k\ell_j}\Big]\,,\;\; x\in(x_j,x_{j+1})\,,$$

Example again: a single flux altered

We suppose that the field is modified on a single ring, i.e. $A = \{\dots, A, A_1, A \dots\}$, the we have a single simple eigenvalue in each gap provided [E-Manko'17]

$$\frac{|\cos A_1 \pi|}{|\cos A\pi|} > 1\,,$$

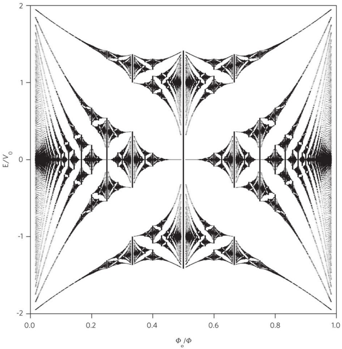
otherwise the spectrum does not change.

In particular, the perturbation may give rise to *no eigenvalues in gaps* at all; note that this happens if the perturbed ring is *'further from the non-magnetic case'*

Note also that the eigenvalue may split from the *ac* spectral band of the unperturbed system and lies between this band and the nearest eigenvalue of infinite multiplicity. When we change the magnetic field, the eigenvalue may absorbed in the same band. On the other hand no eigenvalue emerges from the degenerate band.

Can periodic graphs have "wilder" spectra?

Let us first recall the picture everybody knows



representing the spectrum of the difference operator associated with the *almost Mathieu equation*

$$u_{n+1} + u_{n-1} + 2\lambda \cos(2\pi(\omega + n\alpha))u_n = \epsilon u_n$$

for $\lambda = 1$, otherwise called *Harper equation*, as a function of α

Nice mathematics, but do such things exist?

Fractal nature of spectra for electron on a lattice in a homogeneous magnetic field was conjectured by [Azbel'64] but it caught the imagination only after Hofstadter made the structure visible

It triggered a long and fruitful mathematical quest culminating by the proof of the *Ten Martini Conjecture* by Avila and Jitomirskaya in 2009, that is that the spectrum for an *irrational* field is a *Cantor set*

On the physical side, the effect remained theoretical for a long time and thought of in terms of the mentioned setting, with lattice and and a homogeneous field providing the needed two length scales, generically incommensurable, from the lattice spacing and the cyclotron radius

The first experimental demonstration of such a spectral character was done instead in a microwave waveguide system with suitably placed obstacles simulating the almost Mathieu relation [Kühl et al'98]

Only recently an experimental realization of the original concept was achieved using a graphene lattice [Dean et al'13], [Ponomarenko'13]

Globally non-constant magnetic field

Our goal is now to investigate whether a similar effect can be seen in a 'one-dimensional' system. *The coupling constant will be in this part denoted γ*! To his aim we again employ duality

However, the above version dealing with weak solutions is not sufficient, we need a stronger one proved in [Pankrashkin'13] using boundary triples

We exclude the Dirichlet eigenvalues, $\sigma_D = \{k^2 :\ k \in \mathbb{N}\}$, and introduce

$$s(x;z) = \begin{cases} \frac{\sin(x\sqrt{z})}{\sqrt{z}} & \text{for } z \neq 0, \\ x & \text{for } z = 0, \end{cases} \quad \text{and} \quad c(x;z) = \cos(x\sqrt{z})$$

Theorem (after Pankrashkin'13)

For any interval $J \subset \mathbb{R} \setminus \sigma_D$, the operator $(H_{\gamma,A})_J$ 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 $(L_A q\varphi)_j = 2\cos(A_j\pi)\varphi_{j+1} + 2\cos(A_{j-1}\pi)\varphi_{j-1}$ and

$$\eta(z) := \gamma s(\pi;z) + 2c(\pi;z) + 2s'(\pi;z)$$

Non-constant magnetic field, continued

Corollary

The spectrum of $-\Delta_{\gamma,A}$ *is bounded from below and can be decomposed into the discrete set* $\sigma_D = \{n^2 |\, n \in \mathbb{N}\}$ *of infinitely degenerate eigenvalues and the part* σ_{L_A} *determined by* L_A, $\sigma(-\Delta_{\gamma,A}) = \sigma_p \cup \sigma_{L_A}$, *where* σ_{L_A} *can be written as the union*

$$\sigma_{L_A} = \bigcup_{n=0}^{\infty} \sigma_n$$

with $\sigma_n = \eta^{(-1)}\big(\sigma(L_A)\big) \cap I_n$ *for* $n \geq 0$, $I_n = \eta^{(-1)}\big([-4,4]\big) \cap \big(n^2, (n+1)^2\big)$ *for* $n > 0$, *and* $I_0 = \eta^{(-1)}\big([-4,4]\big) \cap \big(-\infty, 1\big)$.

When $\gamma \neq 0$, *the spectrum has always gaps between the* σ_n*'s. For* $\gamma > 0$, *the spectrum is positive. For* $\gamma < -8\pi$, *the spectrum has a negative part and does not contain zero. Finally,* $0 \in \sigma(-\Delta_{\gamma,A})$ *holds if and only if* $\gamma\pi + 4 \in \sigma(L_A)$.

Pay attention: In general, the σ_n's may *very different* from absolutely continuous spectral bands!

A linear field growth

Suppose now that $A_j = \alpha j + \theta$ holds for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. We denote the corresponding operator L_A by $L_{\alpha,\theta}$, i.e.

$$(L_{\alpha,\theta}\varphi)_j = 2\cos\big(\pi(\alpha j + \theta)\big)\varphi_{j+1} + 2\cos\big(\pi(\alpha j - \alpha + \theta)\big)\varphi_{j-1}$$

for all $j \in \mathbb{Z}$. The rational case, $\alpha = p/q$, is easily dealt with.

Proposition

Assume that $\alpha = p/q$, where p and q are relatively prime. Then

(a) If $\alpha j + \theta + \frac{1}{2} \notin \mathbb{Z}$ for all $j = 0, \dots, q-1$, then $L_{\alpha,\theta}$ has purely ac spectrum that consists of q closed intervals possibly touching at the endpoints. In particular, $\sigma(L_{\alpha,\theta}) = \big[-4|\cos(\pi\theta)|, 4|\cos(\pi\theta)|\big]$ holds if $q = 1$.

(b) If $\alpha j + \theta + \frac{1}{2} \in \mathbb{Z}$ for some $j = 0, \dots, q-1$, then the spectrum of $L_{\alpha,\theta}$ is of pure point type consisting of q distinct eigenvalues of infinite degeneracy. In particular, $\sigma(L_{\alpha,\theta}) = \{0\}$ holds if $q = 1$.

An irrational slope

On the other hand, if $\alpha \notin \mathbb{Q}$ the spectrum of $L_{\alpha,\theta}$ is closely related to that of the almost Mathieu operator $H_{\alpha,\lambda,\theta}$ in the critical situation, $\lambda = 2$, acting as

$$\left(H_{\alpha,\theta,\lambda}\varphi\right)_j = \varphi_{j+1} + \varphi_{j-1} + \lambda \cos(2\pi\alpha j + \theta)\varphi_j$$

for any $\varphi \in \ell^2(\mathbb{Z})$ and all $j \in \mathbb{Z}$.

From the mentioned deep results of Avila, Jitomirskaya, and Krikorian we know that for any $\alpha \notin \mathbb{Q}$, the spectrum of $H_{\alpha,2,\theta}$ does not depend on θ and it is a *Cantor set of Lebesgue measure zero*

In the same way as in [Shubin'94] one can demonstrate an unitary equivalence which means, in particular, that the spectra of $H_{\alpha,\theta,2}$ and $L_{\alpha,\theta}$ coincide

Combining all these results we can describe the spectrum of our original operator in case the magnetic field varies linearly along the chain

The linear-field spectrum

Theorem (E-Vašata'17)

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

a. *If $\alpha, \theta \in \mathbb{Z}$ and $\gamma = 0$, then $\sigma(-\Delta_{\gamma,A}) = \sigma_{ac}(-\Delta_{\gamma,A}) \cup \sigma_{pp}(-\Delta_{\gamma,A})$ where $\sigma_{ac}(-\Delta_{\gamma,A}) = [0, \infty)$ and $\sigma_{pp}(-\Delta_{\gamma,A}) = \{n^2 |\, n \in \mathbb{N}\}$.*
b. *If $\alpha = p/q$ with p and q relatively prime, $\alpha j + \theta + \frac{1}{2} \notin \mathbb{Z}$ for all $j = 0, \dots, q-1$ and assumptions of (a) do not hold, then $-\Delta_{\gamma,A}$ has infinitely degenerate ev's at the points of $\{n^2 |\, n \in \mathbb{N}\}$ and an ac part of the spectrum in each interval $(-\infty, 1)$ and $\big(n^2, (n+1)^2\big)$, $n \in \mathbb{N}$ consisting of q closed intervals possibly touching at the endpoints.*
c. *If $\alpha = p/q$, where p and q are relatively prime, and $\alpha j + \theta + \frac{1}{2} \in \mathbb{Z}$ for some $j = 0, \dots, q-1$, then the spectrum $-\Delta_{\gamma,A}$ is of pure point type and such that in each interval $(-\infty, 1)$ and $\big(n^2, (n+1)^2\big)$, $n \in \mathbb{N}$ there are exactly q distinct eigenvalues and the remaining eigenvalues form the set $\{n^2 |\, n \in \mathbb{N}\}$. All the eigenvalues are infinitely degenerate.*

The linear-field spectrum, continued

Theorem (E-Vašata'17, cont'd)

(d) *If $\alpha \notin \mathbb{Q}$, then $\sigma(-\Delta_{\gamma,A})$ 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 $\big(n^2, (n+1)^2\big)$, $n \in \mathbb{N}$. Moreover, the overall Lebesgue measure of $\sigma(-\Delta_{\gamma,A})$ is zero.*

Using a fresh result of [Last-Shamis'16] we can also show

Proposition

Let $A_j = \alpha j + \theta$ for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. There exist a dense G_δ set of the slopes α for which, and all θ, the Haussdorff dimension

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

Remark: If you regard a linear field *unphysical*, you may either view it as an *idealization* or to replace it a *quasiperiodic function* with the *same slope* leading to *the same result*.

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

Let us be more precise, If you open [Berkolaiko-Kuchment'13] you will see they recall how things look like for 'ordinary' Schrödinger operators where the dimension is known to be decisive:the 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* to which we have nowadays an affirmative answer in a large number of cases

The reasoning relies on the behavior of the spectral bands, i.e. ranges of the dispersion curves/surfaces. They typically overlap if $\nu \geq 2$ making opening of gaps more and more difficult as the energy increases

Berkolaiko and Kuchment say that the situation with graphs is similar, however, they add immediately that *this is not a strict law* and illustrate this claim on resonant gaps created by a graph 'decoration', see also [Schenker-Aizenman'00]

The question: is it a 'law' after all?

More exactly, 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 the standard coupling conditions

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

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

Theorem ([E-Turek'17])

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

Proof idea

The spectrum is determined by *secular equation* [B-K'13]: we define

$$F(k;\vec{\vartheta}) := \det\left(\mathsf{I} - \mathrm{e}^{i(\mathsf{A}+k\mathsf{L})}\mathsf{S}(k)\right),$$

where the $2E \times 2E$ matrices A, L, and S are as follows: the diagonal matrix L is given by the lengths of the directed edges (bonds) of Γ, the diagonal A has entries $\mathrm{e}^{\pm i\vartheta_l}$ at points of the 'Brillouin torus identification', all the others are zero, and finally, S is the *bond scattering matrix*

Then $k^2 \in \sigma(H)$ holds if there is a quasimomentum values $\vec{\vartheta} \in (-\pi,\pi]^\nu)$ such that the equation $F(k;\vec{\vartheta}) = 0$ is satisfied

We note that $F(k;\vec{\vartheta}$ depends on $\vec{\vartheta}$ and $(k\ell_0, k\ell_1, \dots, k\ell_d)$, where $\{\ell_0, \ell_1, \dots, \ell_d\}$, $d+1 \le E$ are the mutually different edge lengths of Γ. If the ℓ's are rationally related, the function is *periodic* in k, hence if there is a gap, there are *infinitely many of them*

Proof idea, and an extension

If the lengths are *not* rationally related, their ratios can be *approximated by rationals* with an arbitrary precision.

If k^2 is in a gap, i.e. $|F(k;\vec{\vartheta})| > \delta$ for some $\delta > 0$ and all $\vec{\vartheta} \in (-\pi, \pi]^\nu$) – recall that $|F(k;\cdot))|$ has a minimum at the torus – then its value will *remain separated from zero* when the ℓ's are replaced by the rational approximants and k is large enough. $\square$

Recall next that the vertex conditions can be equivalently written as

$$\begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi$$

for certain r, S, and T, where $I^{(r)}$ is the identity matrix of order r; the coupling is scale-invariant if and only if the square matrix $S = 0$

We will consider two *associated* quantum graph Hamiltonians, H with the above vertex coupling, and H_0 where we replace S by zero

A result for this associated pair

Proposition ([E-Turek'17])

For the spectra $\sigma(H)$ and $\sigma(H_0)$ the following claims hold true:

(i) *If $\sigma(H_0)$ has an open gap, then $\sigma(H)$ has infinitely many gaps.*

(ii) *If the edge lengths are rationally dependent, then the gaps of $\sigma(H)$ asymptotically coincide with those of $\sigma(H_0)$.*

Proof idea: The argument is based on the following observation: the on-shell S-matrix for H

$$\mathcal{S}(k) = -I^{(n)} + 2 \begin{pmatrix} I^{(r)} \\ T^* \end{pmatrix} \left(I^{(r)} + TT^* - \frac{1}{ik} S \right)^{-1} \begin{pmatrix} I^{(r)} & T \end{pmatrix}$$

Hence the scale-invariant part is, naturally, independent of k, and *the Robin part is $\mathcal{O}(k^{-1})$*

The same is true for $\mathrm{S}(k)$, and as consequence, the spectrum at high energies is mostly determined by the scale-invariant part. □

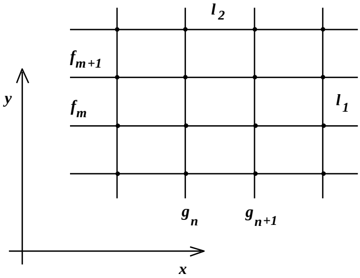
So, are there any BS graphs?

Our next goal is to give an affirmative answer:

Theorem ([E-Turek'17])

Bethe–Sommerfeld graphs exist.

As usual with existence claims, it is enough to demonstrate an example. With this aim we are going to revisit the model of a *rectangular lattice graph* introduced in [E'96, E-Gawlista'96]



Spectral condition

According to [E'96], a number $k^2 > 0$ belongs to a gap if and only if $k > 0$ satisfies the gap condition, which reads

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

and

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

where we denote the edge lengths ℓ_j, $j = 1, 2$, as a, b; 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

What is known

The spectrum depends on the ratio $\theta = \frac{\ell_1}{\ell_2}$. If θ is rational, $\sigma(H)$ has 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 continuous 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

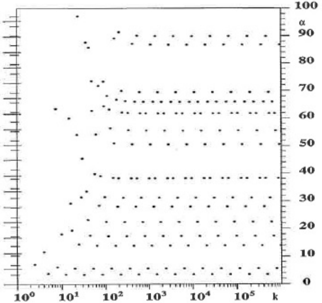
$$\mu(\theta) := \inf \left\{ c > 0 \;\middle|\; (\exists_\infty (p, q) \in \mathbb{N}^2) \left(\left| \theta - \frac{p}{q} \right| < \frac{c}{q^2} \right) \right\};$$

we note that $\mu(\theta) = \mu(\theta^{-1})$

The golden mean situation

Let us start with the *golden mean*, $\phi = \frac{\sqrt{5}+1}{2} = [1;1,1,\dots]$, which can be regarded as the 'worst' irrational

The answer is not a priori clear: let us plot the minima of the function appearing in the first gap condition, i.e. for $\alpha > 0$



Note that they approach the limit values *from above*, also that the series open at $\frac{\pi^2}{\sqrt{5ab}}\phi^{\pm 1/2}|n^2 - m^2 - nm|,\ n, m \in \mathbb{N}$ [E-Gawlista'96]

But a closer look shows a more complex picture

Theorem ([E-Turek'17])

Let $\frac{a}{b} = \phi = \frac{\sqrt{5}+1}{2}$*, 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 Bethe–Sommerfeld 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:

Theorem ([E-Turek'17])

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

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

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

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

More general result

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

Theorem ([E-Turek'17])

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.

BS property does not need a definite sign of α

Proposition ([E-Turek'17])

Let the edge ratio be

$$\theta = \frac{2t^3 - 2t^2 - 1 + \sqrt{5}}{2(t^4 - t^3 + t^2 - t + 1)} \quad \text{for} \;\; t \in \mathbb{N},\; t \geq 3\,;$$

then there is a nonzero and finite number of gaps in the positive spectrum for some $\alpha > 0$ and for some $\alpha < 0$ as well

Note that the above number θ can be written as $\theta = \frac{t\phi+1}{(t^2+1)\phi+t}$ with $\phi = \frac{1+\sqrt{5}}{2}$, and moreover, the continued-fraction representation of θ is $[0; t, t, 1, 1, 1, 1, \dots]$. Furthermore, we have $\mu(\theta) = \mu(\phi) = \frac{1}{\sqrt{5}}$.

The talk was based on

[EM15] P.E., Stepan Manko: Spectra of magnetic chain graphs: coupling constant perturbations, *J. Phys. A: Math. Theor.* **48** (2015), 125302 (20pp)

[EM17] P.E., Stepan Manko: Spectral properties of magnetic chain graphs, *Ann. H. Poincaré* **18** (2017), 929–953.

[EV17] P.E., Daniel Vašata: Cantor spectra of magnetic chain graphs, *J. Phys. A: Math. Theor.* **50** (2017), 165201 (13pp)

[EY17] P.E., Ondřej Turek: Periodic quantum graphs from the Bethe-Sommerfeld point of view, *in preparation*

as well as the other papers mentioned in the course of the presentation.

It remains to say, albeit a bit belatedly

Happy birthday, Petr!

Biz hundert un tsvantsik!