Spectra of periodic quantum graphs and the effect of local perturbations

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Talk overview

In this talk I am going to discuss several recent results on spectral properties of periodic quantum graphs:

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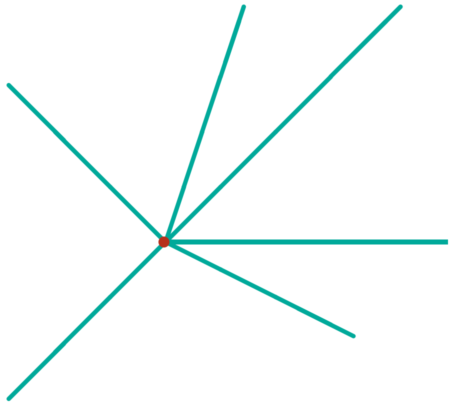
- *Gap structure,* in particular, the high-energy behaviour of the spectrum
- *Dispersion functions,* in particular, location of the band edges in the Brillouin zone
- *Local perturbations:* eigenvalues in gaps and resonances they produce, in a simple model framework

Quantum graphs: vertex coupling



The most simple example is a *star graph* with the state Hilbert space $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and the particle Hamiltonian acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j''$

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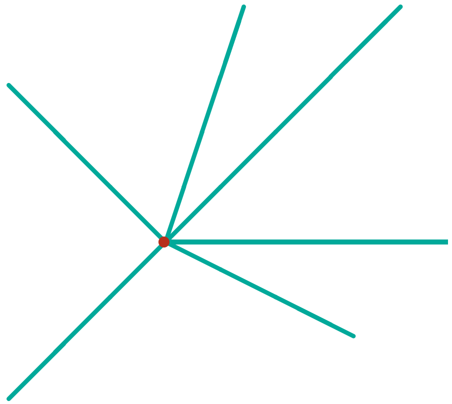

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Since it is second-order, the boundary condition involve $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$ being of the form

$$A\Psi(0) + B\Psi'(0) = 0\,;$$

by [Kostrykin-Schrader'99] the $n \times n$ matrices A, B give rise to a self-adjoint operator if they satisfy the conditions

- $\operatorname{rank}(A, B) = n$
- AB^* is self-adjoint

Unique boundary conditions

The non-uniqueness of the above b.c. can be removed:

Proposition [Harmer'00, K-S'00]: Vertex couplings are uniquely characterized by unitary $n \times n$ matrices U such that

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One can derive them modifying the argument used in [Fülöp-Tsutsui'00] for generalized point interactions, $n = 2$

Self-adjointness requires vanishing of the boundary form,

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

which occurs *iff* the norms $\|\Psi(0) \pm i\ell\Psi'(0)\|_{\mathbb{C}^n}$ with a fixed $\ell \neq 0$ coincide, so the vectors must be related by an $n \times n$ unitary matrix; this gives $(U - I)\Psi(0) + i\ell(U + I)\Psi'(0) = 0$

Examples of vertex coupling

- Denote by $\mathcal{J}$ the $n \times n$ matrix whose all entries are equal to one; then $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ corresponds to the standard δ *coupling*,

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

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- $\alpha = 0$ corresponds to the "free motion", the so-called *free boundary conditions* (better name than Kirchhoff)

- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the δ_s' *coupling*

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

with $\beta \in \mathbb{R}$; for $\beta = \infty$ we get *Neumann* decoupling, etc.

Periodic quantum graphs

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- the spectrum has in general a *gap structure*
- it *need not be absolutely continuous* since the unique continuation principle may not hold, in particular, if graph edge lengths are rationally related
- local perturbations can produce *eigenvalues*, in the gaps or embedded, and *resonances*

Gap structure

The first question is about the *gap structure*:

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From lattice-graph models [E'96, E-Gawlista'96] we know

- A rectangular lattice with Kirchhoff coupling has *no gaps* above the spectral threshold
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Can a *more general vertex coupling* produce other types of gap behaviour at high energies?

Square-lattice graphs

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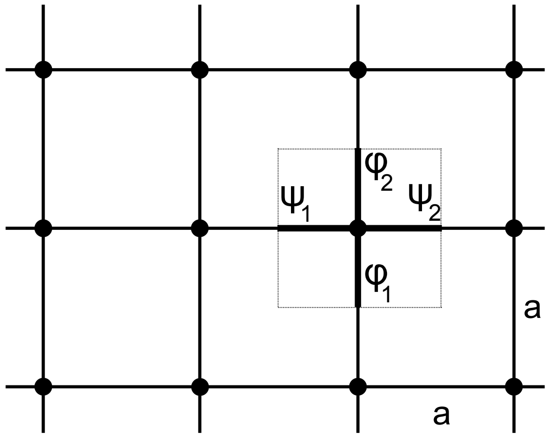
(b) The high-energy asymptotics of bands and gaps w.r.t. the band index n includes the following classes:

- *flat bands*, i.e. infinitely degenerate point spectrum,
- *bands* behaving as $\mathcal{O}(n^j),\ j = 1, 0, -1, -2, -3$, $n \to \infty$,
- *gaps* behaving as $\mathcal{O}(n^j),\ j = 1, 0$, as $n \to \infty$.

Depending on U the high-energy asymptotics of the spectrum may be a combination of the above listed types.

Proof outline

One has to perform Floquet analysis



for solutions with energy $E = k^2,\ k > 0$,

$$\begin{aligned}
\psi_1(x) &= C_1^+ \mathrm{e}^{\mathrm{i}kx} + C_1^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [-a/2, 0] \\
\psi_2(x) &= C_2^+ \mathrm{e}^{\mathrm{i}kx} + C_2^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0, a/2] \\
\varphi_1(x) &= D_1^+ \mathrm{e}^{\mathrm{i}kx} + D_1^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [-a/2, 0] \\
\varphi_2(x) &= D_2^+ \mathrm{e}^{\mathrm{i}kx} + D_2^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0, a/2]
\end{aligned}$$

Proof outline, continued

We introduce the following matrices,

$$\left\{ \begin{array}{c} M \\ N \end{array} \right\} := \begin{pmatrix} \pm e^{-\frac{i}{2}(\theta_1 - ak)} & e^{-\frac{i}{2}(\theta_1 + ak)} & 0 & 0 \\ e^{\frac{i}{2}(\theta_1 - ak)} & \pm e^{\frac{i}{2}(\theta_1 + ak)} & 0 & 0 \\ 0 & 0 & \pm e^{-\frac{i}{2}(\theta_2 - ak)} & e^{-\frac{i}{2}(\theta_2 + ak)} \\ 0 & 0 & e^{\frac{i}{2}(\theta_2 - ak)} & \pm e^{\frac{i}{2}(\theta_2 + ak)} \end{pmatrix}$$

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then the spectral condition becomes $\det(AM + ikBN) = 0$ where the KS matrices are

$$-A = \begin{pmatrix} S & 0 \\ -T^* & I^{(4-m)} \end{pmatrix}, \quad B = \begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix},$$

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then the spectral condition becomes $\det(AM + ikBN) = 0$ where the KS matrices are chosen as [Cheon-E.-Turek'10]

$$-A = \begin{pmatrix} S & 0 \\ -T^* & I^{(4-m)} \end{pmatrix}, \quad B = \begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix},$$

The claim comes from a straightforward but rather tedious analysis of the particular cases $m = 0, 1, 2, 3, 4$ $\square$

Remarks

- The generic situation corresponds to $m = 4$ with all the edges coupled and gaps growing linearly with n

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- Each case with a fixed m covers a situations with flat bands corresponding to lattice decoupling into separated edges, or pairs of edges
- The lattice can separate into 'one-dimensional' subsets describing generalized Kronig-Penney models on lines or zigzag curves, or to 'combs'
- From the spectral point of view the case $m = 3$ is the richest, including situations with a power-like shrinking bands that occur for the graph decomposed into 'combs'

Spectral edges positions

Next we address another ‘dimension-related’ question. It is known that looking for band edges of one-dimensional periodic Schrödinger operator it is enough to check *endpoints of the Brillouin zone*

The same is often done in higher dimensions even if numerical counterexamples hint that caution is needed

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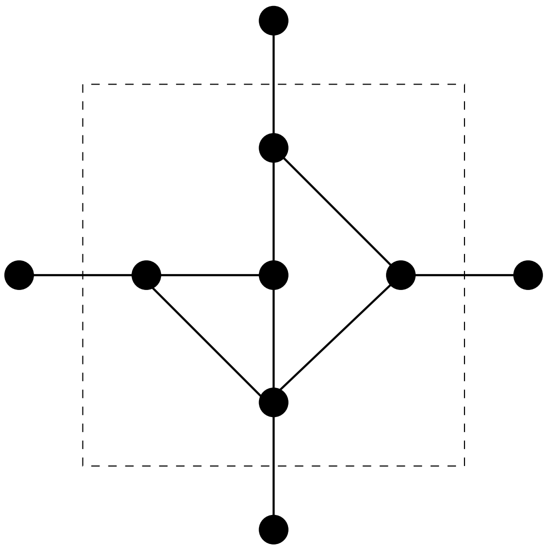
[Harrison-Kuchment-Sobolev-Winn’07] provided example of a periodic graph with the following basic cell



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They demonstrated that in this and some other examples spectral edges correspond to quasimomentum values *inside the Brillouin zone*

Graphs in those examples were $\mathbb{Z}^2$-periodic and some people kept believing that in case of $\mathbb{Z}$-periodicity it is sufficient to check periodic and antiperiodic solutions

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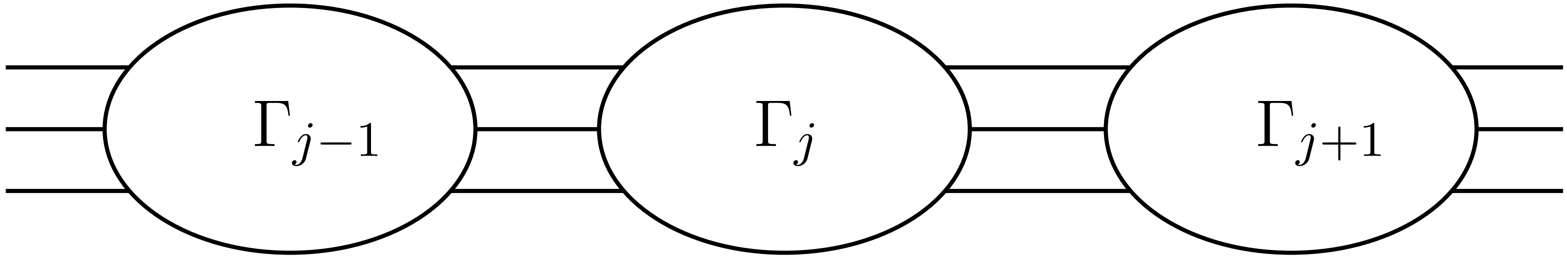
In order to see for which periodic systems such a claim can be made, let us look at periodic *chain graphs*



Formulation of the problem

Graph G consists of a chain of identical copies Γ_j of some graph Γ, consecutive copies being connected by m edges. The internal structure of Γ is not important

We equip G with a Laplacian is the way described above; for simplicity we assume that the edge coupling is *Kirchhoff*

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The standard Floquet theory applies. For quasimomentum $k \in [-\pi, \pi]$ we consider the fiber operator $H(k)$ defined by means of the condition $f(\tau_n x) = \mathrm{e}^{ikn} f(x)$ for $(n, x) \in \mathbb{Z} \times \Gamma$. Note that values $k = 0, \pm\pi$ refer to periodic and antiperiodic solutions, respectively

Spectrum of $H(k)$ is discrete consisting of eigenvalues $\lambda_j(k)$, $j = 1, 2, \ldots$. We look for values of k where extrema of the *band functions* $\lambda_j(\cdot)$ are attained

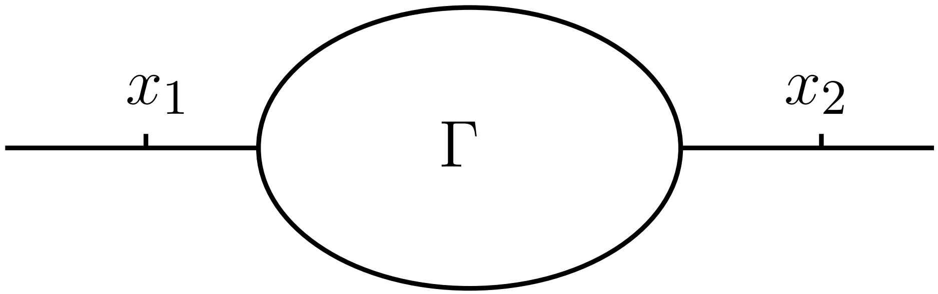
The result

Theorem [E-Kuchment-Winn'10]: Let G be a $\mathbb{Z}$-periodic "chain" graph G with m connecting edges and H be the corresponding Hamiltonian operator acting on $L^2(G)$. Then

(a) If $m = 1$, the endpoints of the bands $I_j = \lambda_j([-\pi, \pi])$, i.e. the extrema of the band functions, are *attained at the points* $k = 0, k = \pm\pi$ (although, they might be attained at some other points as well). In other words, the spectra of the periodic and anti-periodic problems provide the ends of the bands of the spectrum

(b) If $m > 1$, this is *not always true*

The case $m = 1$



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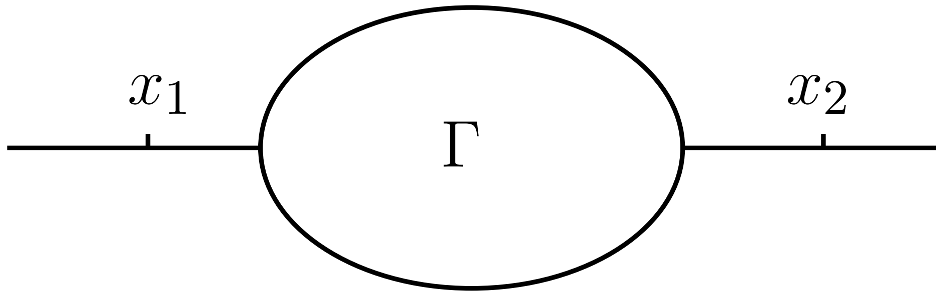

Lemma: Assume that $m = 1$.

(i) If some value λ is attained by the band functions $\lambda_j(k)$ at more than two points k in the segment $[-\pi, \pi]$, then there is a constant branch $\lambda(k) \equiv \lambda$ for all k, and thus this value is attained at all points of the segment

(ii) The set D of all such values λ is discrete (possibly empty)

(iii) If $\lambda \notin D$, then in a neighborhood of this value all band functions are strictly monotonous on $[0, \pi]$

The case $m = 1$, continued

Proof of the Lemma, outline: Suppose that a value λ is taken by $\lambda_j(k)$ at more than two points $k \in [-\pi, \pi]$. Then the solution space of $(H - \lambda)u = 0$ on G is more than two-dimensional, so there is a non-trivial solution u vanishing with its first derivative at a point x_1 on the connecting edge, and consequently, u vanishes on the whole edge containing x_1.

Using general results from Floquet theory we infer from here that $\sigma(H)$ contains the flat branch $\lambda_j(k) \equiv \lambda$ and that this can occur only at a discrete set D of values of λ

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Consider now $\lambda \notin D$. Due to the invariance of H w.r.t. complex conjugation, the band functions $\lambda_j(\cdot)$ are even, $\lambda_j(-k) = \lambda_j(k)$. This, together with $\lambda \notin D$ implies that all values near λ are attained by the (continuous) function $\lambda_j(\cdot)$ only once on $[0, \pi]$, so the function is monotonous there

Proof of the theorem

Suppose that λ is an extremum of a band function $\lambda_j(\cdot)$. If $\lambda \in D$, then the statement (i) of the Lemma claims that this value λ is attained at all values of k, in particular for $k = \pi, 0$ that correspond to the (anti)periodic problems

Let next $\lambda \notin D$. Then the statement (iii) of the Lemma implies that the corresponding value of k cannot be in the interior $(0, \pi)$ of the segment $[0, \pi]$. Thus, either $k = 0$ and λ belongs to the spectrum of the periodic problem, or $k = \pi$ and λ belongs to the spectrum of the anti-periodic problem

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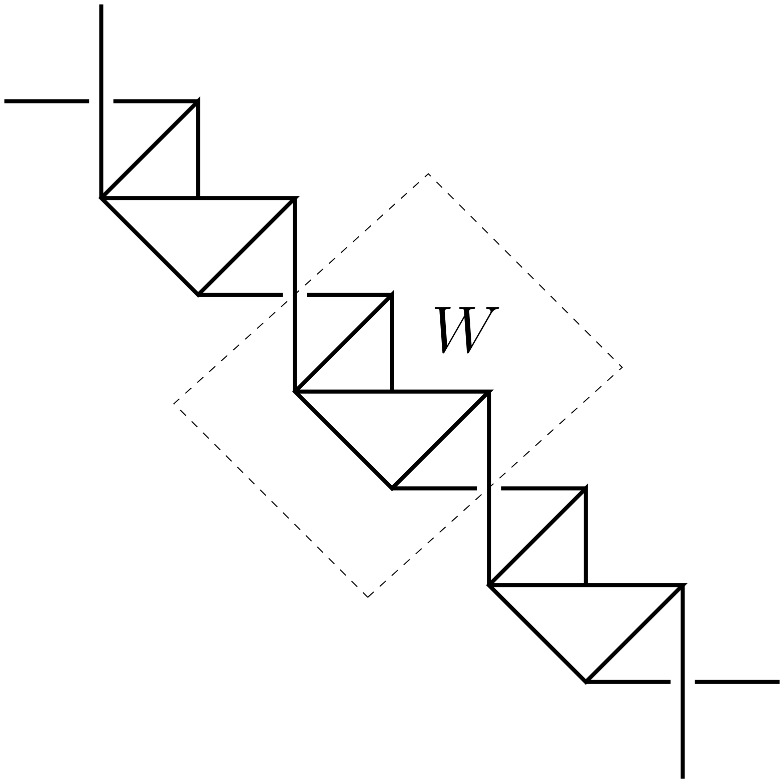
To prove the other part we construct an *example* of a chain with $m = 2$ by a suitable *folding of the $\mathbb{Z}^2$ periodic graph* from the paper [Harrison-Kuchment-Sobolev-Winn'07] we have mentioned above

Proof of the theorem, continued

By folding we get the following $\mathbb{Z}$ periodic graph with $m = 2$



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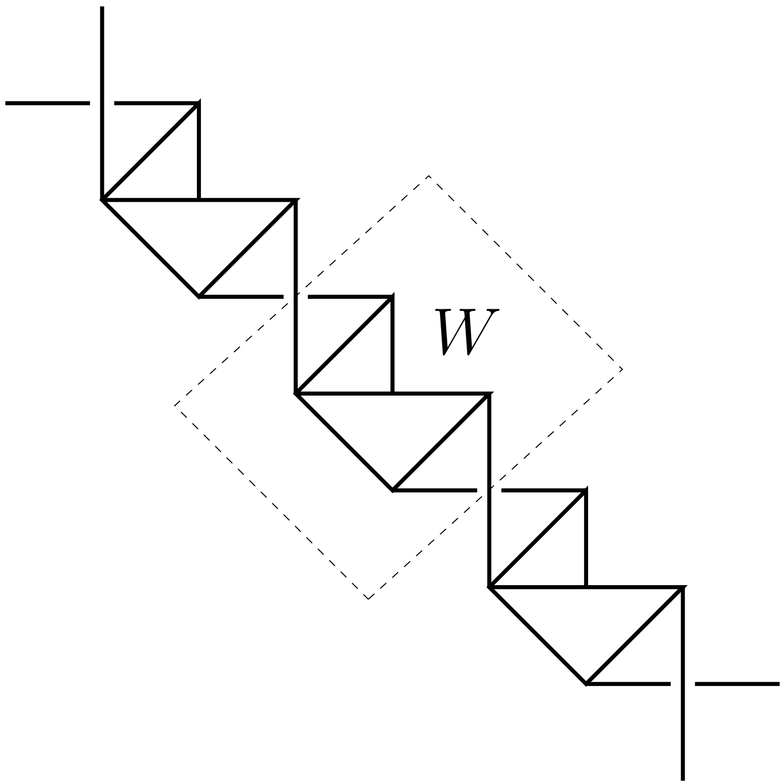

The second element of the proof is the *duality* between quantum (metric) graphs and combinatorial graphs [E'97]

Proof of the theorem, continued

The easiest thing is to assume that the above graph is *equilateral* then folding its spectrum (by $k \mapsto \cos k$) we get the spectrum of the discrete Laplace-Beltrami operator Δ on functions defined on the vertices of G, given by

$$(\Delta f)(v) := \frac{1}{\sqrt{d_v}} \sum_{u \sim v} \frac{1}{\sqrt{d_u}} f(u)\,,$$

where u and v are vertices, d_u is the degree of u, and the sum is taken over all vertices u adjacent to v

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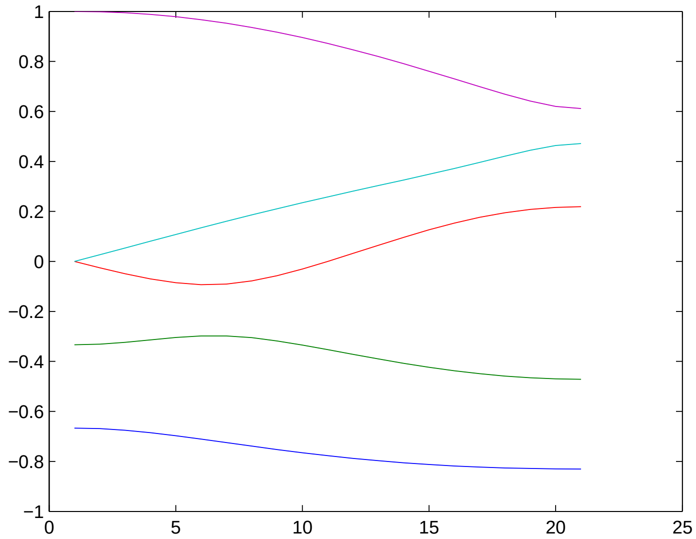
We arrive thus at the spectral problem for the matrix

$$\Delta(k) = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 3^{-1/2} & \mathrm{e}^{ik}/2 & 0 & 3^{-1/2} \\ 3^{-1/2} & 0 & 1/2 & \mathrm{e}^{ik}/3^{1/2} & 0 \\ \mathrm{e}^{-ik}/2 & 1/2 & 0 & 1/2 & 1/2 \\ 0 & \mathrm{e}^{-ik}/3^{1/2} & 1/2 & 0 & 3^{-1/2} \\ 3^{-1/2} & 0 & 1/2 & 3^{-1/2} & 0 \end{pmatrix}$$

Proof of the theorem, completed

It is straightforward to see that two spectral branches out of five have extremum *inside the Brillouin zone*



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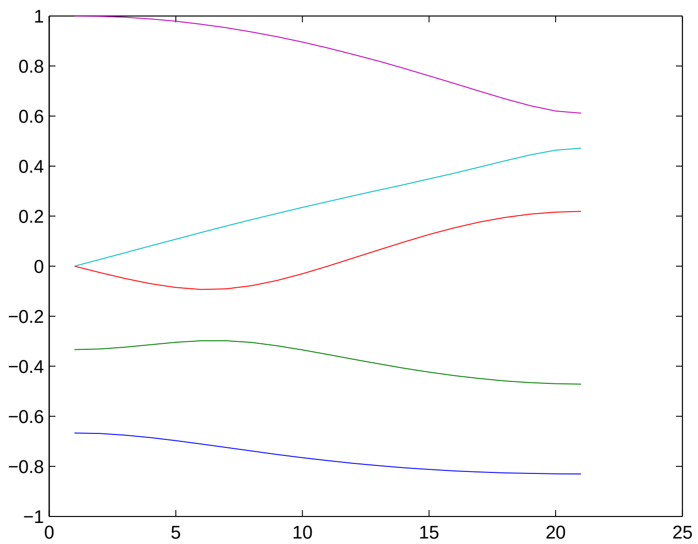

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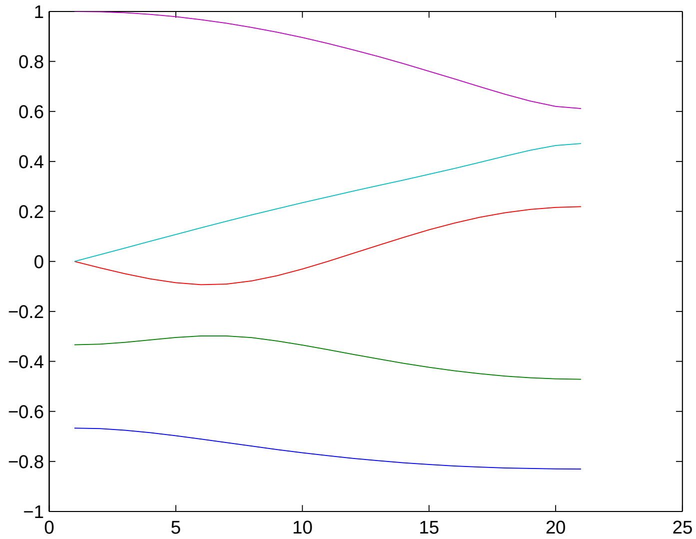

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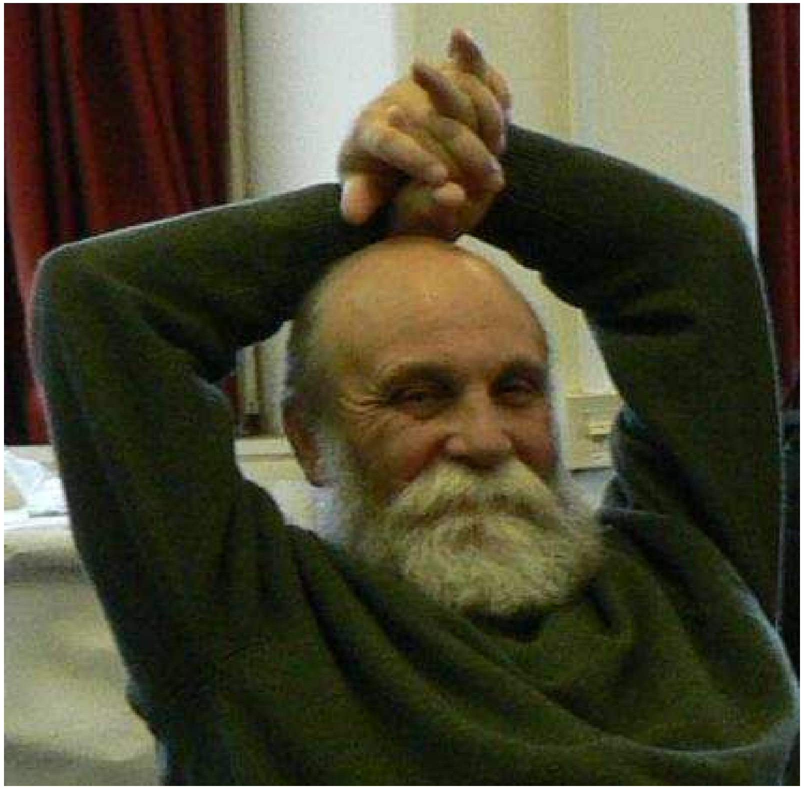
Remark: Conclusions can be extended to more general Schrödinger operators on $\mathbb{Z}$-periodic graphs

Remembering Pierre



Since this meeting is dedicated to the memory of Pierre Duclos it is appropriate to mention one of his last works

Local perturbations

Instead of attempting general claims we will try to analyze the effect in a simple *model setting* in which the effect mentioned in the introduction will be seen

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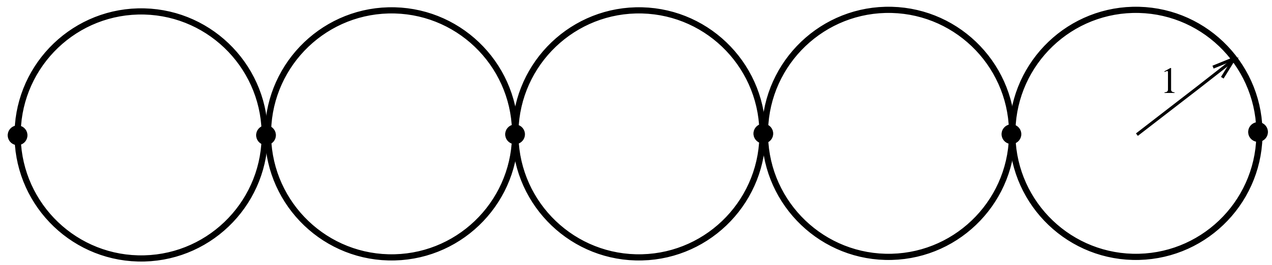
Instead of attempting general claims we will try to analyze the effect in a simple *model setting* in which the effect mentioned in the introduction will be seen

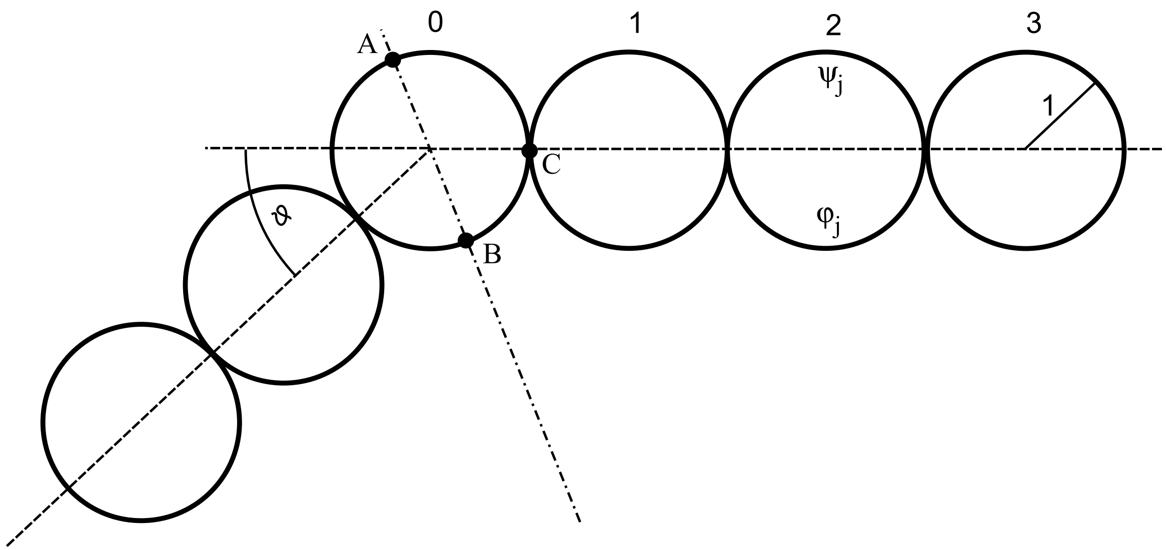
The model: we will analyze the *influence of a “bending” deformation* on a a “chain graph” which exhibits a one-dimensional periodicity



Without loss of generality we assume unit radii; the rings are connected by the δ-*coupling* of a strength $\alpha \neq 0$

Bending the chain

We will suppose that the chain is deformed as follows



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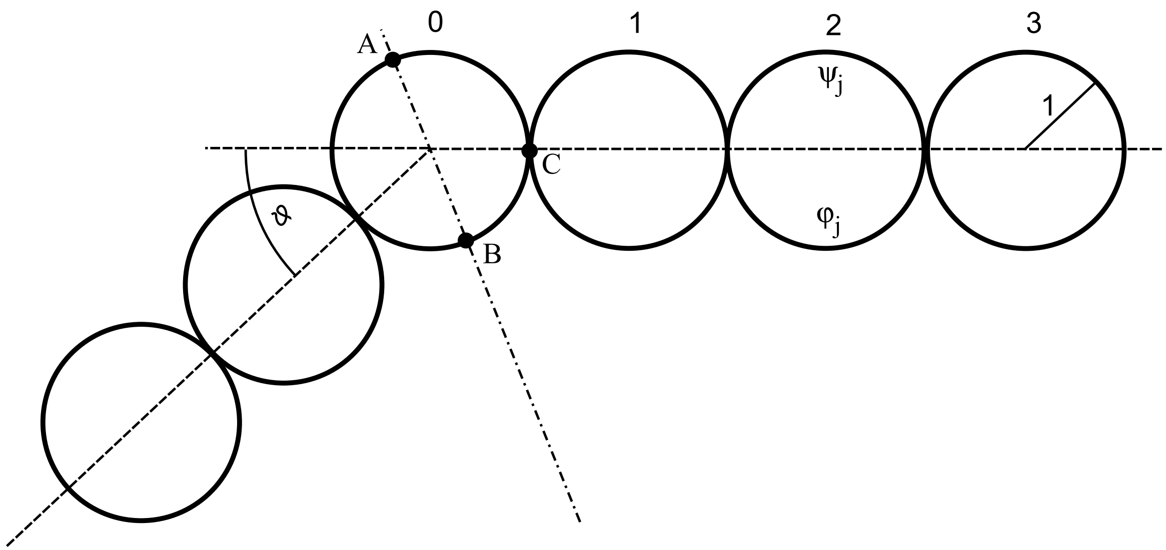
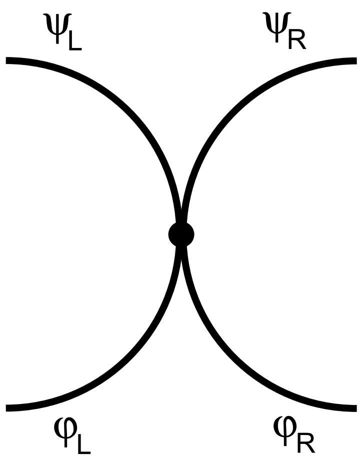


Our aim is to show that

- the band spectrum of the straight Γ is preserved
- there are *bend-induced eigenvalues*, we analyze their behavior with respect to model parameters
- the bent chain exhibits also *resonances*

An infinite periodic chain

The "straight" chain Γ_0 can be treated as a periodic system analyzing the spectrum of the elementary cell



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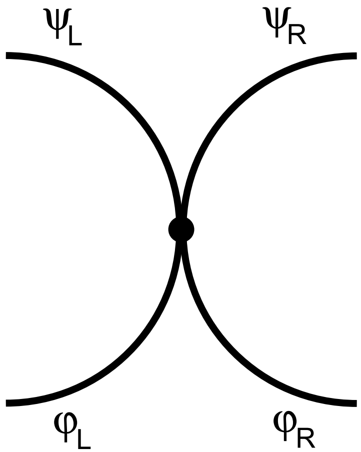

with Floquet-Bloch boundary conditions with the phase $\mathrm{e}^{2\mathrm{i}\theta}$

This yields the condition

$$\mathrm{e}^{2\mathrm{i}\theta} - \mathrm{e}^{\mathrm{i}\theta}\left(2\cos k\pi + \frac{\alpha}{2k}\sin k\pi\right) + 1 = 0$$

Straight chain spectrum

A straightforward analysis leads to the following conclusion:

Proposition: $\sigma(H_0)$ consists of *infinitely degenerate eigenvalues* equal to n^2 with $n \in \mathbb{N}$, and *absolutely continuous spectral bands* such that

If $\alpha > 0$, then every spectral band is contained in $(n^2, (n+1)^2]$ with $n \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, and its upper edge coincides with the value $(n+1)^2$.

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If $\alpha < 0$, then in each interval $[n^2, (n+1)^2)$ with $n \in \mathbb{N}$ there is exactly one band with the lower edge n^2. In addition, there is a band with the lower edge (the overall threshold) $-\kappa^2$, where κ is the largest solution of

$$\left| \cosh \kappa\pi + \frac{\alpha}{4} \cdot \frac{\sinh \kappa\pi}{\kappa} \right| = 1$$

Straight chain spectrum

Proposition, cont'd: The upper edge of this band depends on α. If $-8/\pi < \alpha < 0$, it is k^2 where k solves

$$\cos k\pi + \frac{\alpha}{4} \cdot \frac{\sin k\pi}{k} = -1$$

in $(0,1)$. On the other hand, for $\alpha < -8/\pi$ the upper edge is negative, $-\kappa^2$ with κ being the smallest solution of the condition, and for $\alpha = -8/\pi$ it equals zero.

Finally, $\sigma(H_0) = [0, +\infty)$ holds if $\alpha = 0$.

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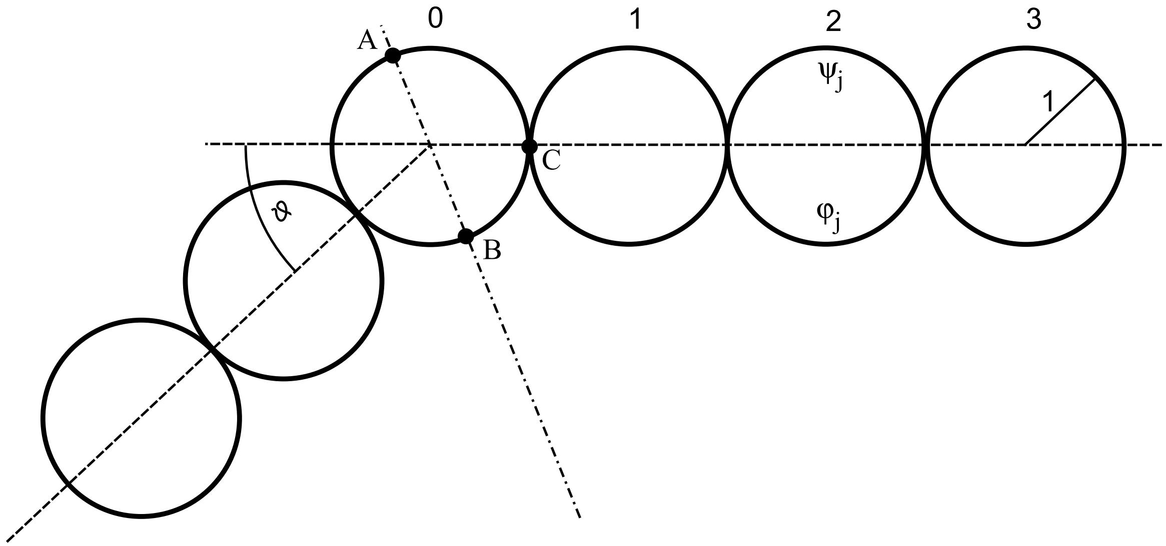
Let us add a couple of *remarks*:

- The bands correspond to *Kronig-Penney model* with the coupling $\frac{1}{2}\alpha$ instead of α, in addition one has here the *infinitely degenerate point spectrum*
- It is also an example of *gaps coming from decoration*

The bent chain spectrum

Now we pass to the bent chain denoted as Γ_ϑ:



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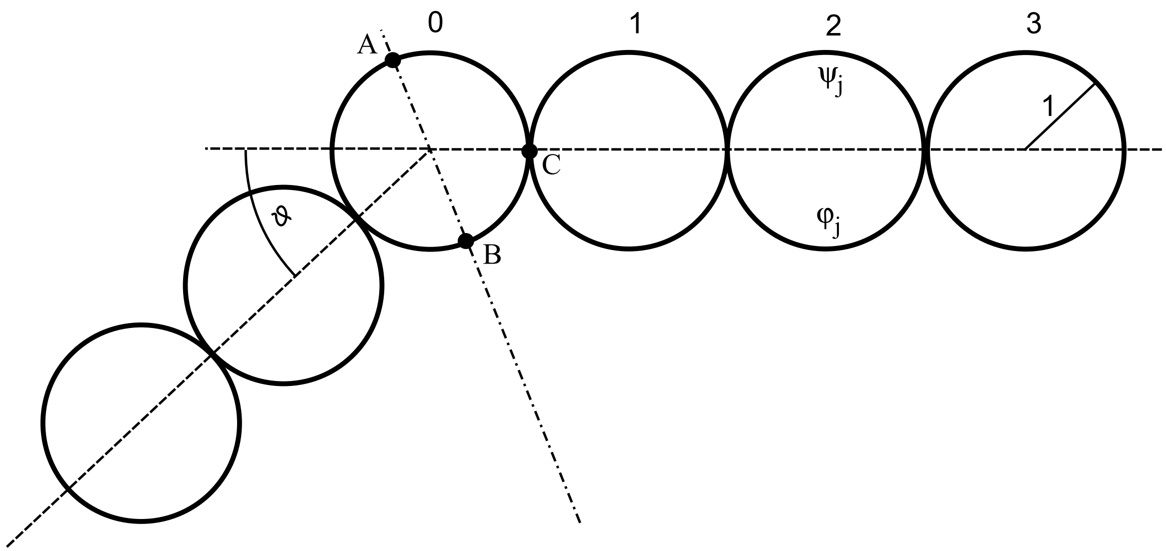

Since Γ_ϑ has mirror symmetry, the operator H_ϑ can be reduced by parity subspaces into a direct sum of an even part, H^+, and odd one, H^-; we drop mostly the subscript ϑ

Equivalently, we analyze the half-chain with *Neumann* and *Dirichlet* conditions at the points A, B, respectively

Eigenfunction components

At the energy k^2 they are are linear combinations of $\mathrm{e}^{\pm\mathrm{i}kx}$,

$$\begin{aligned} \psi_j(x) &= C_j^+\mathrm{e}^{\mathrm{i}kx} + C_j^-\mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0,\pi]\,, \\ \varphi_j(x) &= D_j^+\mathrm{e}^{\mathrm{i}kx} + D_j^-\mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0,\pi] \end{aligned}$$

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There are δ-couplings in the points of contact, i.e.

$$\psi_j(0) = \varphi_j(0)\,, \quad \psi_j(\pi) = \varphi_j(\pi)\,, \quad \text{and}$$

$$\psi_j(0) = \psi_{j-1}(\pi)\,; \quad \psi_j'(0) + \varphi_j'(0) - \psi_{j-1}'(\pi) - \varphi_{j-1}'(\pi) = \alpha \cdot \psi_j(0)$$

Transfer matrix

Using the above relations we get for all $j \geq 2$

$$\begin{pmatrix} C_j^+ \\ C_j^- \end{pmatrix} = \underbrace{\begin{pmatrix} \left(1 + \frac{\alpha}{4\mathrm{i}k}\right) \mathrm{e}^{\mathrm{i}k\pi} & \frac{\alpha}{4\mathrm{i}k}\mathrm{e}^{-\mathrm{i}k\pi} \\ -\frac{\alpha}{4\mathrm{i}k}\mathrm{e}^{\mathrm{i}k\pi} & \left(1 - \frac{\alpha}{4\mathrm{i}k}\right) \mathrm{e}^{-\mathrm{i}k\pi} \end{pmatrix}}_{M} \cdot \begin{pmatrix} C_{j-1}^+ \\ C_{j-1}^- \end{pmatrix},$$

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Remark: By general arguments, σ_{ess} is preserved, and there are at most two eigenvalues in each gap

Spectrum of H^+

Combining the above with the Neumann condition at the mirror axis we get the spectral condition in this case,

$$\cos k\vartheta = -\cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}}$$

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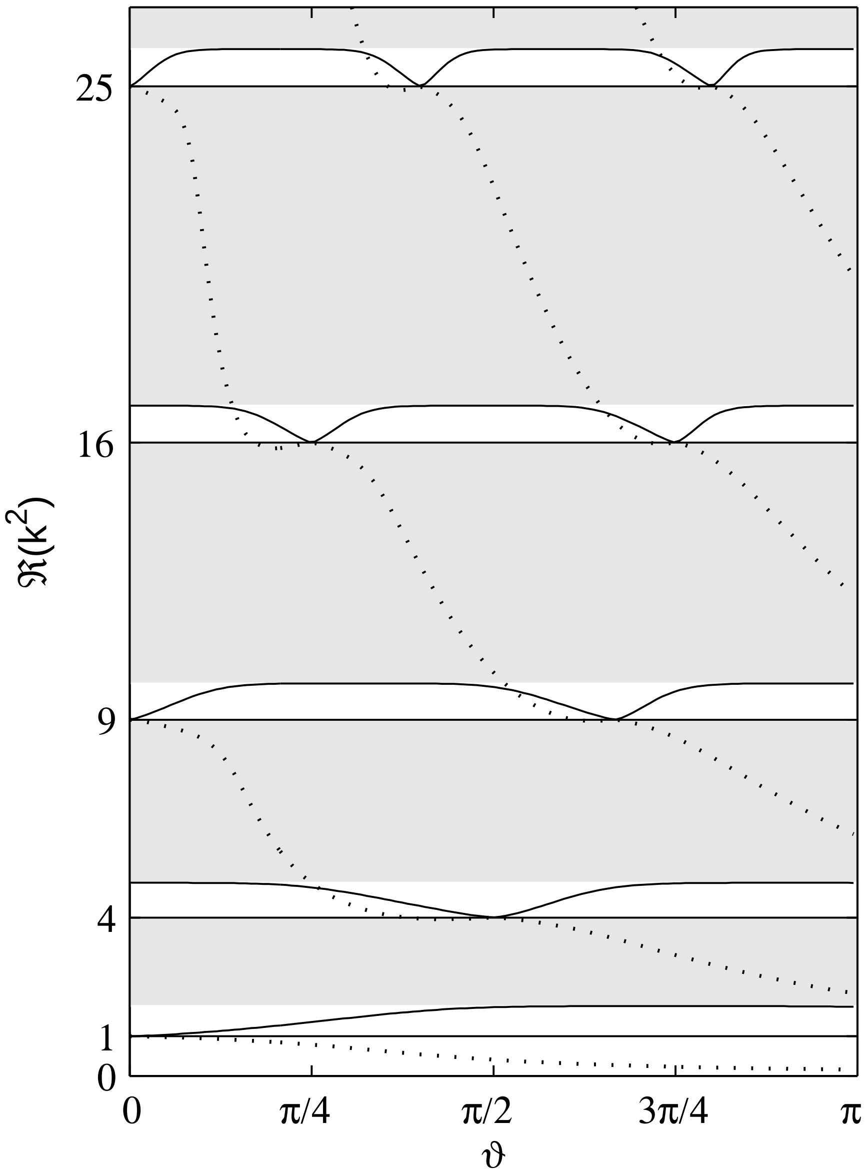
After a tiresome but straightforward analysis one arrives then at the following conclusion:

Proposition: If $\alpha \geq 0$, then H^+ has no negative eigenvalues. On the other hand, for $\alpha < 0$ the operator H^+ has at least one negative eigenvalue which lies under the lowest spectral band and above the number $-\kappa_0^2$, where κ_0 is the (unique) solution of $\kappa \cdot \tanh \kappa\pi = -\alpha/2$

Spectrum of H^+ for $\alpha = 3$



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Replacing Neumann condition by Dirichlet at the mirror axis we get the spectral condition in this case,

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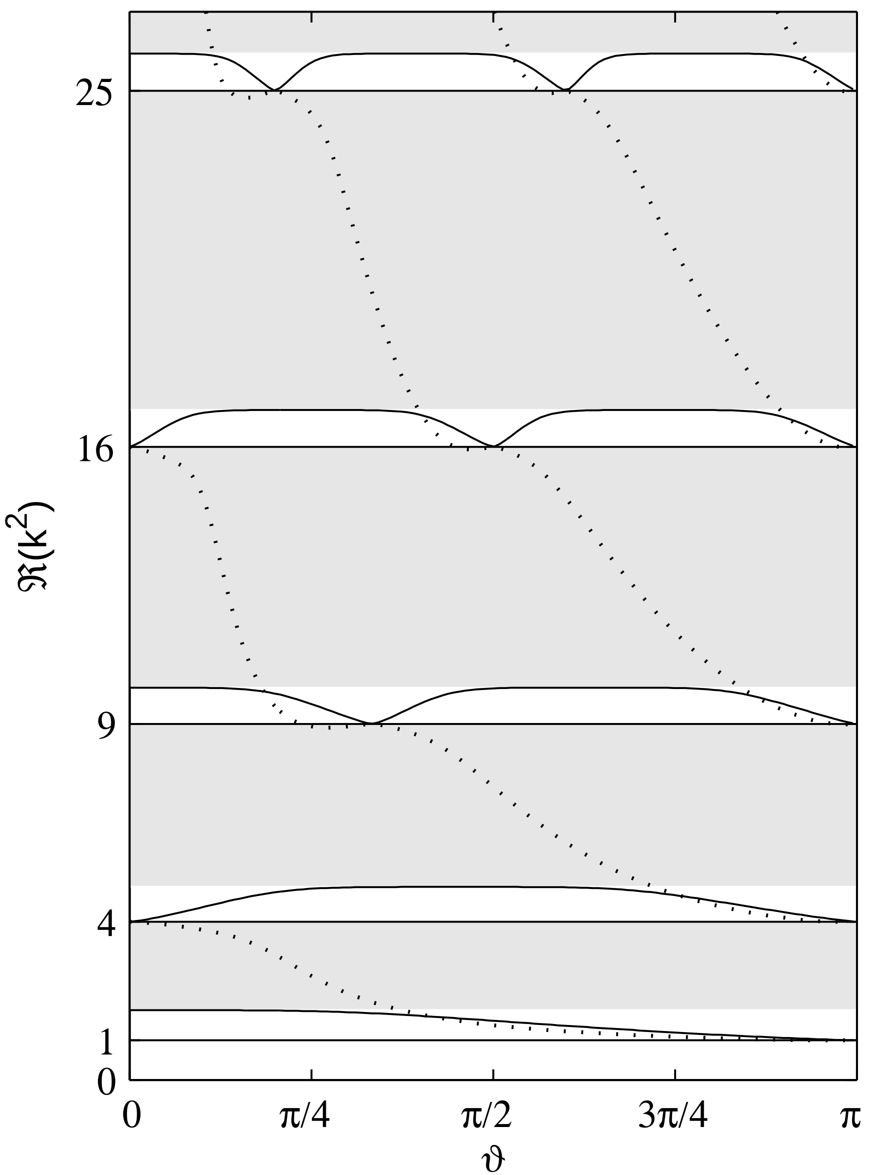
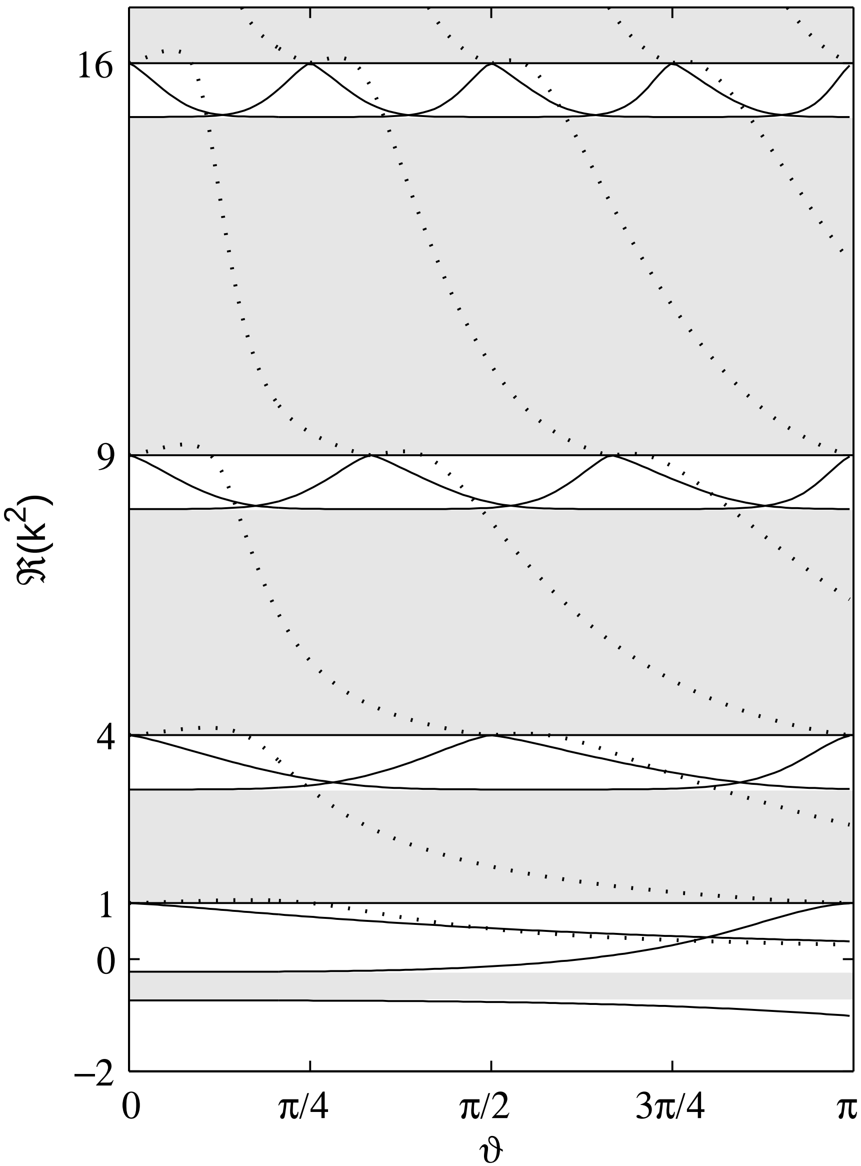
Summarizing, for each of the operators $H^\pm$ there is at least one eigenvalue in every spectral gap closure. It can lapse into a band edge n^2, $n \in \mathbb{N}$, and thus be in fact absent. The ev's of H^+ and H^- may coincide, becoming a single ev of multiplicity two; this happens only if

$$k \cdot \tan k\pi = \frac{\alpha}{2}$$

Spectrum of H^- for $\alpha = 3$



$\sigma(H)$ for attractive coupling, $\alpha = -3$



Resonances, analyticity

The above eigenvalue curves are not the only solutions of the spectral condition. There are also *complex solutions* representing *resonances* of the bent-chain system

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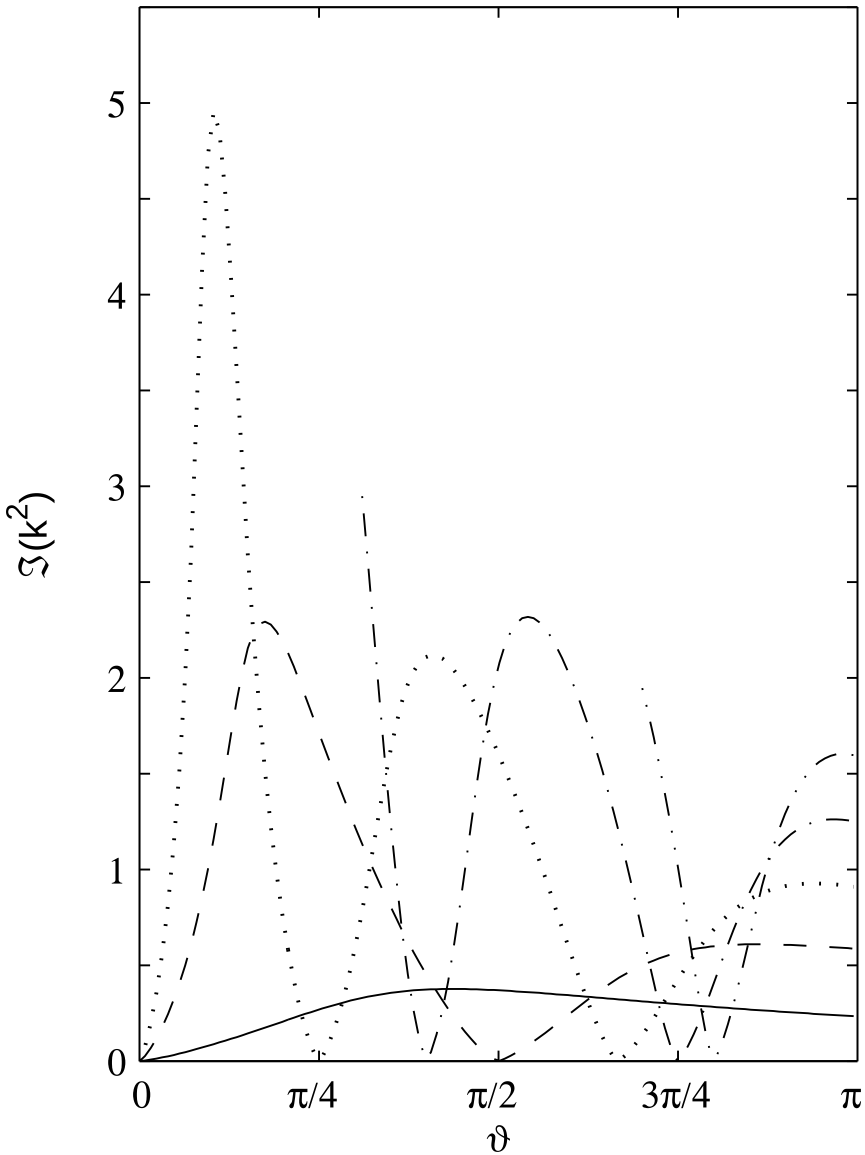
A further analysis of the spectral condition gives

Proposition: The eigenvalue and resonance curves for H^+ are *analytic* everywhere except at $(\vartheta, k) = (\frac{n+1-2\ell}{n}\pi, n)$, where $n \in \mathbb{N}$, $\ell \in \mathbb{N}_0$, $\ell \leq \left[\frac{n+1}{2}\right]$. Moreover, the real solution in the n-th spectral gap is given by a function $\vartheta \mapsto k$ which is *real-analytic*, except at the points $\frac{n+1-2\ell}{n}\pi$. Similar claims can be made for the odd part for H^-.

Imaginary parts of H^+ resonances, $\alpha = 3$



More on the angle dependence

For simplicity we take H^+ only, the results for H^- are analogous. Ask about the behavior of the curves at the points whe they touch bands and where eigenvalues and resonances may cross

If $\vartheta_0 := \frac{n+1-2\ell}{n}\pi > 0$ is such a point we find easily that in is vicinity we have

$$k \approx k_0 + \sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\,|\vartheta - \vartheta_0|^{4/3}$$

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However, H^+ has an eigenvalue near $\vartheta_0 = 0$ also in the gaps adjacent to even numbers, when the curve starts at $(0, k_0)$ for k_0 solving $|\cos k\pi + \frac{\alpha}{4k}\sin k\pi| = 1$ in $(n, n+1)$, n even

Even threshold behavior

Proposition: Suppose that $n \in \mathbb{N}$ is even and k_0 is as described above, i.e. k_0^2 is the right endpoint of the spectral gap adjacent to n^2. Then the behavior of the solution in the vicinity of $(0, k_0)$ is given by

$$k = k_0 - C_{k_0,\alpha} \cdot \vartheta^4 + \mathcal{O}(\vartheta^5)\,,$$

where $C_{k_0,\alpha} := \frac{k_0^2}{8\pi} \cdot \left(\frac{\alpha}{4}\right)^3 (k_0\pi + \sin k_0\pi)^{-1}$

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Remark: Note that the analogous problem for *bent leaky wires* studied in [E-Ichinose'01] remains open.

The results discussed here come from

[DET08] P. Duclos, P.E., O. Turek: On the spectrum of a bent chain graph, *J. Phys. A: Math. Theor.* **A41** (2008), 415206

[EKW10] P.E., P. Kuchment, B. Winn: On the location of spectral edges in $\mathbb{Z}$-periodic media, *J. Phys. A: Math. Theor.* **A41** (2008), 474022

[ET10] P.E., O. Turek: High-energy asymptotics of the spectrum of a periodic square-lattice quantum graph, *J. Phys. A: Math. Theor.* **A41** (2008), 474024

and also

[CET10] T. Cheon, P.E., O. Turek Approximation of a general singular vertex coupling in quantum graphs, *Ann. Phys.* **325** (2010), 548-578

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[E97] P.E.: A duality between Schrödinger operators on graphs and certain Jacobi matrices, *Ann. Inst. H. Poincaré: Phys. Théor.* **66** (1997), 359-371

[EG96] P.E., R. Gawlista: Band spectra of rectangular graph superlattices, *Phys. Rev.* **B53** (1996), 7275-728

[HKSW07] 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.* **A40** (2008), 7597-7618

Thank you for your attention!