Constrained quantum dynamics

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Transport in quantum graphs

Spectral properties of quantum graphs depend in the first place on their *topology* and *geometry*. If the graph is *finite* – meaning a finite number of edges of finite lengths – its spectrum is *discrete*.

On the other hand, in *infinite* graphs there is typically has an (absolutely) continuous spectral component – although there are exceptions – and as a consequence, particles 'living' on such a graph may be transported; this is the main topic of this lecture.

There are different setting in which transport can be studied, for instance:

- The graph has a *compact 'core'* and to some its vertices *semiinfinite 'leads'* are attached. This is a natural framework to investigated *scattering*, and of a particular interest are *resonances in such systems*.
- The graph is *periodic*, then its spectrum typically consists of *bands* allowing for transport unless they are *flat*, they are separated by *gaps*.
- One may ask general questions, for instance, about the *number of gaps* or about mutual relations between the *band and gap widths*.
- A periodic graphs may be *locally perturbed* which typically gives rise to *localized states*.

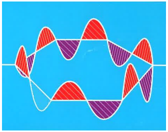
Resonances in quantum graphs

Our first topic will be *resonances* on graphs consisting of a compact 'core' and semiinfinite 'leads'. Let us start from some general observations:

- There are *different definitions* of what a resonance is; the to most common identify it with a *complex singularity* of either the *resolvent* of the Hamiltonian or of the on-shell *scattering matrix*.
- They are often the same things but one has to check this identification in each particular case; keep in mind that the to concept are different: in the first case it is a property of a *single operator*, in case of scattering we compare operators H and H_0, the full and the free Hamiltonian.
- In both cases the singularity is situated on the *'unphysical sheet'* of energy, that, in an *analytical continuation* of the resolvent/S-matrix.
- In QM, resonances most often come from *perturbations of embedded eigenvalues*; the nontrivial topology of quantum graphs means that they exhibit resonances frequently.

Resonances in quantum graphs

Concerning the last claim, in view of a nontrivial topology, the *unique continuation property* does not hold in general, in particular, a quantum graphs Hamiltonian may have *compactly supported eigenfunctions* as this example shows:



Courtesy: Peter Kuchment

The conditions that make them possible, for instance, *rational relations* between the edge lengths, may be violated; such perturbations then give rise to resonances.

Let us consider a graph Γ consisting of vertices $\mathcal{V} = \{\mathcal{X}_j : j \in I\}$, finite edges $\mathcal{L} = \{\mathcal{L}_{jn} : (\mathcal{X}_j, \mathcal{X}_n) \in I_{\mathcal{L}} \subset I \times I\}$, and semiinfinite edges (leads) $\mathcal{L}_\infty = \{\mathcal{L}_{j\infty} : \mathcal{X}_j \in I_{\mathcal{C}}\}$. The corresponding state Hilbert space is

$$\mathcal{H} = \bigoplus_{L_j \in \mathcal{L}} L^2([0, l_j]) \oplus \bigoplus_{\mathcal{L}_{j\infty} \in \mathcal{L}_\infty} L^2([0, \infty))\,;$$

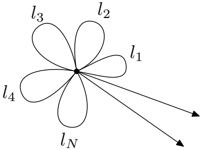
its elements we write as columns $\psi = (f_j : \mathcal{L}_j \in \mathcal{L},\, g_j : \mathcal{L}_{j\infty} \in \mathcal{L}_\infty)^{\mathrm{T}}$.

A useful trick

In the absense of external fields, the Hamiltonian acts as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ on each link on $\mathcal{H}^2_{\mathrm{loc}}$ functions satisfying the boundary conditions

$$(U_j - I)\Psi_j + i(U_j + I)\Psi'_j = 0$$

characterized by unitary matrices U_j at the vertices $\mathcal{X}_j$. A useful trick is to replace Γ *'flower-like' graph* with one vertex by putting all the vertices to a single point,



Its degree is, of course, $2N + M$, where $N := \mathrm{card}\,\mathcal{L}$ and $M := \mathrm{card}\,\mathcal{L}_\infty$.

The coupling in the 'master vertex' is then described by the condition

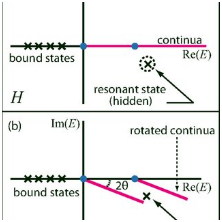
$$(U - I)\Psi + i(U + I)\Psi' = 0,$$

where the unitary $(2N + M) \times (2N + M)$ matrix U is block-diagonal with the blocks U_j reflecting *the true topology of* Γ.

Different resonance definitions

Consider first the *resolvent resonances*. A powerful method method to reveal them is based on *complex scaling*.

The method is common in atomic and molecular physics, recall e.g. *helium autoionization effect*; it is illustrated in the attached picture.



Source: wikipedia

Quantum graphs we consider are ell suited for application of an *exterior* complex scaling. Looking for complex eigenvalues of the scaled operator we preserve the compact part of the graph using the wave function Ansatz $f_j(x) = a_j \sin kx + b_j \cos kx$ on the j-th internal edge.

On the other hand, functions on the semi-infinite edges are scaled by $g_{j\theta}(x) = \mathrm{e}^{\theta/2} g_j(x\mathrm{e}^{\theta})$ with an imaginary θ; the poles of the resolvent on the second sheet become 'uncovered' for *θ large enough*. The 'exterior' boundary values of $g_j(x) = g_j \mathrm{e}^{ikx}$ referring to energy k^2 thus equal to

$$g_j(0) = \mathrm{e}^{-\theta/2} g_j, \quad g_j'(0) = ik\mathrm{e}^{-\theta/2} g_j.$$

Resolvent and scattering resonances

Substituting these boundary values to the matching condition we get

$$\left[(U-I)C_1(k)+ik(U+I)C_2(k)\right]\psi=0,$$

where $\psi=(a_1,b_1,a_2,\dots,b_N,\mathrm{e}^{-\theta/2}g_1,\dots,\mathrm{e}^{-\theta/2}g_M)^{\mathrm{T}}$ and $C_j(k)$ are block- diagonal, $C_j:=\mathrm{diag}\,(C_j^{(1)}(k),C_j^{(2)}(k),\dots,C_j^{(N)}(k),i^{j-1}I_{M\times M})$ with

$$C_1^{(j)}(k)=\begin{pmatrix} 0 & 1\\ \sin kl_j & \cos kl_j \end{pmatrix},\qquad C_2^{(j)}(k)=\begin{pmatrix} 1 & 0\\ -\cos kl_j & \sin kl_j \end{pmatrix}$$

Naturally, this systems of linear equations is solvable if and only if

$$\det\left[(U-I)\,C_1(k)+ik(U+I)\,C_2(k)\right]=0.$$

Passing to *scattering resonances*, we choose a combination of two planar waves, $g_j=c_j\mathrm{e}^{-ikx}+d_j\mathrm{e}^{ikx}$, as an Ansatz on the external edges; we ask about poles of the matrix $S=S(k)$ which maps the amplitudes of the incoming waves, $c=\{c_n\}$, into the amplitudes of their outgoing counterparts, $d=\{d_n\}$, through the linear relation $d=Sc$.

Resolvent and scattering resonances

Matching the functions at the vertices where the leads are attached, we get

$$(U-I)C_1(k)\begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ c_1+d_1 \\ \vdots \\ c_M+d_M \end{pmatrix} + ik(U+I)C_2(k)\begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ d_1-c_1 \\ \vdots \\ d_M-c_M \end{pmatrix} = 0$$

It is an easy exercise to eliminate a_j, b_j from this system arriving at a system of M equations that yields the map $S^{-1}d = c$; this system is *not* solvable, $\det S^{-1} = 0$, under the *same condition* we have obtained above. This allows us to conclude:

Proposition

The two above resonance notions, the resolvent and scattering one, are equivalent for quantum graphs.

P.E., J. Lipovský: Resonances from perturbations of quantum graphs with rationally related edges, *J. Phys. A: Math. Theor.* **43** (2010), 105301.

Effective coupling on the compact subgraph

The problem can be reduced to the graph core only rephrasing it as a *non-selfadjoint* spectral problem on the *'flower'* without the M-fold *'stalk'*.

To this aim, we write U in the block form, $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$, where U_1 in the $2N \times 2N$ matric referring to the compact subgraph, U_4 is the $M \times M$ matrix related to the exterior part, and the off-diagonal U_2 and U_3 are rectangular matrices connecting the two.

Eliminating the external part leads to an effective coupling on the compact subgraph expressed by the condition

$$(\tilde{U}(k) - I)(f_1, \dots, f_{2N})^{\mathrm{T}} + i(\tilde{U}(k) + I)(f_1', \dots, f_{2N}')^{\mathrm{T}} = 0,$$

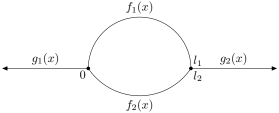
where the corresponding coupling matrix

$$\tilde{U}(k) := U_1 - (1-k)U_2[(1-k)U_4 - (k+1)I]^{-1}U_3$$

is obviously *energy-dependent* and, in general, *non-unitary*.

This is another nice illustration of a simple formula know already to *Schur*, often attributed to *Feshbach*, or *Grushin*, or other people.

Example: a loop with two leads



In each vertex we use a four-parameter family of boundary conditions assuming *continuity on the loop*, $f_1(0) = f_2(0)$, together with

$$f_1(0) = \alpha_1^{-1}(f_1'(0) + f_2'(0)) + \gamma_1 g_1'(0),$$
$$g_2(0) = -\bar{\gamma}_2(f_1'(l_1) + f_2'(l_2)) + \tilde{\alpha}_2^{-1} g_2'(0),$$

and similarly in the other vertex with $\alpha_j \in \mathbb{R}$, $\tilde{\alpha}_j \in \mathbb{R}$, and $\gamma_j \in \mathbb{C}$.

Writing the loop edge lengths as $l_1 = l(1-\lambda)$ and $l_2 = l(1+\lambda)$ with $\lambda \in [0,1]$, which effectively means shifting one of the connections points around the loop as λ is changing, one arrives at the resonance condition

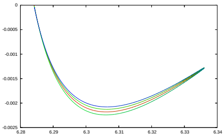
$$\sin kl(1-\lambda) \sin kl(1+\lambda) - 4k^2 \beta_1^{-1}(k)\beta_2^{-1}(k) \sin^2 kl + k[\beta_1^{-1}(k) + \beta_2^{-1}(k)] \sin 2kl = 0,$$

where $\beta_i^{-1}(k) := \alpha_i^{-1} + \frac{ik|\gamma_i|^2}{1-ik\tilde{\alpha}_i^{-1}}$.

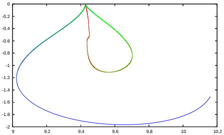
Example: a loop with two leads

It is easy to see that there are embedded eigenvalues if the parameter λ characterizing the shift is *rational*, and also that the singularities become complex if we move away from such a point; we can then solve the resonance condition perturbatively.

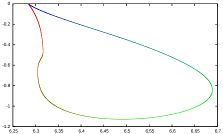
For larger changes of λ one can still solve the condition *numerically* to determine the *pole trajectories*. In order to make the dependence on λ visible, we color code them, moving from red ($\lambda = 0$) to blue ($\lambda = 1$).



$n = 2$ and $\tilde{\alpha}_1^{-1} = -2$, $\alpha_2^{-1} = 0$, $\alpha_1^{-1} = \tilde{\alpha}_2^{-1} = |\gamma_j|^2 = 1$

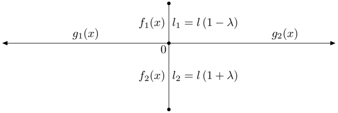


$n = 3$ and all the $\alpha_j^{-1} = \tilde{\alpha}_j^{-1} = |\gamma_j|^2 = 1$



$n = 2$ and the same parameter values

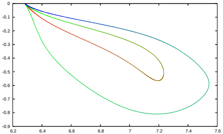
Another example: a cross-shaped graph

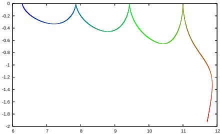


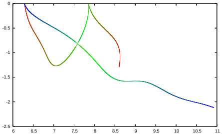
This time we restrict ourselves to the δ coupling combined with Dirichlet conditions at the loose ends; this yields the resonance condition

$$2k \sin 2kl + (\alpha - 2ik)(\cos 2kl\lambda - \cos 2kl) = 0$$

The examples correspond to resonances associated with the embedded eigenvalue for $n = 2$ and $\alpha = 10,\ 1,\ 2.596$, respectively.







The last one shows an *avoided crossing* of resonance trajectories, the last two also illustrate an effect called *quantum holonomy*.

T. Cheon, A. Tanaka: New anatomy of quantum holonomy, *EPL* **85** (2009), 20001.

High-energy asymptotics

Now something more general. We know that at high energies the *number of bound states* is give semiclassically by the *Weyl formula*; in open systems like our graphs with leads the same is true for the number of *eigenvalues and resonances* taken together.

Brian Davies and Sasha Pushnitski inspected the number of eigenvalues and resonances in a circle of radius R and made an intriguing observation: if the coupling is *Kirchhoff* and some vertices are *balanced*, meaning that they connect the *same number* of *internal* and *external edges*, then the leading term in the asymptotics may be *less than Weyl formula prediction*.

E.B. Davies, A. Pushnitski: Non-Weyl resonance asymptotics for quantum graphs, *Anal. PDE* **4**(5) (2011), 729–756.

To understand what is happening it is useful to look at graphs with a general vertex coupling. Denoting $e_j^\pm := \mathrm{e}^{\pm ikl_j}$ and $e^\pm := \Pi_{j=1}^N e_j^\pm$, we can write the secular equation determining the singularities is

$$0 = \det\Big\{\frac{1}{2}[(U-I)+k(U+I)]E_1(k)+\frac{1}{2}[(U-I)+k(U+I)]E_2+k(U+I)E_3 + (U-I)E_4 + [(U-I)-k(U+I)]\,\mathrm{diag}\,(0,\dots,0,I_{M\times M})\Big\},$$

High-energy asymptotics

where $E_i(k) = \mathrm{diag}\,\Big(E_i^{(1)}, E_i^{(2)}, \dots, E_i^{(N)}, 0, \dots, 0\Big)$, $i = 1, 2, 3, 4$, consists of a trivial $M \times M$ part and N nontrivial 2×2 blocks

$$E_1^{(j)} = \begin{pmatrix} 0 & 0 \\ -ie_j^+ & e_j^+ \end{pmatrix},\; E_2^{(j)} = \begin{pmatrix} 0 & 0 \\ ie_j^- & e_j^- \end{pmatrix},\; E_3^{(j)} = \begin{pmatrix} i & 0 \\ 0 & 0 \end{pmatrix},\; E_4^{(j)} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Fortunately, mathematics is eternal; we have an almost century old result:

Theorem

Let $F(k) = \sum_{r=0}^{n} a_r(k)\, \mathrm{e}^{ik\sigma_r}$, where $a_r(k)$ are rational functions of the complex variable k with complex coefficients, and the numbers $\sigma_r \in \mathbb{R}$ satisfy $\sigma_0 < \sigma_1 < \dots < \sigma_n$. Let us assume that $\lim_{k\to\infty} a_0(k) \neq 0$ and $\lim_{k\to\infty} a_n(k) \neq 0$. Then there are a compact $\Omega \subset \mathbb{C}$, real numbers m_r and positive K_r, $r = 1, \dots, n$, such that the zeros of $F(k)$ outside Ω lie in the logarithmic strips bounded by the curves $-\mathrm{Im}\, k + m_r \log|k| = \pm K_r$ and the counting function of the zeros behaves in the limit $R \to \infty$ as

$$N(R, F) = \frac{\sigma_n - \sigma_0}{\pi} R + \mathcal{O}(1).$$

R.E. Langer: On the zeros of exponential sums and integrals, *Bull. Amer. Math. Soc.* **37** (1931), 213–239.

Application of Langer theorem

Rewriting the secular equation as $F(k) = 0$, we need to find the senior and junior coefficients; by a straightforward computation one can find that $e^{\pm} = \mathrm{e}^{\pm ikV}$, where $V := \sum_{j=1}^{N} l_j$ is the size of the graph core.

Lemma

$e^{\pm} = \left(\frac{i}{2}\right)^N \det\left[(\tilde{U}(k) - I) \pm k(\tilde{U}(k) + I)\right]$ *with* $\tilde{U}(k)$ *defined above.*

Theorem

Given a quantum graph (Γ, H_U) *with finitely many edges and the vertex coupling given by matrices* U_j*, the resonance counting function behaves as*

$$N(R, F) = \frac{2W}{\pi} R + \mathcal{O}(1) \quad \text{for} \quad R \to \infty,$$

where W *is the effective size of* Γ *satisfying* $0 \leq W \leq V := \sum_{j=1}^{N} l_j$*. Moreover,* $W < V$ *(graph is non-Weyl) if and only there is a vertex such that the matrix* $\tilde{U}_j(k)$ *has an eigenvalue* $(1-k)/(1+k)$ *or* $(1+k)/(1-k)$*.*

E.B. Davies, P.E., J. Lipovský: Non-Weyl asymptotics for quantum graphs with general coupling conditions, *J. Phys. A: Math. Theor.* **43** (2010), 474013.

Permutation-invariant couplings

Vertex couplings *invariant w.r.t. edge permutations* are described by matrices $U_j = a_j J + b_j I$, where number $a_j,\, b_j \in \mathbb{C}$ such that $|b_j| = 1$ and $|b_j + a_j \deg v_j| = 1$; matrix J has all the entries equal to one. Note that both the δ and δ'_{s} are particular cases of such a coupling.

For a vertex with p internal and q external edges and such a coupling U_j, the effective matrix matrix $\tilde{U}_j(k)$ is easily calculated; this allows us to make the following conclusion:

Corollary

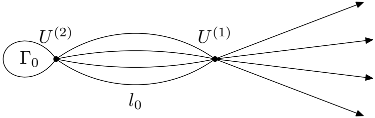
If (Γ, H_U) has a vertex with a permutation-invariant coupling which is balanced, $p = q$, the graph is non-Weyl if and only if the coupling at this vertex is either of Kirchhoff or anti-Kirchhoff type,

$$f_j = f_n,\;\; \forall j, n \le 2p, \quad \sum_{j=1}^{2p} f'_j = 0 \quad \text{or} \quad f'_j = f'_n,\;\; \forall j, n \le 2p, \quad \sum_{j=1}^{2p} f_j = 0$$

If one drops the requirement of permutation symmetry, it is possible to construct *examples of non-Weyl graphs* in which *no vertex is balanced*.

What is the cause of a non-Weyl asymptotics?

We want to show that (anti-)Kirchhoff conditions at balanced vertices are easy to decouple diminishing thus effectively the graph size.



Suppose that a balanced vertex v_1 connects p internal edges of the same length l_0 (we can always add 'dummy' Kirchhoff vertices) and p external edges, coupled by a $U^{(1)} = aJ_{2p\times 2p} + bI_{2p\times 2p}$. The coupling to the rest of the graph, denoted as Γ_0, is described by a $q \times q$ matrix $U^{(2)}$ with $q \geq p$.

The idea is to use a *unitary equivalence*. Given a unitary $p \times p$ matrix V we define $V^{(1)} := \mathrm{diag}\,(V, V)$ and $V^{(2)} := \mathrm{diag}\,(I_{(q-p)\times(q-p)}, V)$, then it is straightforward to check that the original graph Hamiltonian is *unitarily equivalent* to the one in which matrices $U^{(1)}$ and $U^{(2)}$ are replaced by $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ and $[V^{(2)}]^{-1}U^{(2)}V^{(2)}$, respectively.

If the columns of V are *orthonormal eigenvectors* of $U^{(1)}$, beginning with $\frac{1}{\sqrt{p}}(1, 1, \dots, 1)^{\mathrm{T}}$, then $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ decouples then into $2\times$ *blocks*.

What is the cause of a non-Weyl asymptotics?

The first one of those corresponds to the *symmetrization* of all the external u_j's and internal f_j's, thus leading to the 2×2 coupling matrix $U_{2\times 2} = apJ_{2\times 2} + bI_{2\times 2}$; in the complement the internal and external edges are *separated* satisfying Robin conditions, $(b-1)v_j(0) + i(b+1)v_j'(0) = 0$ and $(b-1)g_j(0) + i(b+1)g_j'(0) = 0$ for $j = 2, \dots, p$.

The 'overall' Kirchhoff/anti-Kirchhoff condition at v_1 is transformed into the *'line' Kirchhoff/anti-Kirchhoff condition* in the subspace of permutation-symmetric functions, and since this is *no coupling at all* (recall that anti-Kirchhhoff and Kirchhoff on line are unitarily equivalent), this causes non-Weyl behavior by effectively *reducing the graph size by* l_0.

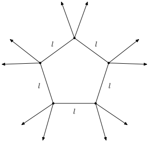
In all the other cases the point interaction corresponding to the matrix $apJ_{2\times 2} + bI_{2\times 2}$ is nontrivial, and consequently, *the graph size is preserved*.

Note that similar trick can used in analysis of *tree graphs* rephrasing the task as an investigation of a family of problems of the line.

A.V. Sobolev, M.Z. Solomyak: Schrödinger operator on homogeneous metric trees: spectrum in gaps, *Rev. Math. Phys.* **14** (2002), 421–467.

Effective size is a global property

One may ask whether considering the effect of each balanced vertex *separately* allows to to determine the effective size. It is *not* the case, as the following simple example of Kirchhoff graph Γ_n shows:



The symmetry allows to decompose the system w.r.t. the cyclic rotation group $\mathbb{Z}_n$ into segments characterized by numbers ω satisfying $\omega^n = 1$; the resonance condition then reads $-2(\omega^2+1) + 4\omega \mathrm{e}^{-ik\ell} = 0$. Using is, we easily find that the effective size of Γ_n is

$$W_n = \begin{cases} n\ell/2 & \text{if } n \neq 0 \pmod 4, \\ (n-2)\ell/2 & \text{if } n = 0 \pmod 4. \end{cases}$$

Note also that one can demonstrate non-Weyl behavior of graph resonances *experimentally* in a model using *microwave networks*:

M. Ławniczak, J. Lipovský, L. Sirko: Non-Weyl microwave graphs, *Phys. Rev. Lett.* **122** (2019), 140503.

Periodic graphs

Let us no pass to graphs which are truly infinite. There is a number of interesting cases here; we restrict our attention to *periodic graphs*, of a great importance if we think of using graphs to model *material structure*.

The basic method to deal with them is the same as for other periodic system in QM, namely to apply to the Hamiltonian the *Bloch* or *Floquet decomposition* writing it as a direct integral

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

where the fiber operator $H(\theta)$ acts on $L^2(Q)$, where $Q \subset \mathbb{R}^d$ is *period cell* of the graph and the *quasimomentum* θ runs through the *dual cell* Q^* of the lattice usually called the *Brillouin zone*.

Bloch decomposition is commonly used to prove that the spectrum of H

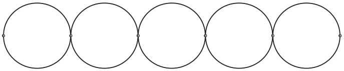
- is *absolutely continuous*
- has a *band-and-gap structure*

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.

Periodic graphs

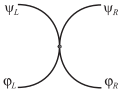
For quantum graphs, however, the spectrum of H *is not necessarily absolutely continuous* since they may exhibit *flat bands* coming from the mentioned violation of the unique continuation property. There are also other differences which we will mention below.

Let us begin with a very simple *example*, a *ring chain* graph



assuming that adjacent rings, supposed to be of perimeter 2π, are connected through a δ *coupling* of strength α

Take the Ansatz $\psi_L(x) = \mathrm{e}^{-iAx}(C_L^+ \mathrm{e}^{ikx} + C_L^- \mathrm{e}^{-ikx})$ 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 $\mathrm{e}^{i\theta}$,

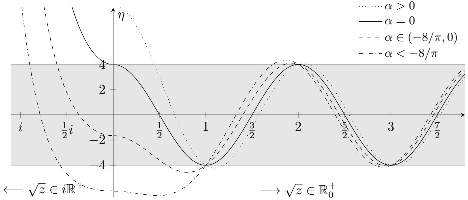
$$\sin k\pi \big(\mathrm{e}^{2i\theta} - \tfrac{1}{2}\eta(k)\mathrm{e}^{i\theta} + 1\big) = 0,$$

Ring chain graphs

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

We see that the system has *flat bands*, that is, infinitely degenerate eigenvalues n^2, $n \in \mathbb{Z}$. The *absolutely continuous part* of the spectrum comes from the second factor.

It yields the condition $|\eta(k)| \le 4$. Its solution can be found *graphically*:



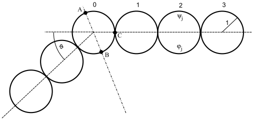
There is an *infinite number of gaps* provided $\alpha \neq 0$, of asymptotically constant widths on the energy scale, and one *negative band* if $\alpha < 0$.

Note that, up to a factor $\frac{1}{2}$, this nothing but the spectrum of the *Kronig-Penney* model as it is clear from the mirror symmetry of the chain.

Local perturbations: a bent chain

We have mentioned that *local perturbations* in general give rise to eigenvalues in the gaps. We shall return to the this question later, for the moment we mention just one example.

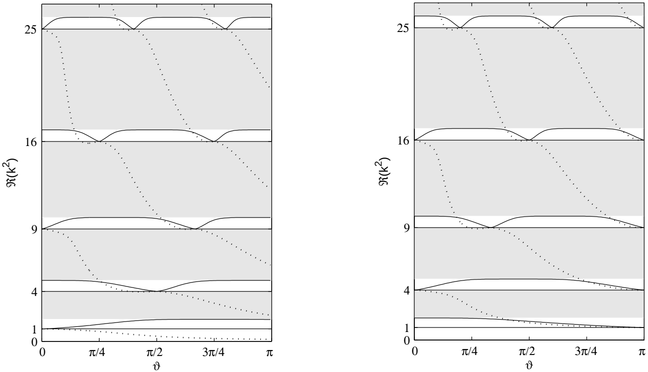
It is related to the previous model with $\alpha \neq 0$: let us assume we perturb it by *bending the chain*, which means shifting the position of a single vertex.



Denote the Hamiltonian as H_ϑ. We note that the *flat bands* (coinciding with the upper or lower edges of *ac* bands) are independent of ϑ.

From the general principles we have *at most to eigenvalues* in each gap, because $H_\vartheta^\pm$ and $H_0^\pm$ have a common symmetric restriction with *deficiency indices* $(2,2)$. Furthermore, the *mirror symmetry* allows us to treat the *even* and *odd* parts separately, that is, the halfchain with the Neumann and Dirichlet cut, respectively.

Example: bent-chain spectrum for $\alpha = 3$



for the even and odd part of the operator, $H_\vartheta^\pm$, respectively.

We see that the eigenvalues in gaps may be absent but only at rational values of ϑ and never simultaneously. Similar pictures we get for other values of α, the dotted lines mark (real values) of *resonance* positions.

P. Duclos, P.E., O. Turek: On the spectrum of a bent chain graph, *J. Phys. A: Math. Theor.* **41** (2008), 415206.

Periodic graphs: the number of gaps

We have seen that the spectrum may have *no gaps* but also an *infinite number* of them. Let us now ask whether there may be *'just a few'* gaps.

Let us recall that 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 $\mathbb{Z}^d$*-periodic systems with* $d \geq 2$ 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, in a sense, are 'mixing' different dimensionalities?

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

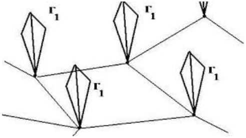
The literature says that – while the situation is similar – the finiteness of the gap number *is not a strict law*, and topology is the reason.

Graph decoration

An infinite number of gaps in the spectrum of a periodic graph can be created 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*.

Theorem

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

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

Worse than that, it was shown that 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*:

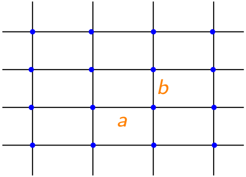
Theorem

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

The Bloch analysis is not difficult in this case. In particular, we find that a number $k^2 > 0$ belongs to a gap if and only if $k > 0$ satisfies the *gap condition* which 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, $\alpha = 0$, which is trivial from the present point of view, $\sigma(H) = [0, \infty)$.

Note that for $\alpha < 0$ the spectrum extends to the negative part of the real axis and may have a gap there – this happens if $\alpha < -4(a^{-1} + b^{-1})$ – 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 such a quantum graph

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 $q \neq 0$; in that case there are *no gaps* in the spectrum provided that $|\alpha|$ is *small enough*.

Recall that for such numbers one introduces the *Markov constant* by

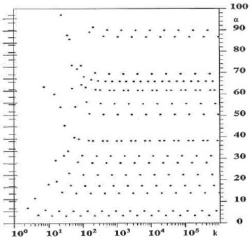
$$\mu(\theta) := \inf \left\{ c > 0 \,\middle|\, (\exists_\infty (p,q) \in \mathbb{N}^2) \left(\left|\theta - \frac{p}{q}\right| < \frac{c}{q^2} \right) \right\};$$

(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' gap series open as the coupling strength α increases; the critical values at which that happens are $\frac{\pi^2}{\sqrt{5ab}}\theta^{\pm 1/2}|n^2 - m^2 - nm|,\ n, m \in \mathbb{N}$, cf. [E-Gawlista'96, loc.cit.].

But a closer look shows a more complex picture

But a detailed analysis, cf. [E-Turek'17, loc.cit.], shows to a different and more subtle picture:

Theorem

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

(i) *If $\alpha > \frac{\pi^2}{\sqrt{5}a}$ or $\alpha \le -\frac{\pi^2}{\sqrt{5}a}$, 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 claim 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; a more refined Diophantine analysis yields the following result:

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

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

Beyond the golden mean case

The used technique allows to derive within the present model a more general result, applicable to *any* α badly approximable by rationals:

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.

Choosing, for instance, $\theta = [0; t, t, 1, 1, \dots]$ with $t \geq 3$, one can check that the BS property may also hold in lattices with *repulsive* δ *coupling*, $\alpha > 0$.

Nevertheless, the BS behavior is exceptional and one wonders whether and how often it could be observed in other quantum graph situations.

What to bring home from Lecture III

- Transport in infinite quantum graphs may take many forms.
- Graphs with leads are suitable for investigations of *resonance effects*.
- In resonance scattering on graphs, semiclassical considerations must be taken with caution as, e.g., the *Weyl asymptotics* may not hold.
- The spectrum of periodic quantum graphs may contain *flat bands*.
- Local perturbations of periodic graphs do not change the essential spectrum, in other words, the *bands*, but they typically give rise to *eigenvalues in the gaps*.
- Periodic graphs can exhibit *Bethe-Sommerfeld behavior* having a finite but nonzero open gaps in the spectrum.