Quantum mechanics on graphs: why is it interesting?

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A Della Pietra Lecture in the Simons Center for Geometry and Physics

Stony Brook, June 7, 2022

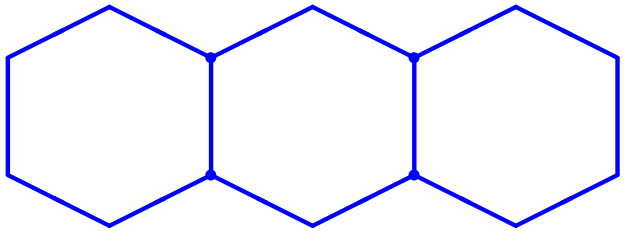
Why QM on graphs is of interest?

The answer to this question is like a kaleidoscope showing different facets when turned; let us look at some of them:

- The *birth* and *rebirth* of the quantum graph concept
- Graph *vertices*: how to match the wavefunctions?
- The *meaning* of different vertex couplings
- *Duality* between discrete and metric graphs
- Quantum graphs may violate the *Weyl asymptotics*
- Even *linear graphs* may behave nontrivially
- *Listening* to the graph shape
- Graphs are a natural environment to study *quantum chaos*
- There are also *different quantum graphs*

Quantum graph origin: Pauling's insight

The notion first appeared in early days of QM when *Linus Pauling* suggested that the Kekulé pictures describing molecules of *aromatic hydrocarbons*, like benzene, napfthalene, anthracene sketched here



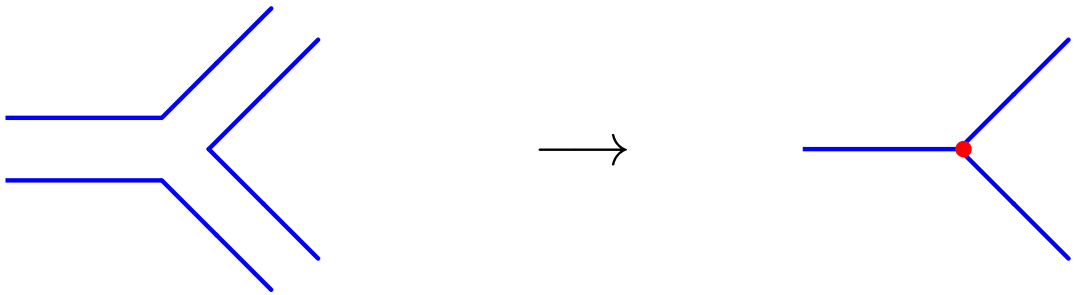
and others – ignoring the double edges marking the bond type – are more than symbols. He conjectured that some electrons form a *graph-shaped frame* in which the remaining ones move.

Using this idea, he managed to calculate spectra of such molecules with $\sim$10% accuracy, a remarkable feat for such a primitive model.

Doing so, he had to decide how the electron wave functions match at the graph vertices. He choose the simplest possible way assuming that they are *continuous* and the *sum of their derivatives vanishes*, that is, what people today mostly call *Kirchhoff conditions*.

Vertex coupling

This choice requires a justification as it is *not the only possibility*. An insight was proposed seventeen years later – science was slower those days and there a world war in between – using another natural idea:



Ruedenberg and Scherr, *J. Chem. Phys.* **21** (1953), 1565

By a *formal use* of Green's formula, they showed that the *squeezing limit* of free motion in a branched tube with *Neumann boundary* yields nothing but the Kirchhoff conditions used by Pauling.

The idea looks simple indeed, however, mathematically it proved to be *quite a hard problem*; I will return to it later.

After that, the quantum graphs concept was forgotten and existed, at most, as an *obscure textbook example* for more than three decades.

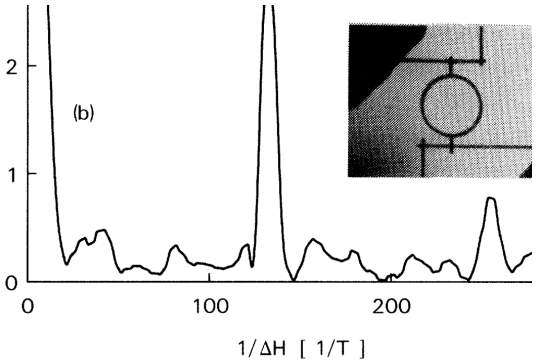
Rebirth of the concept

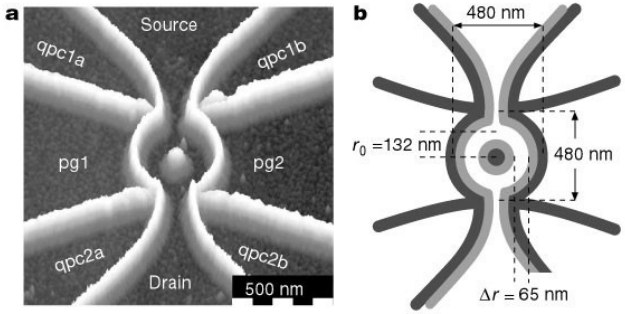
In fact, the idea of such a way to describe *atomic lattices* returned recently in connection with *graphene* and other 2D materials described by *Schrödinger* or *Dirac* equation on graphs.

Kuchment and Post, *Commun. Math. Phys.* **275** (2007), 805

Oliveira and Rocha, *Rep. Math. Phys.* **89** (2022), 231

In the meantime, however, a new inspiration came from a different area, namely from the progress in solid state physics. Since the 1980s the fabrication techniques improved allowing us to produce structure so tiny and clean that the *electron transport is coherent*.





Examples: a ring of diameter diameter 784nm made of *gold wire* of width 41nm, and a ring-type *heterostructure made of AlGaAs-GaAs*.

Webb et al., *Phys. Rev. Lett.* **54** (1985), 2696

Fuhrer et al., *Nature* **413** (2001), 822

Rebirth of the concept

Recall that metallic ring graphs were one of the first systems on which the existence of *Aharonov-Bohm effect* was demonstrated experimentally.

There are numerous materials of which such graph-like systems are constructed. Apart from *semiconductors* and *metals* already mentioned, one can use, for instance, *carbon nanotubes*.

From the stationary point of view, it is not surprising that properties of such systems can be simulated and studied using *microwave networks* built of optical cables.

Hul et al., *Phys. Rev.* **E69** (2004), 056205

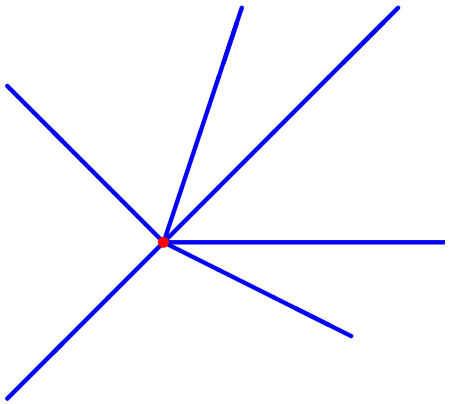
From the mathematical point of view, graphs can support a number of other equations coming both quantum and classical physics. I addition to Schrödinger and Dirac mentioned, for instance *wave equation*, undamped and damped, *elasticity equation*. Also, nonlinear equations such as *Schrödinger* and *Korteweg de Vries* have been studied.

Thirty five years after their rebirth, *quantum graphs are everywhere.*

How to match the wave functions

The choice made by Pauling was not the only possible. Recall that to define a QM Hamiltonian, in general it is not sufficient to specify its differential symbol. To qualify as an observable, the operator must be *self-adjoint*, $H = H^*$, which for an unbounded operator is a considerably stronger requirement than mere *symmetry*, $H \subset H^*$.

In physicist's language this means to demand that that the *probability current must be preserved*. Let us illustrate that on an example:



The most simple case 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 $\psi_j \mapsto -\psi_j''$ (to make things easy, we use the units in which $\hbar = 2m = 1$)

Self-adjoint vertex couplings

Since the operator is of second order, the boundary condition involve the values of functions and the first *outward* derivatives at the vertex.

These boundary values can be written as columns, $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$, the entries understood as left limits at the endpoint; then the most general self-adjoint matching conditions are of the form

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

where the $n \times n$ matrices A, B satisfy the conditions

- $\mathrm{rank}\,(A, B) = n$
- AB^* is *Hermitean*

 Kostrykin and Schrader, *J. Phys.* **A32** (1999), 595  Rofe-Beketov, *Teor. Funkc., Funkc. Anal. Pril.* **8** (1969), 3

Naturally, these conditions are non-unique, as A, B can be replaced by CA, CB with a *regular* C. This non-uniqueness can be removed by using

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

where U is a *unitary $n \times n$ matrix*, hence depending on n^2 real parameters

Self-adjoint vertex couplings

The claim is easy to verify. To see that it is enough to express the squared norms $\|\Psi(0) \pm i\ell\Psi'(0)\|^2_{\mathbb{C}^n}$ and subtract them from each other; the difference is nothing but the *boundary form*,

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

which has to vanish to make the operator self'adjoint.

Note that each term of the sum is, up to the factor $\frac{1}{2}$, nothing but the *probability current* in the jth edge, taken in the outward direction.

As a consequence, the two vectors having the same norm must be related by an $n \times n$ unitary matrix; this gives $(U-I)\Psi(0) + i\ell(U+I)\Psi'(0) = 0$.

It seems that we have one more parameter, but it is not important because the matrices corresponding to two different values are related by

$$U' = \frac{(\ell+\ell')U + \ell - \ell'}{(\ell-\ell')U + \ell + \ell'}.$$

Thus we can set $\ell = 1$, which means just a *choice of the length scale*.

Why we should care about different couplings?

The answer to this question is: from the simple reason – because they describe a *different physics*. Consider again the example of a star graph of n edges, denoting its different Hamiltonians as H_U.

One of them is H_{D} corresponding to $U = -I$, in other words, each edge component of H_U is a halfline Laplacian with *Dirichlet* boundary condition, $\psi_j(0) = 0$. The spectrum of of such a *disconnected graph* is easily found, being $\sigma(H_{\mathrm{D}}) = \mathbb{R}_+$ of multiplicity n.

For any U we have $\sigma_{\mathrm{ess}}(H_U) = \mathbb{R}_+$, because the difference of the resolvents, $(H_U - z)^{-1} - (H_{\mathrm{D}} - z)^{-1}$, is an operator of *finite rank* (equal to n) but in addition, there may be *negative eigenvalues*.

It is easy to check the number of these eigenvalues coincides with the number of eigenvalues of U *in the open upper complex halfplane*.

Common 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 so-called *δ coupling*,

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

  with 'coupling strength' $\alpha \in \mathbb{R}$; $\alpha = \infty$ gives the Dirichlet $U = -I$
- On the other hand, $\alpha = 0$ gives *Kirchhoff condition* mentioned above.
- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the *δ'_{s} coupling*,

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

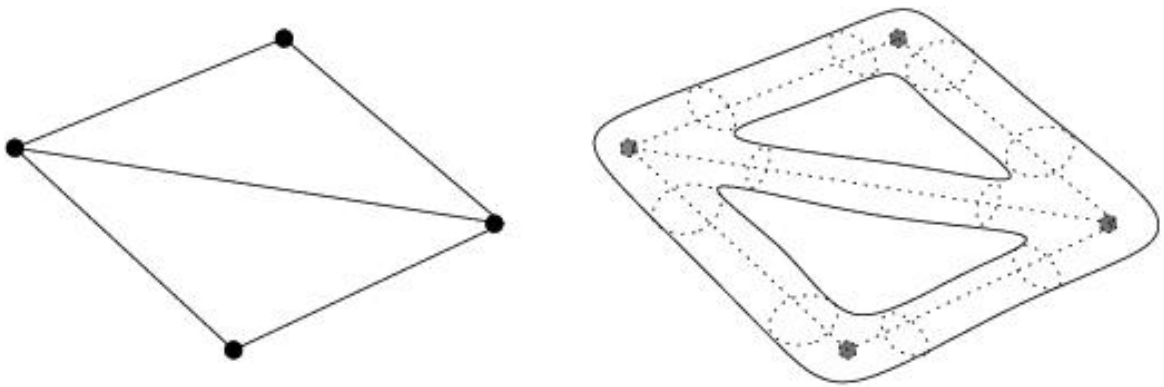
  with $\beta \in \mathbb{R}$. For $\beta = \infty$ we get the *Neumann* decoupling; the case $\beta = 0$ is sometimes referred to as *anti-Kirchhoff condition*.
- Another generalization of the 1D δ' interaction is the *δ' coupling*:

$$\sum_{j=1}^{n} \psi_j'(0) = 0, \quad \psi_j(0) - \psi_k(0) = \frac{\beta}{n}(\psi_j'(0) - \psi_k'(0)),\ 1 \le j,k \le n$$

  with $U = \frac{n-i\alpha}{n+i\alpha}I - \frac{2}{n+i\alpha}\mathcal{J}$ and Neumann edge decoupling for $\beta = \infty$.
- There many other couplings, of course, some of physical interest

Can any s-a coupling be given meaning?

Let us return to the *squeezing network* idea of Ruedenberg and Scher and ask under which conditions one can approximate Hamiltonian of a quantum graphs by the Laplacian – or more general operator – of the appropriate *'fat graph'*



For *Neumann* network the approximation of [RS'53] can be made rigorous, leading to *Kirchhoff coupling* at the vertices.

Kuchment and Zeng, *J. Math. Anal. Appl.* **258** (2001), 671

Rubinstein and Schatzman, *Arch. Rat. Mech. Anal.* **160** (2001), 271

Saito, *Electron. J. Diff. Eq.* **31** (2000), 1

Exner and Post, *J. Geom. Phys.* **54** (2005), 77

What about the other vertex couplings?

The *δ-coupling* is not difficult: in the star graph example we replace the Laplacian with the Schrödinger operator acting as $\psi_j \mapsto -\psi_j'' + V_j\psi_j$ on the graphs edges.

Given a family $W_{\varepsilon,j} := \frac{1}{\varepsilon} W_j\left(\frac{x}{\varepsilon}\right)$, $j = 1, \ldots, n$, of *scaled potentials*, one can prove that – under appropriate assumptions – we have

$$H_0(V + W_\varepsilon) \longrightarrow H_\alpha(V)$$

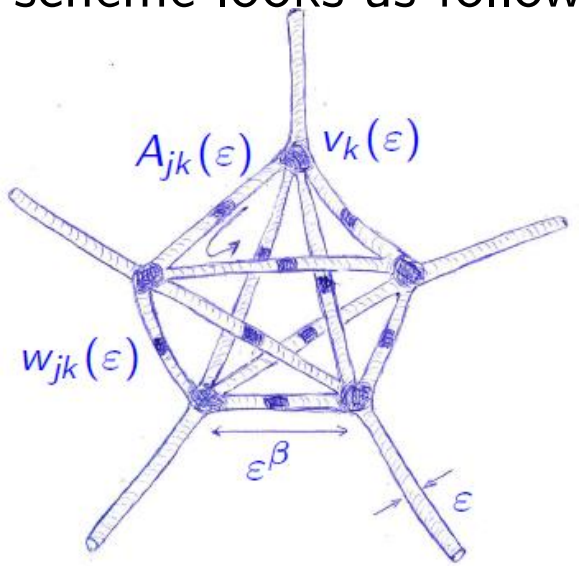
as $\varepsilon \to 0+$ in the *norm resolvent sense*, with the coupling parameter $\alpha := \sum_{j=1}^n \int_0^\infty W_j(x)\,\mathrm{d}x$ representing the 'total' value of the potential.

This result is then easy to 'lift' squeezing networks with scaled potentials.

This is, however, still a small subset in the family of all self-adjoint couplings, and one has to ask whether we can do better.

A general coupling approximation

The answer is affirmative; the scheme looks as follows:



Exner and Post, *Commun. Math. Phys.* **322** (2013), 207

While this is an interesting – a rather involved – mathematics, the result has only the existence meaning and in practice one proceeds pragmatically choosing the coupling *ad hoc* to fit the physics of the problem.

Remark: The squeezing limit of *Dirichlet* networks is completely different. It is generically trivial, but gives a nontrivial result if there is a *resonance at threshold*. The principle is known but no analogue to the above general result has been derived so far.

There are other graphs

The graphs we have considered so far were *metric* meaning that their edges were identified with line segments.

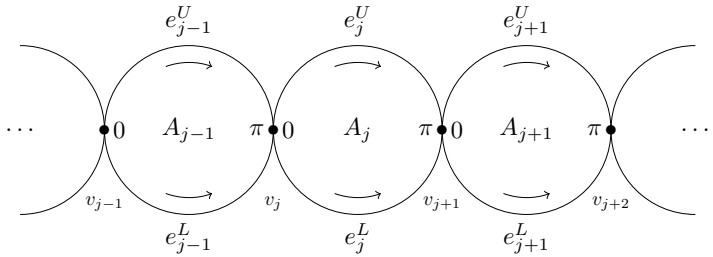
In mathematics, however, graph theory usually means something different; it is a venerable discipline which roots can be traced back at least to 1736 when Leonhard Euler answered the question about the *seven bridges of Königsberg*. A graph is in this setting understood as a collection of *vertices* and of *edges* connecting them in accordance with the graph *adjacency matrix*. The literature on these graphs is immense.

The two theories can be related. It is particularly useful as it allows us to rephrase the spectral analysis of quantum graphs, which is a *differential operator* problem, in terms of a *difference equation*.

The idea proposed in the 1980's by physicists, Alexander and de Gennes, followed by mathematicians. It is particularly simple if the graph in question is *equilateral*. To explain it, we have to exclude first the part σ_{D} consisting of *Dirichlet eigenvalues* with eigenfunctions supported by a *single edge* and *vanishing at its endpoints*.

The duality: a magnetic chain example

As an example, consider an *array of rings*, each of circumference 2π, exposed to a magnetic field perpendicular to the graph plane,



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

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

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

Kostrykin and Schrader, *Commun. Math. Phys.* **237** (2003), 161

If the magnetic field is homogeneous, the spectrum is found by *Floquet decomposition*. It is not purely continuous because of the Dirichlet eigenvalues; if $A - \frac{1}{2} \in \mathbb{Z}$ it consists of *flat bands only*.

The duality: a magnetic chain example

If the field is *non-homogeneous*, the task is more complicated. Apart from the Dirichlet eigenvalues, the spectral problem of the Hamiltonian $-\Delta_{\alpha,A}$ means to solve the differential equation $(-\Delta_{\alpha,A} - k^2)\begin{pmatrix}\psi(x,k)\\ \varphi(x,k)\end{pmatrix} = 0$ with the indicated matching condition at the vertices.

Since we know solutions on the edges, this leads to the *difference* equation

$$2\cos(A_j\pi)\psi_{j+1}(k) + 2\cos(A_{j-1}\pi)\psi_{j-1}(k) = \eta(k)\psi_j(k)\,, \quad k \notin \mathbb{Z}\,,$$

where $\psi_j(k) := \psi(j\pi, k)$ and $\eta(k) := 4\cos k\pi + \frac{\alpha}{k}\sin k\pi$ for $k > 0$, and $\eta(k) := 4 + \alpha\pi$ for $k = 0$.

What is important, this is a two-way correspondence; we can *reconstruct* the solution of the original problem from that of the difference one. This establishes a *two-way connection* between the weak solutions of the two equations preserving their L^p/ℓ^p properties.

The duality: a magnetic chain example

But we can do much better: the restriction $(-\Delta_{\alpha,A}) \restriction J$ to an interval $J \subset \mathbb{R} \setminus \sigma_D$ is *unitarily equivalent* to the *pre-image* $\eta^{(-1)}\big(L_A \restriction \eta(J)\big)$, where L_A is the operator on $\ell^2(\mathbb{Z})$ acting as

$$(L_A\varphi)_j = 2\cos(A_j\pi)\varphi_{j+1} + 2\cos(A_{j-1}\pi)\varphi_{j-1}.$$

Hence the spectrum of $-\Delta_{\alpha,A}$ is obtained by 'unfolding' of $\sigma(L_A)$ by $\eta^{(-1)}$; recall that the function $\eta(k) = 4\cos k\pi + \frac{\alpha}{k}\sin k\pi$ is *monotonous* between any pair of adjacent Dirichlet eigenvalues.

Note also that this claim is a particular case of a general duality result valid for any *equilateral* graph.

Pankrashkin, *J. Math. Anal. Appl.* **396** (2012), 640

To illustrate how the duality can be useful consider an example in which the magnetic field is nonconstant varying *linearly* along the chain, namely $A_j = \mu j + \theta$ for some $\mu, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$.

A chain with linear magnetic field

First of all, you may say that in nature one never meets a (globally) linear magnetic field. A pragmatic answer is that the unbounded character of the sequence $\{A_j\}$ need not bother us because only the *fractional part of each A_j matters.*

But there is a deeper reason why we can consider such a model, nicely expressed by Bratelli and Robinson:

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

Let us thus look how the spectrum of such a chain looks like. It appears that the *character of the slope* μ is important. If it is *rational* the system is *periodic* and by Floquet analysis we find that its spectrum is a combination of *absolutely continuous bands* and *flat bands*; if $\mu j + \theta + \frac{1}{2} \in \mathbb{Z}$ holds for some $j = 0, \ldots, q-1$, the spectrum consists of *flat bands only*.

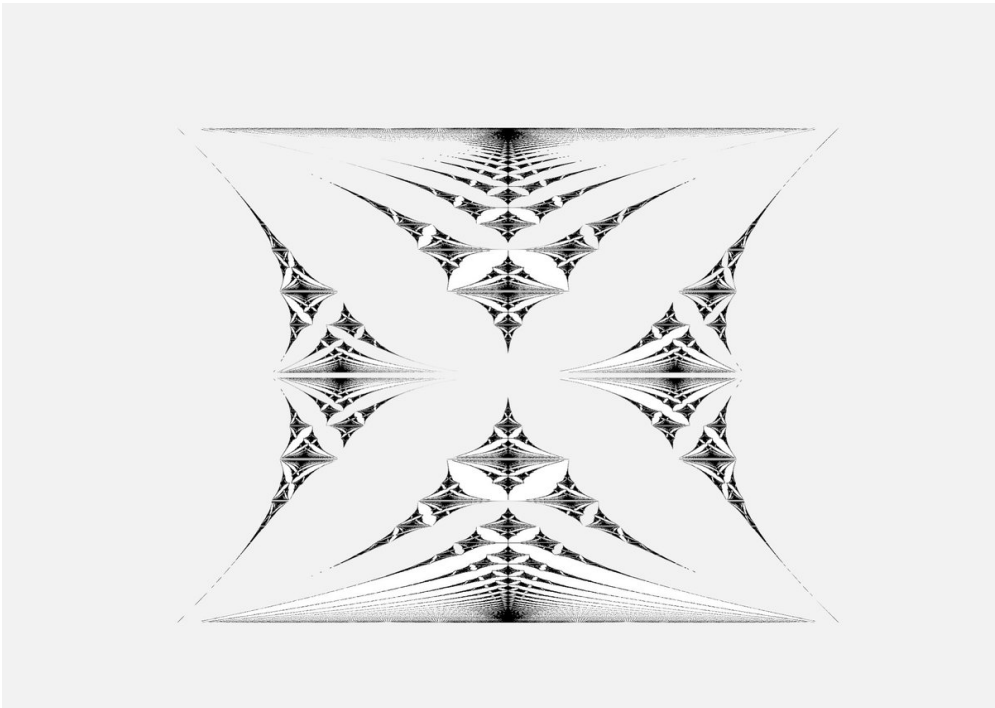
Does it remind you something?

For *irrational* μ the Floquet method cannot be applied but the role the (ir)rationality plays here may bring to your mind a famous problem, the *almost Mathieu equation*

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

in particular its *critical case*, $\lambda = 2$, often also dubbed *Harper equation*.

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



Source: Fermat's Library

The Ten Martini Problem

The spectrum of operator $H_{\mu,2,\theta}$ is easily seen to consists of absolutely continuous bands for any rational value of μ.

On the other hand, the case $\mu \notin \mathbb{Q}$ appeared to be quite difficult and kept mathematicians busy – under the name *Ten Martini Problem* proposed by B. Simon – for more than two decades.

The conjecture saying that the spectrum of $H_{\mu,2,\theta}$ does not depend on θ and it is for any irrational μ a *Cantor set of Lebesgue measure zero* was finally proved to be correct.

Avila and Jitomirskaya, *Ann. Math.* **170** (2009), 303

Note that a complicated spectral behavior exhibited by systems with *incommensurate length scales* was anticipated earlier but it attracted serious attention only after Hofstadter's result ignited the imagination.

Azbel, *J. Exp. Theor. Phys.* **19** (1964), 634

Note also manifestations of such a behavior were found recently by several groups observing graphene lattices in a homogeneous magnetic field.

And how is this related to our problem?

Using an operator algebra trick proposed by Shubin we can establish *unitary equivalence* between $H_{\mu,2,\theta}$ and the operator L_A dual to our quantum graph Hamiltonian. This allows one to determine the spectral character of $-\Delta_{\alpha,A}$ the fact that the function η is *locally analytic*:

 Shubin, *Commun. Math. Phys.* **164** (1994), 259  Exner and Vašata, *J. Phys.* **A50** (2017), 165201

$\sigma(-\Delta_{\alpha,A})$ does not depend on θ and if $\alpha \neq 0$ and $\mu \notin \mathbb{Q}$, 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 $\sigma(-\Delta_{\alpha,A})$ *is zero*.

Translating other almost Mathieu results to this setting, one is able to conclude, e.g., that there is a *dense G_δ set of the slopes μ* for which, and all θ, the Haussdorff dimension $\dim_H \sigma(-\Delta_{\alpha,A}) = 0$. At the same time, there is *another dense set* of the slopes μ, for which, on the contrary, one has $\dim_H \sigma(-\Delta_{\alpha,A}) > 0$.

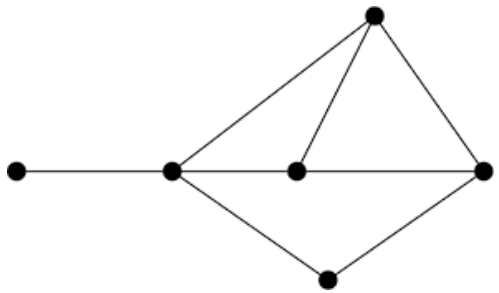
 Last and Shamis, *Commun. Math. Phys.* **348** (2016), 729  Helffer et al., *Commun. Math. Phys.* **368** (2019), 369

Quantum graphs may violate Weyl asymptotics

I hope the example illustrated that quantum graphs – besides their 'practical use – can exhibit intriguing properties.

The list of those is long and in the rest of the talk I am going to show you several other situations where quantum graphs make us think.

One such question concerns the *semiclassical behavior* of the spectrum. Asking about the *eigenvalue counting function* of a finite graph,



$L := \sum_j \ell_j$

our QM intuition suggests – correctly! – that it should be

$$N(k) = \frac{2L}{\pi} k + \mathcal{O}(1)$$

as $k \to \infty$ irrespective of a (nontrivial) vertex coupling; on purpose we *doublecount* considering separately values $\pm k$ giving rise to the energy k^2.

Davies and Pushnitski observation

The situation is similar if we attach to vertices of our finite graph *semi-infinite leads*. Naturally, eigenvalues of the 'core graph' are now embedded in the continuous spectrum of the leads, and a nontrivial coupling turns (some or all of) them into *resonances* to which resolvent poles in the *lower complex halfplane* correspond.

Consequently, one has to count now singularities in the *closed semicircle* $\{z : |z| \leq k, \operatorname{Im} z \leq 0\}$; in the Weyl spirit one expects their number to behave again as $N(k) = \frac{2L}{\pi} k + \mathcal{O}(1)$ when $k \to \infty$.

Alas, this may not be the case! Davies and Pushnitski noted that 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 *smaller than Weyl formula prediction*.

Davies and Pushnitski, *Anal. PDE* **4**(5) (2011), 729

Effective coupling on the 'core graph'

To explain the effect we note that there is a way to consider the 'core graph' only, without the leads. To this aim, we write the matrix U at each vertex where leads are attached in the *block form*, $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$, where U_1 refers to the core, U_4 to the exterior part, and the off-diagonal U_2 and U_3 are rectangular matrices connecting the two.

Then the external part can be eliminated by considering the core only with the *effective coupling* given by

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

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

Note that this is another nice illustration of a simple formula known already to *Schur*, often attributed to *Feshbach*, *Grushin*, and other people.

We also need a tool to count zeros of functions $F(k) = \sum_{r=0}^{n} a_r(k)\,\mathrm{e}^{ik\sigma_r}$. Fortunately, mathematics is eternal and one can use an old result by which the asymptotics is given by the difference of the largest and smallest σ_j.

Langer, *Bull. Amer. Math. Soc.* **37** (1931), 213

The counting function

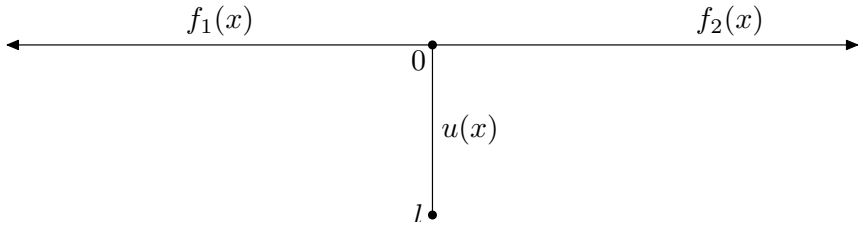
Putting this together we conclude that the counting function for a graph with the *core* Γ and *leads* behaves asymptotically as

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

where W is the *effective size* of Γ satisfying $0 \le W \le L$. Moreover, $W < V$ (we say that graph is *non-Weyl*) if and only there is a vertex such that one of $(1 \mp k)/(1 \pm k)$ is an eigenvalue of the matrix $\tilde{U}_j(k)$.

Davies et al., *J. Phys.* **A43** (2010), 474013

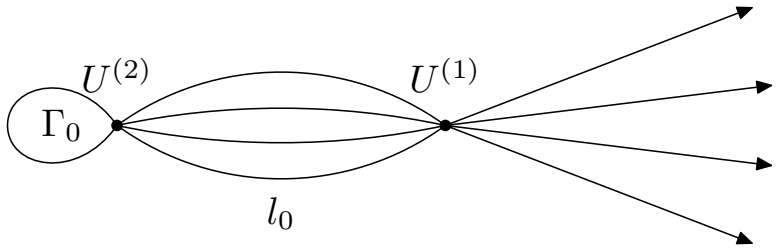
Note that for non-Kirchhoff coupling the vertex *need not be balanced*:



Assuming $f_1(0) = f_2(0) =: f(0)$, $u(\ell) = 0$, together with $u(0) = bf(0)$ and $f_1'(0) + f_2'(0) = -bu'(0)$, we get Weyl graph, $W = \ell$ if $b \neq \sqrt{2}$, but $W = \frac{1}{2}\ell$ if $b = \sqrt{2}$ (the resonance pole escapes then to infinity).

Why balanced vertices matter?

This may look as mathematics, let us try to understand why balanced Kirchhoff vertices diminish the effective size of the core graph. The reason comes from the *symmetry*:

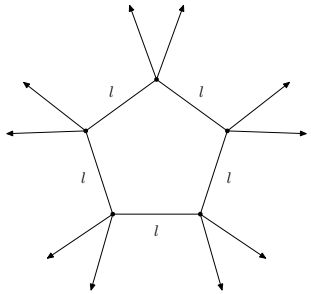


Suppose that a balanced vertex v_1 connects p internal edges of the same length l_0 (we can always add 'dummy' Kirchhoff vertices) and p external edges. Without going into computations, we claim that one can pass to an *unitarily equivalent* graph with the couplings $\tilde{U}^{(2)}$ and $\tilde{U}^{(1)}$ with the latter split into the *one-dimensional symmetric part* and its complement.

However, Kirchhoff coupling at a balanced vertex of *degree one* means *the absence of a coupling*, hence the new graph sees the segment of length ℓ_0 as a *part of the lead*, diminishing thus the effective size.

However, the 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 $(0\,.\,\mathrm{e}^{ik\ell}) - 2(\omega^2+1) + 4\omega\mathrm{e}^{-ik\ell} = 0$. Using it, we easily find that the effective size of Γ_n is

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

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

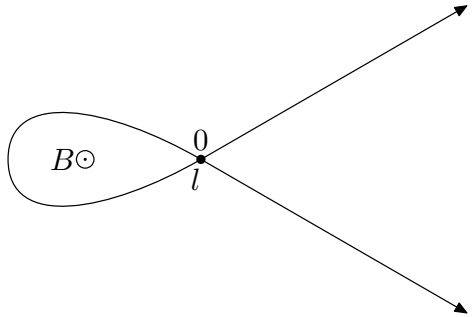
Ławniczak et al., *Phys. Rev. Lett.* **122** (2019), 140503

Magnetic field effects

We saw that a magnetic field can significantly influence quantum graph properties. Let us thus ask what happens with the effective size if such a graph with leads is exposed to a field described by a vector potential A.

By the same technique, reducing the problem to analysis of the core graph with energy-dependent boundary conditions at the 'outer' vertices, one can check that if Γ is *Weyl*, $W = L$, then Γ_A is *also Weyl*.

On the other hand, for *non-Weyl* graphs the field may change their effective size. Here is a simple example:



This (Kirchhoff) graph is non-Weyl for $A = 0$, and thus *for any* A.

Magnetic field effects

The resonance condition for such a graph is easily found to be

$$\text{the missing } \mathrm{e}^{ik\ell} \text{ term } -2\cos\phi + \mathrm{e}^{-ik\ell} = 0,$$

where $\phi = A\ell$ is the magnetic flux through the loop. As the senior term is absent, by Langer theorem the effective size is $W = \frac{1}{2}\ell$ provided that the *ℓ-independent term is nonzero*.

However, for $\phi = \pm\pi/2 \pmod{\pi}$, this term *disappears*. The effective size of the graph is then zero; it is straightforward to see that in the present case there are *no resonances at all*.

Exner and Lipovský, *Phys. Lett.* **A375** (2011), 805

Recall that (in the used units) the *flux quantum* is 2π, hence resonances are absent for *odd multiples* of *a quarter* of the quantum. One could compare it with the ring chain where the absolutely continuous spectrum disappeared for *odd multiples* of *one half* of the quantum.

Even linear graphs may behave nontrivially

To begin with, recall that the first who seriously studied *crystals in a electric field* was Wannier using a natural model combining a periodic and linear potential, often referred to as a *washboard potential*.

He originally thought that such a system may have bound states but this was not the case. If the periodic component was supposed to be regular, the spectrum proved to be *absolutely continuous*, however, exhibiting *resonance ladders*.

The question naturally arose what happens if the interaction is *singular*, in the simplest case given by an equidistant array of *point interactions*, with the Hamiltonian

$$H_{\alpha,F} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \alpha \sum_{n\in\mathbb{Z}} \delta(x - na) - Fx$$

on $L^2(\mathbb{R})$ with some nonzero α and F and an $a > 0$.

Of course, this is nothing but a periodic *line graph* with the δ-coupling.

Wannier-Stark KP ladder

In the absence of the electric field this is nothing but the standard *Kronig-Penney model* the spectrum of which is a textbook matter.

Albeverio et al.: Solvable Models in Quantum Mechanics, 2nd ed., AMS Chelsea 2005

It might this seem that the problem is not difficult to solve but nothing can be farther from the reality!

We know that if the δ interaction is replaced with a *strongly singular one* usually (not very luckily) called δ', defined by the boundary conditions $f'(na+) = f'(na-) =: f'(na)$ and $f(na+) - f(na-) = \beta f'(na)$ – this again a line graph, now with a different self-adjoint coupling – we have

$$\sigma_{\mathrm{ac}}(H_{\delta',\beta,F}) = \emptyset$$

and spectrum is *pure point*, dense or not depending on the properties of F.

Avron et al., *Phys. Rev. Lett.* **72** (1994), 896

Duclos et al., Helv. Phys. Acta **71** (1998), 133

The reason is the *high-energy gap behavior* of the periodic system.

Wannier-Stark KP ladder

The gaps are *shrinking* for a regular potential, while for δ' their widths are *increasing* as $k \to \infty$. And if the gaps are *tilted* by the electric field, they represent *classically forbidden zones*!

The δ case represents a *borderline situation* as in this case the gaps are *asymptotically constant* (in the energy variable). Treatments – of a various degree of rigor – were suggesting that there may be a transition from pure point spectrum for *small* $|F|$ to *continuous* one for strong field was conjectured, and that the *rationality* of the field intensity may play role.


Berezhkovskii and Ovchinnikov, *Sov. Phys. Solid State* **18** (1976), 1908


Ao, *Phys. Rev.* **B41** (1990), 2998


Borysowicz, *Phys. Lett.* **A231** (1997), 240


Buslaev, *AMS Translations*, vol. 189, 1999

This seemed to be supported by the result about the *random WS ladder* in which the constant strength α is replaced by *i.i.d. variable* $\{\alpha_n\}$ of *zero mean*; with *probability one* we have here a transition from pure point to continuous spectrum.


Delyon et al., *Phys. Rev. Lett.* **52** (1984), 2187

Wannier-Stark KP ladder

The last result was very recently strengthened by Frank and Larson: putting $\alpha^2 := \mathbb{E}[\alpha_n^2]$ they proved under some technical assumptions that $\sigma(H_{\alpha,F}) = \mathbb{R}$ holds almost surely being

- singularly continuous if $F > \alpha^2/2a^2$
- dense pure point if $F > \alpha^2/2a^2$

Frank and Larson, *Prob. Math. Phys.* (2022), to appear; arXiv:2104.10256

However, they also proved – at that was a true *tour de force!* – that in the *deterministic case* things look differently, namely:

If $Fa^2/\pi^2 \in \mathbb{Q}_+$ and $F = \frac{q}{3p}$ with $p, q \in \mathbb{N}$, one has

$$\sigma_{\mathrm{ac}}(H_{\alpha,F}) = \mathbb{R}\,,\ \sigma_{\mathrm{sc}}(H_{\alpha,F}) = \emptyset\,,\ \sigma_{\mathrm{pp}}(H_{\alpha,F}) \subset \left\{ \frac{\pi^2}{3pa^2} m + \alpha :\ m \in \mathbb{Z} \right\}.$$

The question about the *irrational field slope* remains open!

Can one hear the shape of a graph?

So far we dealt with spectral (and transport) properties of a single graph, or a class of graphs. One can also ask an *opposite question*: given spectral data of a graph Hamiltonian, can one retrieve information about the graph geometry and topology?

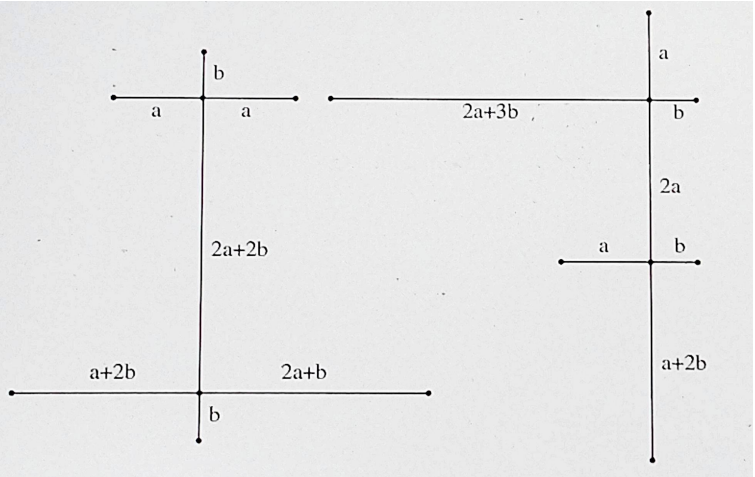
The above question, asked by Gutkin and Smilansky, was of course inspired by the classical question of *Mark Kac* about the *shape of the drum* of which we nowadays know that it is answered negatively, although there are classes of regions for which the answer is affirmative.

Gutkin and Smilansky, *J. Phys.* **34** (2001), 6061

In the case of graphs it was no surprise that the answer, in general, was negative. Examples of isospectral *combinatorial* graphs were known for long, and in view of the duality we have discussed, one could naturally 'translate' these results into the quantum graphs setting.

Isospectral graphs

An example of *isospectral pair* with Kirchhoff vertices, due to [GS'01], is



The example is not a single one, in fact there is a method to construct isospectral graphs which, similarly to construction of isospectral Dirichlet domains addressing Kac's question, has its roots in *Sunada's method* of finding isospectral Riemannian manifolds.

Sunada, *Ann. Math.* **121** (1985), 169

An atlas of isospectral graphs can be found in

Band et al., *J. Phys.* **A42** (2009), 175202

So, which quantum graphs can one hear?

Obviously, to find a class for which the question could be answered affirmatively, one should look 'far away' from equilateral graphs.

The assumptions one has to impose are the following:

- Graph edges are 'fully connected' meaning that the scattering matrix $(S_{jj'})$ at each vertex is *energy-independent* and has *no zero entries*
- The graph has *no loops* and *multiple edges*
- All the edge lengths are *incommensurate*

Under these conditions the spectrum determines *uniquely* the *edge lengths* and the *graph connectivity*.

 Gutkin and Smilansky, *J. Phys.* **34** (2001), 6061  Kurasov and Nowaczyk, *J. Phys.* **A38** (2005), 4901

The reconstruction can be also based on *scattering data*: if we have a graph consisting of a *compact core* and *leads* such that the above assumptions hold for *all the vertices* and *all internal edges*, then the 'edge-to-edge' scattering matrix *determines the graph uniquely*.

The trace formula

The key element of the argument is the formula expressing the *density of states* which can be formally written as

$$d(k) \equiv \sum_n \delta(k - k_n) = \frac{L}{\pi} + \frac{1}{2\pi} \sum_p \left(\mathcal{A}_p \mathrm{e}^{ik\ell_p} + \mathcal{A}_p^* \mathrm{e}^{-ik\ell_p} \right)$$

where the sum runs over all *periodic orbits* in the graph, including those with repetitions, ℓ_p is the *orbit length*, and $\mathcal{A}_p$ is the product of *scattering amplitudes* at the vertices of the path.

It was discovered in the early days and rediscovered repeatedly; it can be made rigorous through averaging with suitable trial functions.

 Roth, *C.R. Acad, Sci.* **296** (1983), 793  Bolte and Endres, *Ann. H. Poincaré* **10** (2009), 189

In view of the incommensurability, one can use the trace formula to find the *length spectrum* of the graph and use it successively to arrange the edges into *metric stars* with the appropriate connectivity.

Quantum chaos in graphs

It is well known that the concepts of *chaotic motion* is classical and quantum physics are widely different. It the former it is manifested by the sensitivity of trajectories to the initial conditions, absence of tori in the phase space, etc.

Chaotic motion of quantum systems, on the other hand, shows in the *distribution of eigenvalues* which looks like that of *large random matrices*. The standard *BGS conjecture* about *billiard dynamics* says that classically chaotic regions exhibit random-type-matrix spectra. Note, however, that the correspondence is not one-to-one, the example of *Šeba billiard* shows that even a classically integrable system may have such a spectrum.

 Bohigas et al., *Phys. Rev. Lett.* **52** (1984), 1

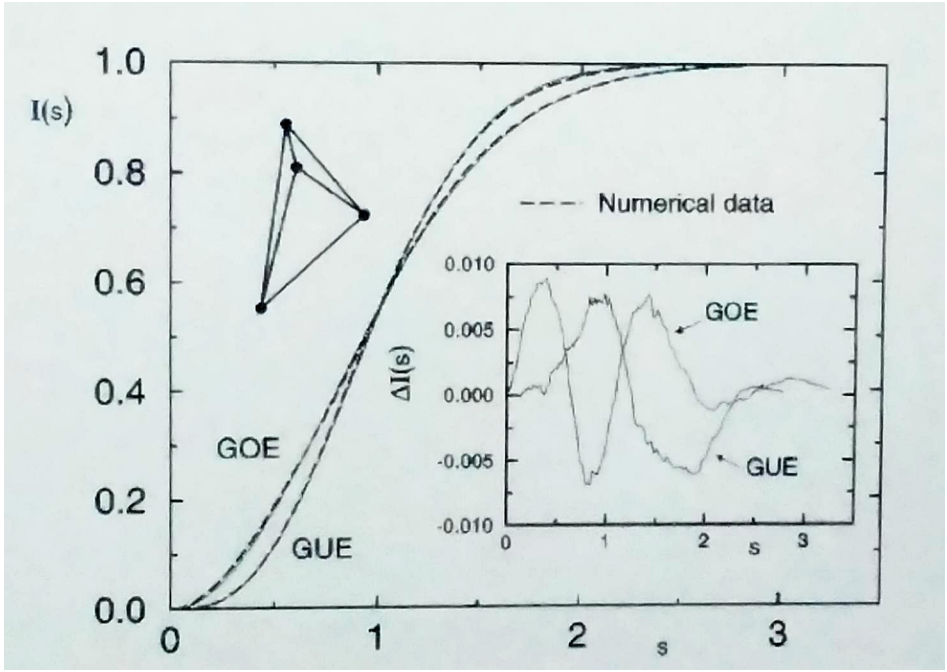
 Šeba, *Phys. Rev. Lett.* **64** (1990), 1855

Kottos and Smilansky proposed to study *quantum chaos on graphs*. It has one obvious advantage: to get a reliable spectral statistics you have to compute a large number of eigenvalues which is much easier here that in the PDE setting.

 Kottos and Smilansky, *Phys. Rev. Lett.* **79** (1997), 4794

A simple example

Adopted from [KS'97] we show here results for a *tetrahedron graph* with *Kirchhoff coupling* at the vertices.



It shows *integrated nearest neighbor distribution* for 80 thousand levels, compared to standard *RMT distributions*, namely *GUE* for the graph with the *magnetic field* and *GOE* for the graph without it.

When and which quantum chaos can we see?

Naturally, now every graph shows a chaotic behavior. To begin with, in analogy with the inverse problem discussed before, a universal behavior is expected in graphs with *incommensurate edges*.

The edges must be connected by *non-separating matching conditions*, otherwise we will obtain *Poissonian distribution* characteristic for independent segments.

This is not sufficient, however, to get an RMT-type result. For instance, a *star graph* with incommensurate edges and Kirchhoff coupling the nearest neighbor distribution shows a *level repulsion* but different from the GOE. We need a 'sufficient connectivity', e.g. the tetrahedron graph is *complete*.


Berkolaiko and Kuchment: Introduction to Quantum Graphs, AMS 2013

In addition to *orthogonal ensembles* of random matrices we saw, one meets also *symplectic* chaotic graphs; this happens when Laplacian on the graph is replaced by the *Dirac operator*.


Bolte and Harrison, *J. Phys.* **A36** (2003), 2747

More chaotic features

The nearest neighbor distribution is not the only characteristics of the chaotic behavior. One also studies the *two-point correlation function*,

$$R_2(x) = \operatorname*{weak–lim}_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \delta(x - (k_j - k_i))$$

and the *form factor* obtained by Fourier transformation,

$$K(\tau) = \int_{\mathbb{R}} \mathrm{e}^{2\pi i x\tau} (R_2(x) - 1)\, \mathrm{d}x\,.$$

The form factor was in various chaotic graphs again found to be in agreement with corresponding quantity of the respective random matrix ensemble.

The form factor can be expressed by means of the trace formula mentioned above. While graphs – in contrast to billiards – have no classical counterpart, *periodic orbits* appearing in the trace formula can be regarded as a certain analogue of classical dynamics.

Leaky graphs

Regarding quantum graphs as model nanowires is in a sense *too idealized*. I reality the confinement of electrons to such a wire is not absolute; the wire boundary is, for instance, an interface between two semiconductor materials, and as result, *tunneling* is possible.

Looking for a more realistic model, let us consider a *planar graph* Γ and choose the singular Schrödinger operator

$$H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma), \quad \alpha > 0,$$

in $L^2(\mathbb{R}^2)$ with *attractive interaction* as its Hamiltonian.

The particle can be now be found in the whole plane. States belonging to the *negative spectral subspace* remain *localized close to* Γ and the set $\mathbb{R}^2 \setminus \Gamma$ is *classically forbidden region*, hence tunneling between parts of Γ is possible with the probability decreasing exponentially with the distance.

We call such models we use the name *leaky (quantum) graphs*. We can also study them in higher dimensions, say with Γ composed of curves and surfaces in $\mathbb{R}^3$ – the only limitation is that the *codimension* of the interaction *must be* ≤ 3 but for simplicity we stay with the 2D situation.

There is more geometry in leaky graphs

In the 'standard' quantum graphs the geometrical information consists of the *lengths* of the edges and their *connectivity*, now we have to take in addition their *shapes* into account.

This seems innocent but it is not. As an example, consider the situation when Γ is a *single infinite curve*. If Γ is a *straight line*, the variable separate and $H_{\alpha,\Gamma}$ has a *purely* ac *spectrum*, $\sigma(H_{\alpha,\Gamma}) = \big[-\frac{1}{4}\alpha^2, \infty\big)$.

Let us look what happens if we *bend the curve* assuming that

- $\Gamma : \mathbb{R} \to \mathbb{R}^2$ is *piecewise C^1-smooth* parametrized by its arc length
- $|\Gamma(s) - \Gamma(s')| \geq c|s - s'|$ holds for some $c \in (0,1)$ excluding, e.g., self-intersections and U-shapes
- Γ is *asymptotically straight*: there are $d > 0$, $\mu > \frac{1}{2}$ such that

$$1 - \frac{|\Gamma(s) - \Gamma(s')|}{|s - s'|} \leq d \left[1 + |s + s'|^{2\mu}\right]^{-1/2}$$

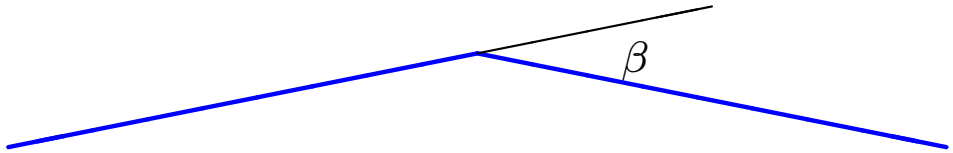
holds in $S_\omega := \left\{(s, s') : \omega < \frac{s}{s'} < \omega^{-1}\right\}$ with some $\omega \in (0,1)$.

Spectrum of a bent curve

In the described situation, the essential spectrum *remains preserved*, $\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}) = [-\frac{1}{4}\alpha^2, \infty)$. What is more interesting, however, that the geometry induces the *existence of discrete spectrum*: if Γ is *not* straight, $H_{\alpha,\Gamma}$ has at least one eigenvalue below the threshold $-\frac{1}{4}\alpha^2$.

Exner and Ichinose, *J. Phys.* **A34** (2001), 1439

The discrete spectrum depends on the geometry being non-void unless Γ is straight. Consider a *broken line* $\Gamma = \Gamma_\beta$ with a small angle β,



which has a single eigenvalue with the asymptotic behavior

$$\frac{-\frac{1}{4}\alpha^2 - \lambda_1(H_{\alpha,\Gamma_\beta})}{-\frac{1}{4}\alpha^2} = -\frac{1}{9\pi^2}\beta^4 + o(\beta^4) \quad \text{as} \quad \beta \to 0.$$

Exner and Kondej, *J. Phys.* **A48** (2015), 495301

More complicated graphs

Geometric effects also appear in more complicated graphs. Some follow directly for the result we quoted. As an example, consider a *star graph* Γ with semiinfinite edges. Except of the trivial case of a straight line, Γ contains *at least one broken line* which we call $\tilde{\Gamma}$.

It is easy to check the essential spectrum of the two is the same,

$$\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}) = \sigma_{\mathrm{ess}}(H_{\alpha,\tilde{\Gamma}}) = \big[-\tfrac{1}{4}\alpha^2, \infty\big)\,,$$

and since $H_{\alpha,\Gamma} \leq H_{\alpha,\tilde{\Gamma}}$, by minimax principle we infer that $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \neq \emptyset$.

Another simple variational argument shows that $\#\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma})$ can be made *arbitrarily large* if we choose one of the angles of the star *sufficiently small*.

This again illustrate the difference between the leaky and 'standard' quantum graphs: for the latter the number of bound states in an infinite-star graph *cannot exceed the vertex degree*.

Leaky graphs with a strong coupling

If the δ interaction is strong, the wave function are concentrated in the small neighborhood of Γ making them *essentially one-dimensional*. Nevertheless, the geometric effect are still there.

To understand what is happening, consider again an *infinite curve*, non-straight but asymptotically straight, this time *smooth enough* so that its *curvature* $\kappa(s)$ and its first two derivatives exist, and ask how the jth eigenvalue of $H_{\alpha,\Gamma}$ behaves as $\alpha \to \infty$. We find that

$$\lambda_j(\alpha) = -\frac{1}{4}\alpha^2 + \mu_j + \mathcal{O}(\alpha^{-1} \ln \alpha)$$

where μ_j is the jth eigenvalue of $S_\Gamma = -\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \frac{1}{4}\kappa(s)^2$, and we know that the operator S_Γ has *at last one negative eigenvalue* whenever $\kappa \neq 0$.

Exner and Yoshitomi, *J. Geom. Phys.* **41** (2002), 344

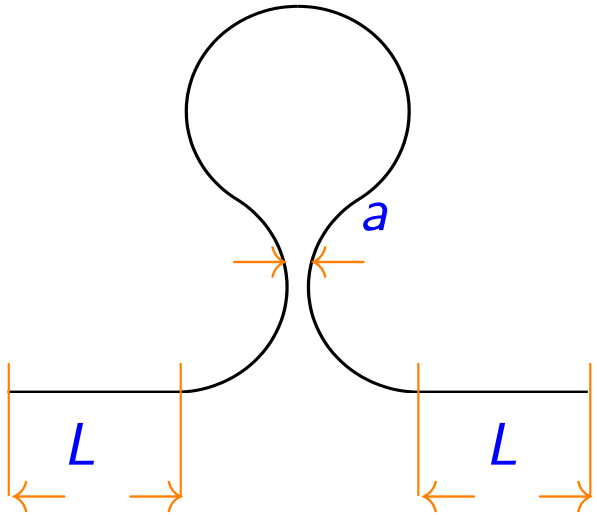
The same technique can be used to show that if Γ is a *smooth periodic curve*, the spectrum of $H_{\alpha,\Gamma}$ has *open gaps* for α large enough.

Yoshitomi, *J. Diff. Eqs* **142** (1998), 12

Scattering on leaky curve

The geometrically induced bound states manifest that parts of a leaky graph 'talk to each other'. Another illustration is provided by *scattering*, even on a *single curve*; we focus on negative energies when the particle is localized in the vicinity of the curve.

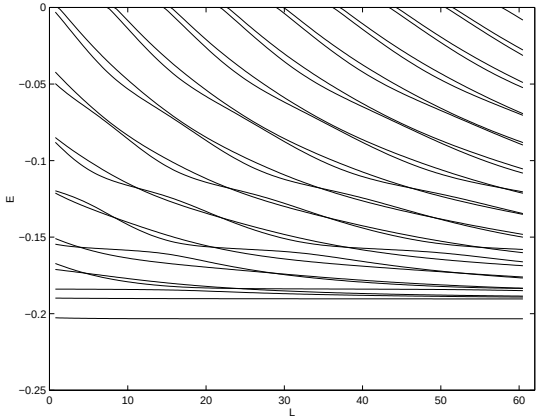
Consider a straight line deformation shaped as an open loop with a bottleneck the width a of which we will vary and ask about *resonances*



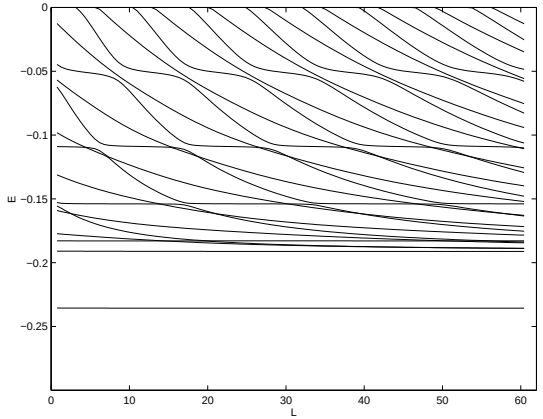
For a straight Γ the transverse eigenfunction is $\mathrm{e}^{-\alpha|y|/2}$, so the distance at which tunneling becomes significant is $\approx 4\alpha^{-1}$. In the example, we choose $\alpha = 1$ and use a well-known physicist's trick to study *resonances* by exploring *spectral properties* of the problem cut to a finite length L and to look for *avoided crossings* in the L eigenvalue dependence.

Hagedorn and B. Meller, *J. Math. Phys.* **41** (2000), 103

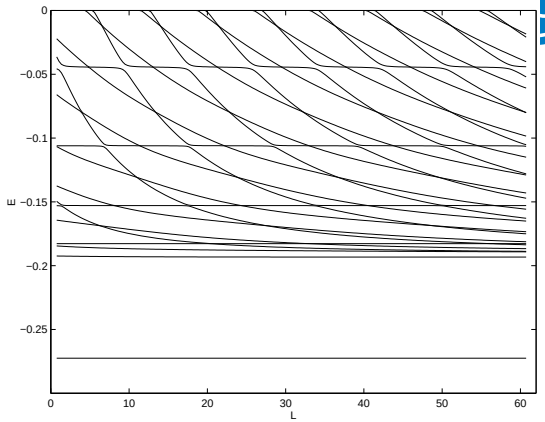
Resonances on bottleneck curve



Wide bottleneck, $a = 5.2$



Narrow bottleneck, $a = 2.9$



Even narrower one, $a = 1.9$

We see that if the bottleneck width is small enough, the system exhibits *resonances*, obviously caused by *tunneling* between adjacent parts.

Those are absent in the 'standard' quantum graph where the curve is *equivalent to a straight line*, and this cannot be changed even if we add a *curvature-induced potential*, say, $-\frac{1}{4}\gamma(s)^2$; to see that, it is enough to 'flip' one half of the curve.

This not the last interesting problem quantum graphs may offer – there are many more – but I am afraid time came to stop.

It remains to say

Thank you for your attention!