Guided quantum dynamics

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With thanks to all my collaborators

A minicourse at the SOMPATY Summer School on Mathematics for the Micro/Nano-World

Samarkand, September 11-16, 2023

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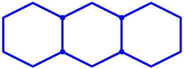
- *Lecture V:* Spectral optimization of graphs and waveguides. Effects of magnetic fields. Summary and outlook.

Where they came from: 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



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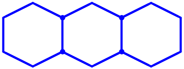

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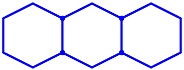

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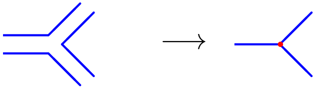
This is not the only choice, though. A formal justification of Kirchhoff coupling was later proposed seventeen years later using a natural idea



K. Ruedenberg, C.W. Scherr: Free–electron network model for conjugated systems, I. Theory, *J. Chem. Phys.* **21** (1953), 1565–1581.

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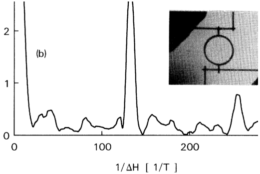

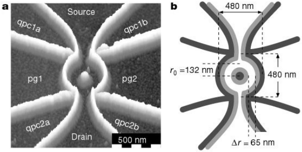

The left figure shows a demonstration of Aharonov-Bohm effect in ring of diameter diameter 784nm made of *gold wire* of width 41nm, the right one a ring-type *heterostructure made of AlGaAs-GaAs*.

R.A. Webb, S. Washburn, C.P. Umbach, R.B. Laibowitz: Observation of h/e Aharonov-Bohm oOscillations in normal-metal rings, *Phys. Rev. Lett.* **54** (1985), 2696–2699.

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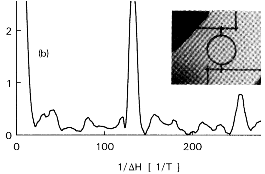

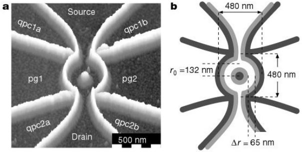

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Quantum graphs appeared be very good models of such systems!

Three decades later graphs are everywhere

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- In addition to Schrödinger, graphs can also support *Dirac operators*. Such models gained importance recently; the reason is that electron motion in *graphene* can be described by *massless Dirac equation*.

  W. Bulla, T. Trenkler : The free Dirac operator on compact and noncompact graphs, *J. Math. Phys.* **31** (1990), 1157–1163.

  J. Bolte, J.M. Harrison: Spectral statistics for the Dirac operator on graphs, *J. Phys. A: Math. Gen.* **36** (2003), 2747–2769.

And the list continues

- Graphs are also used to describe other physical processes governed, for example, by the *wave* or *elasticity* equation.

P. Freitas, J. Lipovský: Eigenvalue asymptotics for the damped wave equation on metric graphs, *J. Diff. Eqs* **263** (2013), 2780–2811.

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- The graph literature is extensive indeed; the best source I can recommend to start with are the monographs

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

  A. Kostenko, N. Nicolussi: *Laplacians on Infinite Graphs*, Mem. EMS, Berlin 2022.

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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*, $H \subset H^*$.

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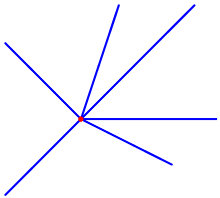
In physicist's language this means to demand that that the *probability current must be preserved*. Let us illustrate that on an example:



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 $\psi_j \mapsto -\psi_j''$

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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

- $\mathrm{rank}\,(A, B) = n$

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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*.

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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*,

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

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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*.

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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 these operators is easily found, it implies that $\sigma(H_{\mathrm{D}}) = \mathbb{R}_+$ of multiplicity n.

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

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Answer: Their number coincides with the number of eigenvalues of U *in the open upper complex halfplane*. Indeed, the matching condition can diagonalized, and on the appropriate subspaces of $\bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ we get n *Robin problems*, $\phi_j'(0) + \tan\frac{\alpha_j}{2}\phi_j(0) = 0$ for the eigenvalue $\mathrm{e}^{i\alpha_j}$ of U.

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*,

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- Another generalization of the 1D δ' interaction is the *δ' coupling*:

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

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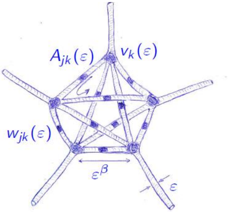

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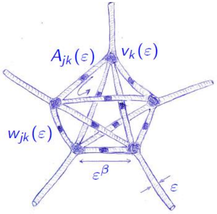

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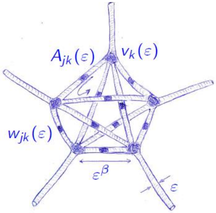

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Transport in quantum graphs

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- 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* in the spectral gaps.

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- 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.

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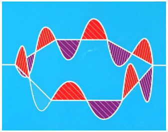

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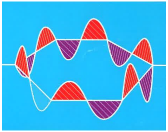

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Let us consider a graph Γ consisting of vertices $\mathcal{V} = \{x_j : j \in I\}$, finite edges $\mathcal{L} = \{\mathcal{L}_{jn} : (x_j, x_n) \in I_{\mathcal{L}} \subset I \times I\}$, and semiinfinite edges (leads) $\mathcal{L}_\infty = \{\mathcal{L}_{j\infty} : x_j \in I_{\mathcal{C}}\}$. 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

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

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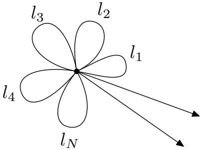

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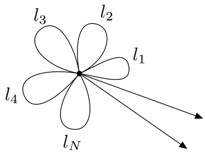

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The coupling in the 'master vertex' is then described by the condition

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

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

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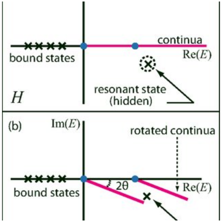

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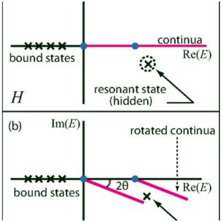

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Quantum graphs we consider are well suited for application of an *exterior* complex scaling. Looking for complex eigenvalues of the scaled operator we preserve the compact part of the graph using the wave function Ansatz $f_j(x) = a_j \sin kx + b_j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

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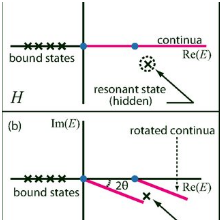

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On the other hand, functions on the semi-infinite edges are scaled by $g_{j\theta}(x) = \mathrm{e}^{\theta/2} g_j(x\mathrm{e}^{\theta})$ with an imaginary θ; the poles of the resolvent on the second sheet become 'uncovered' for *θ large enough*. The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

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

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

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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

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

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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.

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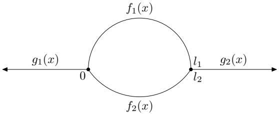
This is another nice illustration of a simple formula know already to *Schur*, often attributed to *Feshbach*, or *Grushin*, or other people.

Example: a loop with two leads



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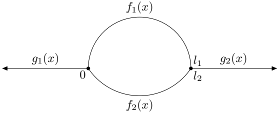

In each vertex we use a four-parameter family of boundary conditions assuming *continuity on the loop*, $f_1(0) = f_2(0)$, together with

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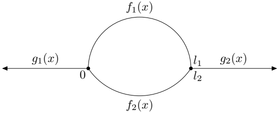

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Writing the loop edge lengths as $l_1 = l(1-\lambda)$ and $l_2 = l(1+\lambda)$ with $\lambda \in [0,1]$, which effectively means shifting one of the connections points around the loop as λ is changing, one arrives at the resonance condition

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

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

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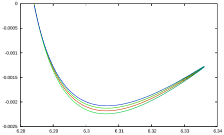

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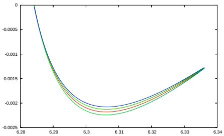

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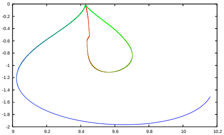

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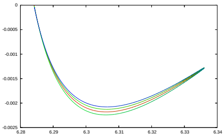

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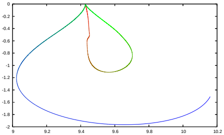

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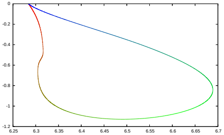

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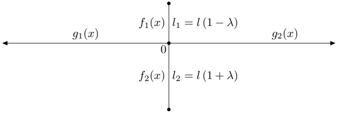
Another example: a cross-shaped graph



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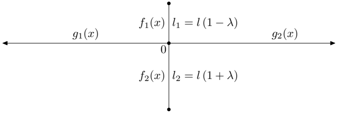

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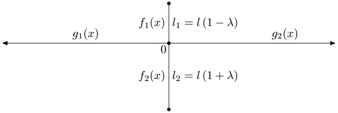

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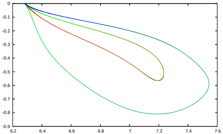

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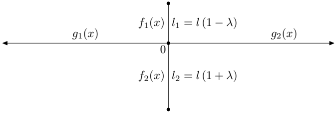

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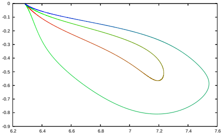

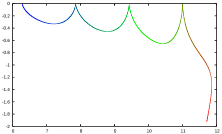

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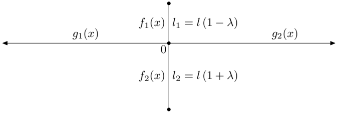

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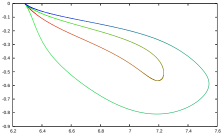

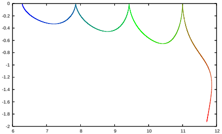

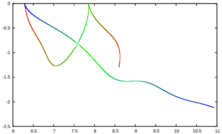

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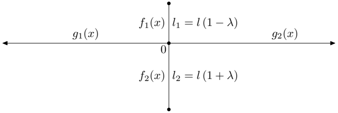

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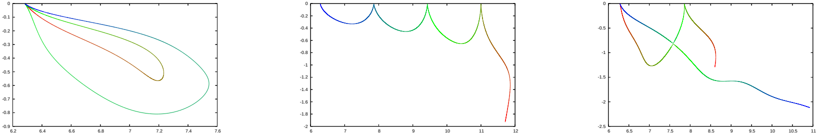

The last one shows an *avoided crossing* of resonance trajectories, the last two also illustrate an effect called *quantum holonomy*.

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

High-energy asymptotics

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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 $e^\pm := \prod_{j=1}^N e_j^\pm$, 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 $E_i(k) = \mathrm{diag}\left(E_i^{(1)}, E_i^{(2)}, \dots, E_i^{(N)}, 0, \dots, 0\right)$, $i = 1, 2, 3, 4$, consists of a trivial $M \times M$ part and N nontrivial 2×2 blocks

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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 $\sigma_0 < \sigma_1 < \cdots < \sigma_n$. 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.

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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.*

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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*

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

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where W *is the effective size of* Γ *satisfying* $0 \le W \le V := \sum_{j=1}^{N} l_j$. *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.

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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:

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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,

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

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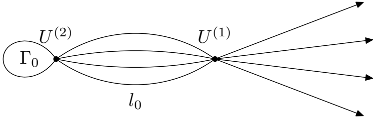
If one drops the requirement of permutation symmetry, it is possible to construct *examples of non-Weyl graphs* in which *no vertex is balanced*.

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.



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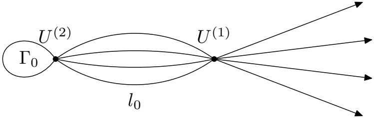

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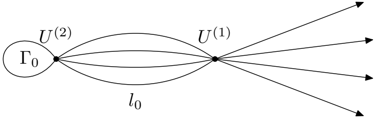

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The idea is to use a *unitary equivalence*. Given a unitary $p \times p$ matrix V we define $V^{(1)} := \mathrm{diag}\,(V, V)$ and $V^{(2)} := \mathrm{diag}\,(I_{(q-p)\times(q-p)}, V)$, then it is straightforward to check that the original graph Hamiltonian 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.

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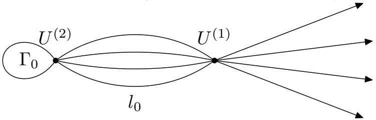

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If the columns of V are *orthonormal eigenvectors* of $U^{(1)}$, beginning with $\frac{1}{\sqrt{p}}(1, 1, \dots, 1)^{\mathrm{T}}$, then $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ decouples then into $2\times$ *blocks*.

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 $j = 2, \ldots, p$.

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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*.

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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

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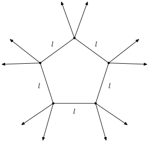

The symmetry allows to decompose the system w.r.t. the cyclic rotation group $\mathbb{Z}_n$ into segments characterized by numbers ω satisfying $\omega^n = 1$; the resonance condition then reads $-2(\omega^2+1)+4\omega\mathrm{e}^{-ik\ell}=0$

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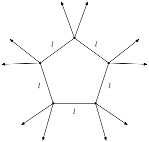

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$$W_n = \begin{cases} n\ell/2 & \text{if } n \neq 0 \ (\mathrm{mod} 4), \\ (n-2)\ell/2 & \text{if } n = 0 \ (\mathrm{mod} 4). \end{cases}$$

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

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

Periodic graphs

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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*.

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

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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.

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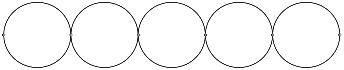

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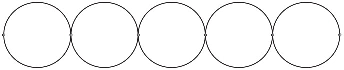

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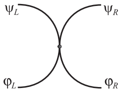

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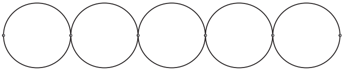

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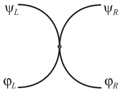

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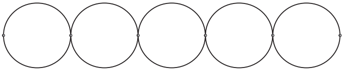

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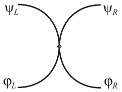

The functions have to be matched through *(a) the δ-coupling* and *(b) Floquet conditions*. This yields equation for the phase factor $\mathrm{e}^{i\theta}$,

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

Ring chain graphs

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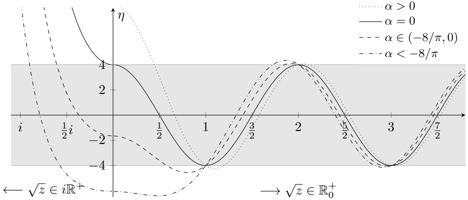

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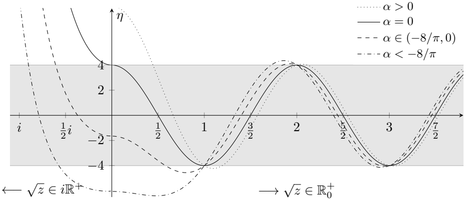

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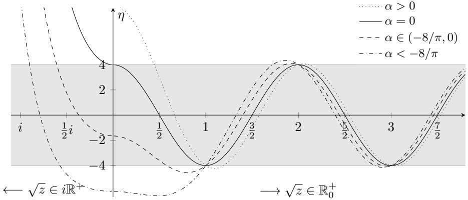

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Note that, up to a factor $\frac{1}{2}$, this nothing but the spectrum of the *Kronig-Penney* model as it is clear from the mirror symmetry of the chain.

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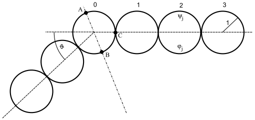

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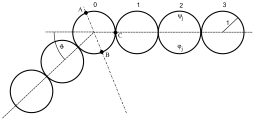

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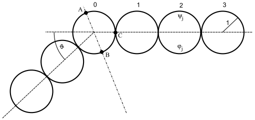

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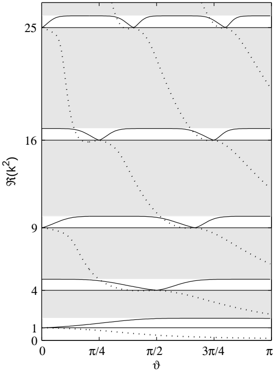
From the general principles we have *at most to eigenvalues* in each gap, because $H_\vartheta^\pm$ and $H_0^\pm$ have a common symmetric restriction with *deficiency indices* $(2,2)$. Furthermore, the *mirror symmetry* allows us to treat the *even* and *odd* parts separately, that is, the halfchain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

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



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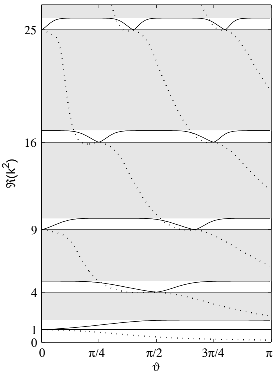

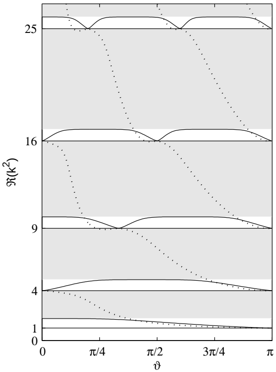

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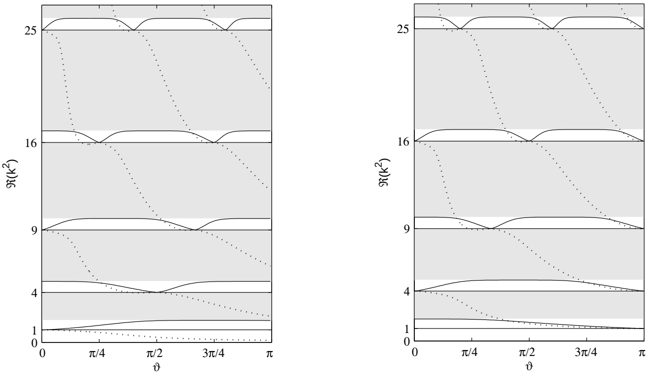

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We see that the eigenvalues in gaps may be absent but only at rational values of ϑ and never simultaneously. Similar pictures we get for other values of α, the dotted lines mark (real values) of *resonance* positions.

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

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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.

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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.

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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.

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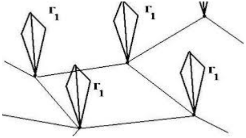

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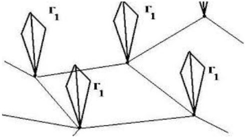

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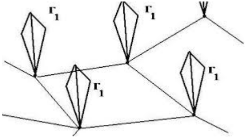

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Thus, instead of 'not a strict law', the question rather is whether *it is a 'law' at all*: do infinite periodic graphs having a *finite nonzero* number of open gaps exist? From obvious reasons we would call them *Bethe-Sommerfeld graphs*.

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

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Theorem

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

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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.

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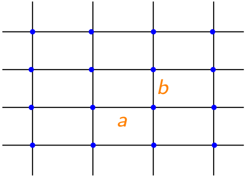
It is sufficient, of course, to demonstrate an example. With this aim we are going to revisit the model of a *rectangular lattice graph* with a δ *coupling* in the vertices introduced in

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

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

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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

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On the other hand, $\theta \in \mathbb{R}$ is *badly approximable* if there is a $c > 0$ such that

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

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

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

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

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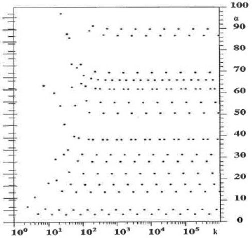

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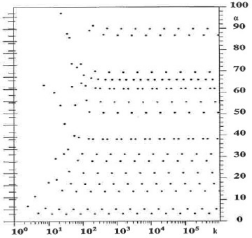

where the points approach the limit values *from above*. Note also that 'higher' gap series open as the coupling strength α increases; the critical values at which that happens are $\frac{\pi^2}{\sqrt{5ab}}\theta^{\pm 1/2}|n^2 - m^2 - nm|,\ n, m \in \mathbb{N}$, cf. [E-Gawlista'96, loc.cit.].

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

(ii) *If*
$$-\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right) \leq \alpha \leq \frac{\pi^2}{\sqrt{5}a},$$
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Corollary

The above claim about the existence of BS graphs is valid.

More about this example

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We are also able to control the number of gaps in the BS regime; a more refined Diophantine analysis yields the following result:

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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

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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

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

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

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- Quantum graphs typically exhibit rich families of *resonances*. Depending on the vertex coupling their semiclassical behavior may *violate Weyl's law*.

What to bring home from Lecture I

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- Quantum graphs offer a nice illustration of the *importance of self-adjointness*, or more specifically, they show that this property is much more than mere 'Hermiticity' of operators supposed to represent observables.
- Quantum graphs typically exhibit rich families of *resonances*. Depending on the vertex coupling their semiclassical behavior may *violate Weyl's law*.
- Periodic quantum graphs often exhibit *flat bands*. There are graphs in which the number of open gaps is *nonzero and finite*.