Quantum graphs and their applications

Part II, following lectures by Peter Kuchment

Pavel Exner

exner@ujf.cas.cz

Doppler Institute

for Mathematical Physics and Applied Mathematics

Prague

Overview of Part II

After you learned how metric graphs are used to model physical systems and what are their properties, we will look into a justification of the model and a modification of it.

- *Lecture IV*
  Our subject today is *the meaning of the vertex coupling*, i.e. ways in which one can understand the parameters in the boundary conditions. We will approach the problem by *approximating a quantum graph* by a family of systems with well defined properties

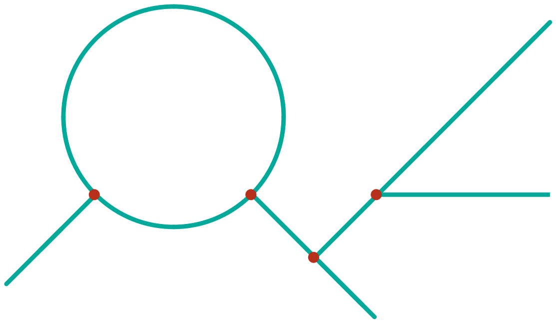
Overview of Part II

After you learned how metric graphs are used to model physical systems and what are their properties, we will look into a justification of the model and a modification of it.

- *Lecture IV*
  Our subject today is *the meaning of the vertex coupling*, i.e. ways in which one can understand the parameters in the boundary conditions. We will approach the problem by *approximating a quantum graph* by a family of systems with well defined properties
- *Lecture V*
  The assumption that a quantum particle is strictly confined to a graph is an idealization. Tomorrow we will discuss the concept of *a leaky graph* a show some properties of such systems

A recollection

Our basic model describes a *non-relativistic quantum confined to a graph*

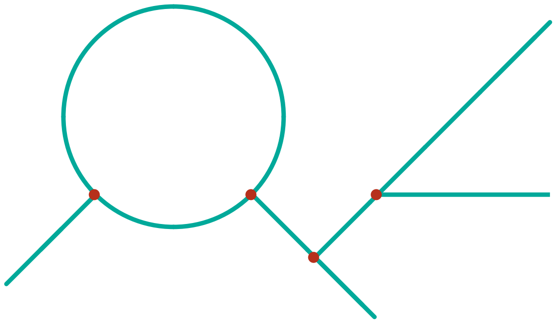


Hamiltonian: $-\frac{\partial^2}{\partial x_j^2} + v(x_j)$
on graph edges,
boundary conditions at vertices

which represents locally a one-dimensional Sturm-Liouville problem. It is the *boundary conditions* through which the graph topology – and its spectral consequences mentioned in the previous lectures – come into play

A recollection

Our basic model describes a *non-relativistic quantum confined to a graph*

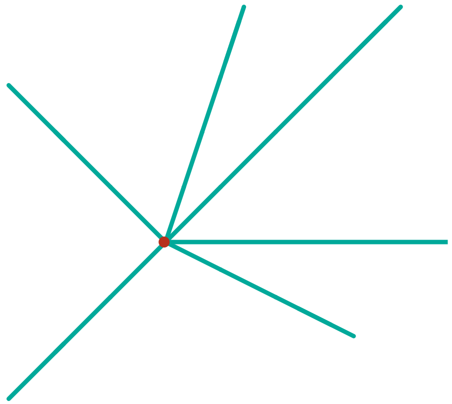


Hamiltonian: $-\frac{\partial^2}{\partial x_j^2} + v(x_j)$
on graph edges,
boundary conditions at vertices

which represents locally a one-dimensional Sturm-Liouville problem. It is the *boundary conditions* through which the graph topology – and its spectral consequences mentioned in the previous lectures – come into play

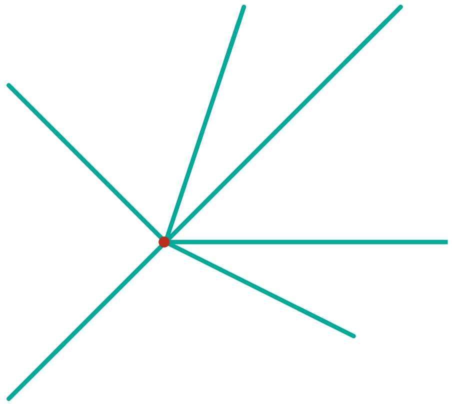
The same is true for other graph models, e.g. *Dirac operators* on graphs, *generalized graphs* whose "edges" are manifold of different dimensions, etc. We will not discuss them in this lecture

Wavefunction coupling at vertices



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

Wavefunction coupling at vertices



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

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

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

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

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

Unique boundary conditions

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

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

$$A = U - I\,, \quad B = i(U + I)$$

Unique boundary conditions

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

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

$$A = U - I\,, \quad B = i(U + I)$$

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

Self-adjointness requires vanishing of the boundary form,

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

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

Examples of vertex coupling

- Let $\mathcal{J}$ be the $n \times n$ matrix with all entries *one*; then $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ corresponds to the standard δ *coupling*,

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

with "coupling strength" $\alpha \in \mathbb{R}$; $\alpha = \infty$ gives $U = -I$.

The *only case* with vertex continuity [E-Šeba'89]

Examples of vertex coupling

- Let $\mathcal{J}$ be the $n \times n$ matrix with all entries *one*; then $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ corresponds to the standard δ *coupling*,

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

  with "coupling strength" $\alpha \in \mathbb{R}$; $\alpha = \infty$ gives $U = -I$.
  The *only case* with vertex continuity [E-Šeba'89]

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

Examples of vertex coupling

- Let $\mathcal{J}$ be the $n \times n$ matrix with all entries *one*; then $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ corresponds to the standard δ *coupling*,

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

  with “coupling strength” $\alpha \in \mathbb{R}$; $\alpha = \infty$ gives $U = -I$.
  The *only case* with vertex continuity [E-Šeba’89]

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

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

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

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

Further examples

- Another generalization of 1D δ' 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 $\beta \in \mathbb{R}$ and $U = \frac{n - i\alpha}{n + i\alpha} I - \frac{2}{n + i\alpha} \mathcal{J}$; the infinite value of β refers again to Neumann decoupling of the edges

Further examples

- Another generalization of 1D δ' 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 $\beta \in \mathbb{R}$ and $U = \frac{n-i\alpha}{n+i\alpha} I - \frac{2}{n+i\alpha}\mathcal{J}$; the infinite value of β refers again to Neumann decoupling of the edges

- Due to *permutation symmetry* the U's are combinations of I and $\mathcal{J}$ in the examples. In general, interactions with this property form a *two-parameter family* described by $U = uI + v\mathcal{J}$ s.t. $|u| = 1$ and $|u + nv| = 1$ giving the b.c.

$$\begin{aligned} (u-1)(\psi_j(0) - \psi_k(0)) + i(u-1)(\psi_j'(0) - \psi_k'(0)) &= 0 \\ (u-1+nv)\sum_{k=1}^{n} \psi_k(0) + i(u-1+nv)\sum_{k=1}^{n} \psi_k'(0) &= 0 \end{aligned}$$

Why are vertices interesting?

Apart of the general mathematical motivation mentioned above, there are various specific reasons, e.g.

- A nontrivial vertex coupling can lead to *number theoretic properties* of graph spectrum; I will show a simple example below

Why are vertices interesting?

Apart of the general mathematical motivation mentioned above, there are various specific reasons, e.g.

- A nontrivial vertex coupling can lead to *number theoretic properties* of graph spectrum; I will show a simple example below
- On the practical side, the conductivity of graph nanostructures is controlled typically by external fields, vertex coupling can serve the same purpose

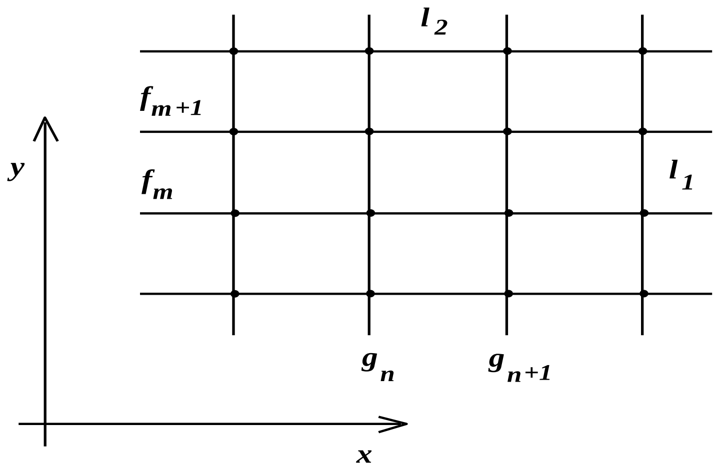
Why are vertices interesting?

Apart of the general mathematical motivation mentioned above, there are various specific reasons, e.g.

- A nontrivial vertex coupling can lead to *number theoretic properties* of graph spectrum; I will show a simple example below
- On the practical side, the conductivity of graph nanostructures is controlled typically by external fields, vertex coupling can serve the same purpose
- In particular, the generalized point interaction has been proposed as a way to realize a *qubit* [Cheon-Tsutsui-Fülöp'04]; vertices with $n > 2$ can similarly model *qudits*

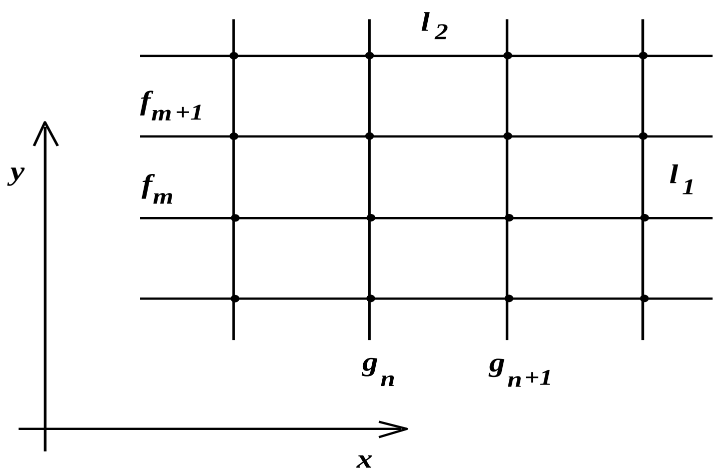
An example: a rectangular lattice graph

Basic cell is a rectangle of sides ℓ_1, ℓ_2, the δ coupling with parameter α is assumed at every vertex



An example: a rectangular lattice graph

Basic cell is a rectangle of sides ℓ_1, ℓ_2, the δ coupling with parameter α is assumed at every vertex



Spectral condition for quasimomentum (θ_1, θ_2) reads

$$\sum_{j=1}^{2} \frac{\cos\theta_j \ell_j - \cos k\ell_j}{\sin k\ell_j} = \frac{\alpha}{2k}$$

Lattice band spectrum

Recall a continued-fraction classification, $\alpha = [a_0, a_1, \dots]$:

- *“good” irrationals* have $\limsup_j a_j = \infty$ (and full Lebesgue measure)
- *“bad” irrationals* have $\limsup_j a_j < \infty$ (and $\lim_j a_j \neq 0$, of course)

Lattice band spectrum

Recall a continued-fraction classification, $\alpha = [a_0, a_1, \dots]$:

- *"good" irrationals* have $\limsup_j a_j = \infty$ (and full Lebesgue measure)
- *"bad" irrationals* have $\limsup_j a_j < \infty$ (and $\lim_j a_j \neq 0$, of course)

Theorem [E'95]: Call $\theta := \ell_2/\ell_1$ and $L := \max\{\ell_1, \ell_2\}$.

(a) If θ is rational or "good" irrational, there are infinitely many gaps for any nonzero α

(b) For a "bad" irrational θ there is $\alpha_0 > 0$ such no gaps open above threshold for $|\alpha| < \alpha_0$

(c) There are infinitely many gaps if $|\alpha|L > \frac{\pi^2}{\sqrt{5}}$

Lattice band spectrum

Recall a continued-fraction classification, $\alpha = [a_0, a_1, \dots]$:

- *"good" irrationals* have $\limsup_j a_j = \infty$ (and full Lebesgue measure)
- *"bad" irrationals* have $\limsup_j a_j < \infty$ (and $\lim_j a_j \neq 0$, of course)

Theorem [E'95]: Call $\theta := \ell_2/\ell_1$ and $L := \max\{\ell_1, \ell_2\}$.

(a) If θ is rational or "good" irrational, there are infinitely many gaps for any nonzero α

(b) For a "bad" irrational θ there is $\alpha_0 > 0$ such no gaps open above threshold for $|\alpha| < \alpha_0$

(c) There are infinitely many gaps if $|\alpha| L > \frac{\pi^2}{\sqrt{5}}$

This illustrates why it is desirable to *understand vertex couplings*. This will be our main task in this lecture

Some references

[CFT'04] T. Cheon, T. Fülöp, I. Tsutsui: Quantum abacus, *Phys. Lett.* **A330** (2004), 338-342

[E'95] P.E.: Lattice Kronig–Penney models, *Phys. Rev. Lett.* **75** (1995), 3503-3506

[EŠ'89] P. Exner, P. Šeba: Free quantum motion on a branching graph, *Rep. Math. Phys.* **28** (1989), 7-26

[FT'00] T. Fülöp, I. Tsutsui: A free particle on a circle with point interaction, *Phys. Lett.* **A264** (2000), 366–374

[Ha'00] M. Harmer: Hermitian symplectic geometry and extension theory, *J. Phys. A: Math. Gen.* **33** (2000), 9193-9203

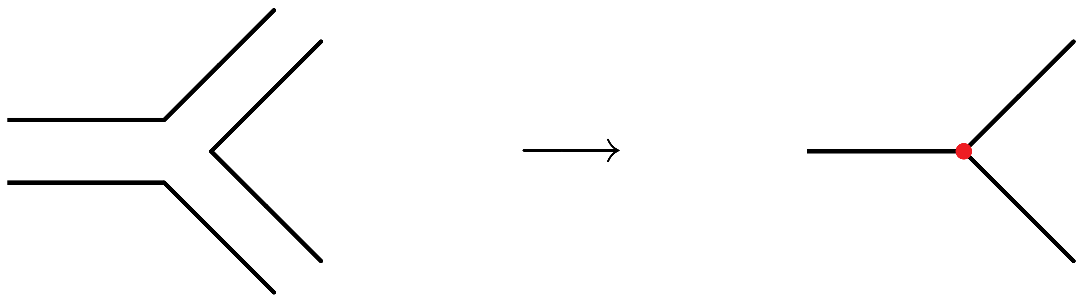
[KS'99] V. Kostrykin, R. Schrader: Kirchhoff's rule for quantum wires, *J. Phys. A: Math. Gen.* **32** (1999), 595-630

[KS'00] V. Kostrykin, R. Schrader: Kirchhoff's rule for quantum wires. II: The inverse problem with possible applications to quantum computers, *Fortschr. Phys.* **48** (2000), 703-716

[Ku'04] P. Kuchment: Quantum graphs: I. Some basic structures, *Waves in Random Media* **14** (2004), S107-S128

A head-on approach

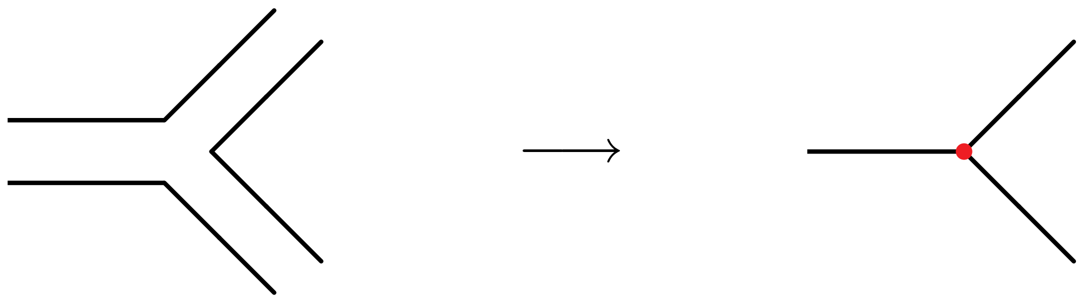
Take a more realistic situation with no ambiguity, such as *branching tubes* and analyze the *squeezing limit*:



Unfortunately, it is not so simple as it looks because

A head-on approach

Take a more realistic situation with no ambiguity, such as *branching tubes* and analyze the *squeezing limit*:



Unfortunately, it is not so simple as it looks because

- after a long effort the *Neumann-like case* was solved [Freidlin-Wentzell'93], [Freidlin'96], [Saito'01], [Kuchment-Zeng'01], [Rubinstein-Schatzmann'01], [E.-Post'05], [Post'06] giving free b.c. only
- there is a recent progress in *Dirichlet case* [Post'05], [Molchanov-Vainberg'06], [Grieser'07]?, but the full understanding has not yet been achieved here

More on the Dirichlet case

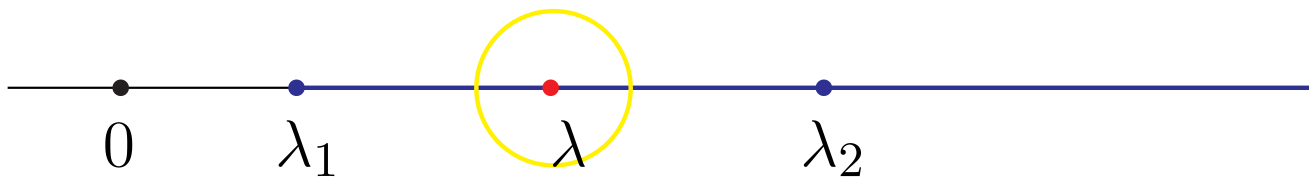
- *Generically* it is expected that that the limit *with the energy around the threshold* gives *Dirichlet decoupling*, but there may be *exceptional cases*

More on the Dirichlet case

- *Generically* it is expected that that the limit *with the energy around the threshold* gives *Dirichlet decoupling*, but there may be *exceptional cases*
- if the vertex regions *squeeze faster* than the “tubes” one gets *Dirichlet decoupling* [Post’05]

More on the Dirichlet case

- *Generically* it is expected that that the limit *with the energy around the threshold* gives *Dirichlet decoupling*, but there may be *exceptional cases*
- if the vertex regions *squeeze faster* than the “tubes” one gets *Dirichlet decoupling* [Post’05]
- on the other hand, if you blow up the spectrum for a fixed point *separated from thresholds*, i.e.



one gets a nontrivial limit with b.c. fixed by scattering on the “fat star” [Molchanov-Vainberg’06]

The Neumann-like case

The simplest situation in [KZ'01, EP'05] (weights left out)

Let M_0 be a finite connected graph with vertices v_k, $k \in K$ and edges $e_j \simeq I_j := [0, \ell_j]$, $j \in J$; the state Hilbert space is

$$L^2(M_0) := \bigoplus_{j \in J} L^2(I_j)$$

and in a similar way Sobolev spaces on M_0 are introduced

The Neumann-like case

The simplest situation in [KZ'01, EP'05] (weights left out)

Let M_0 be a finite connected graph with vertices v_k, $k \in K$ and edges $e_j \simeq I_j := [0, \ell_j]$, $j \in J$; the state Hilbert space is

$$L^2(M_0) := \bigoplus_{j \in J} L^2(I_j)$$

and in a similar way Sobolev spaces on M_0 are introduced

The form $u \mapsto \|u'\|^2_{M_0} := \sum_{j \in J} \|u'\|^2_{I_j}$ with $u \in \mathcal{H}^1(M_0)$ is associated with the operator which acts as $-\Delta_{M_0} u = -u''_j$ and satisfies free b.c.,

$$\sum_{j,\, e_j \text{ meets } v_k} u'_j(v_k) = 0$$

On the other hand, Laplacian on manifold

Consider a Riemannian manifold X of dimension $d \geq 2$ and the corresponding space $L^2(X)$ w.r.t. volume $\mathrm{d}X$ equal to $(\det g)^{1/2}\mathrm{d}x$ in a fixed chart. For $u \in C^\infty_{\mathrm{comp}}(X)$ we set

$$q_X(u) := \|\mathrm{d}u\|_X^2 = \int_X |\mathrm{d}u|^2 \mathrm{d}X\,, \;\; |\mathrm{d}u|^2 = \sum_{i,j} g^{ij} \partial_i u\, \partial_j \overline{u}$$

The closure of this form is associated with the s-a operator $-\Delta_X$ which acts in fixed chart coordinates as

$$-\Delta_X u = -(\det g)^{-1/2} \sum_{i,j} \partial_i((\det g)^{1/2} g^{ij}\, \partial_j u)$$

On the other hand, Laplacian on manifold

Consider a Riemannian manifold X of dimension $d \geq 2$ and the corresponding space $L^2(X)$ w.r.t. volume $\mathrm{d}X$ equal to $(\det g)^{1/2}\mathrm{d}x$ in a fixed chart. For $u \in C^\infty_{\mathrm{comp}}(X)$ we set

$$q_X(u) := \|\mathrm{d}u\|^2_X = \int_X |\mathrm{d}u|^2 \mathrm{d}X\,, \; |\mathrm{d}u|^2 = \sum_{i,j} g^{ij} \partial_i u\, \partial_j \overline{u}$$

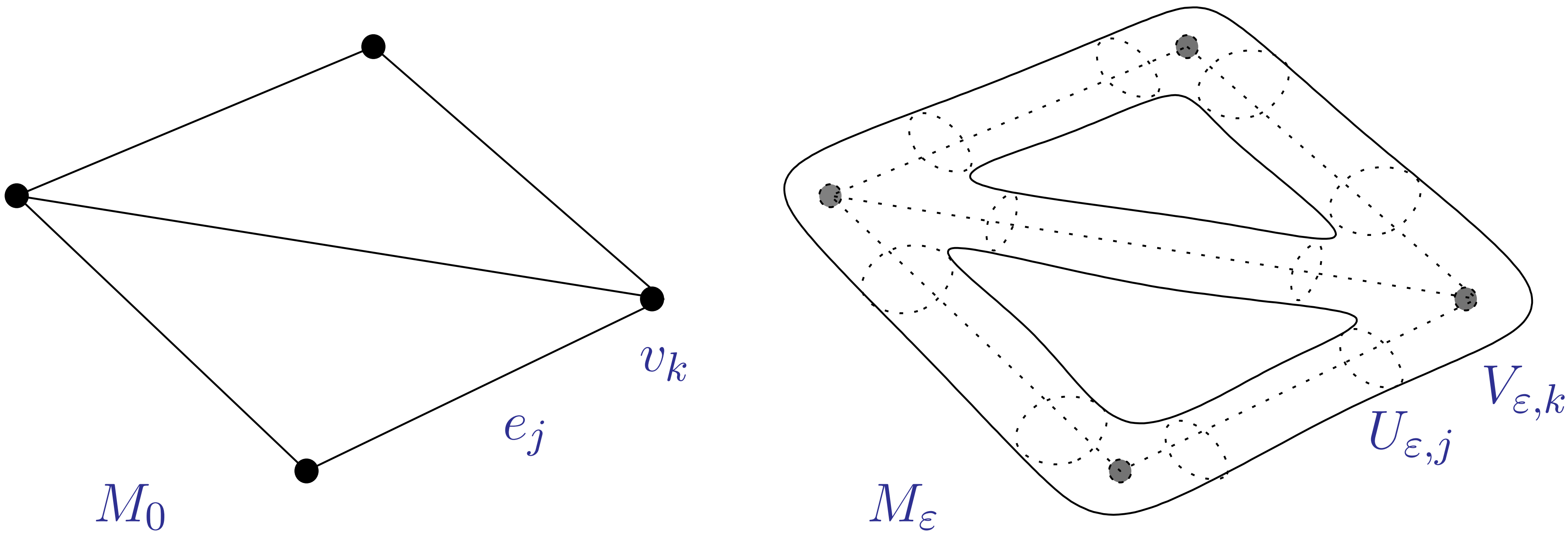
The closure of this form is associated with the s-a operator $-\Delta_X$ which acts in fixed chart coordinates as

$$-\Delta_X u = -(\det g)^{-1/2} \sum_{i,j} \partial_i((\det g)^{1/2} g^{ij}\, \partial_j u)$$

If X is compact with piecewise smooth boundary, one starts from the form defined on $C^\infty(X)$. This yields $-\Delta_X$ as the *Neumann* Laplacian on X and allows us in this way to treat "fat graphs" and "sleeves" on the same footing

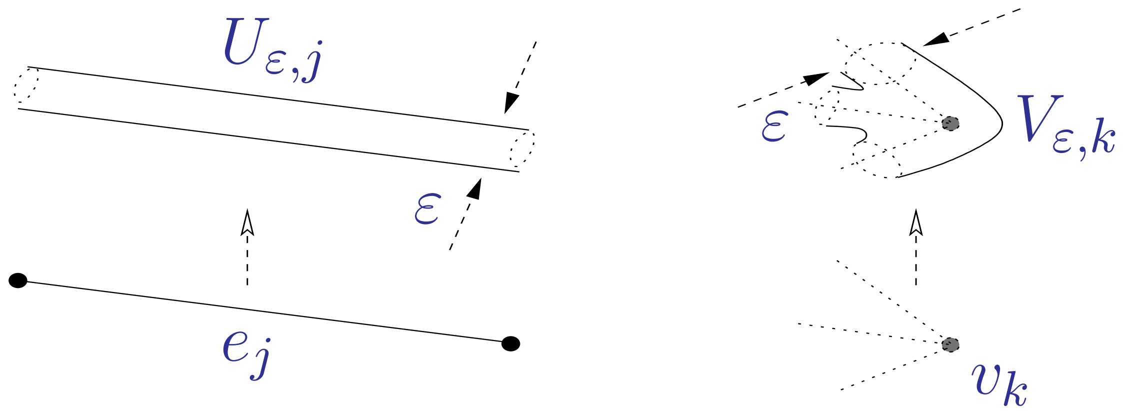
Fat graphs and sleeves: manifolds

We associate with the graph M_0 a family of manifolds M_ε

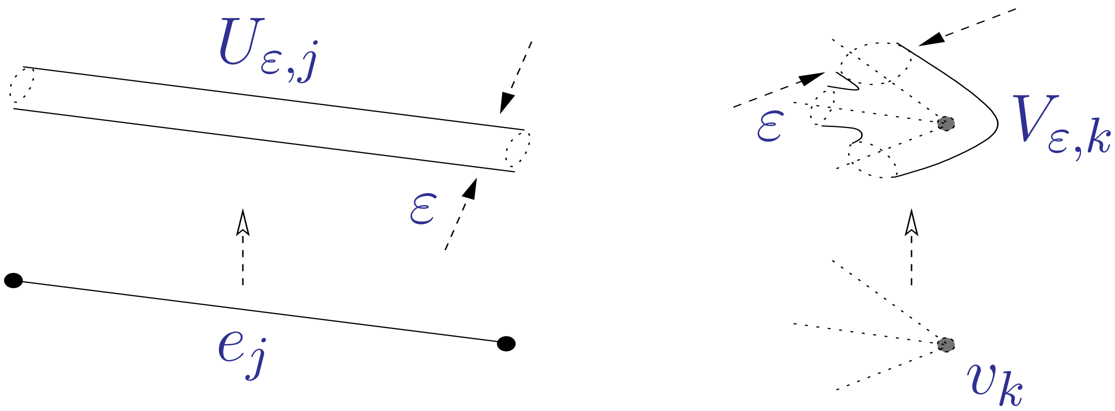


We suppose that M_ε is a union of compact edge and vertex components $U_{\varepsilon,j}$ and $V_{\varepsilon,k}$ such that their interiors are mutually disjoint for all possible $j \in J$ and $k \in K$

Manifold building blocks



Manifold building blocks



However, M_ε *need not be embedded* in some $\mathbb{R}^d$.

It is convenient to assume that $U_{\varepsilon,j}$ and $V_{\varepsilon,k}$ depend on ε only through their metric:

- for edge regions we assume that $U_{\varepsilon,j}$ is diffeomorphic to $I_j \times F$ where F is a compact and connected manifold (with or without a boundary) of dimension $m := d-1$
- for vertex regions we assume that the manifold $V_{\varepsilon,k}$ is diffeomorphic to an ε-independent manifold V_k

Eigenvalue convergence

Let thus $U = I_j \times F$ with metric g_ε, where cross section F is a compact connected Riemannian manifold of dimension $m = d - 1$ with metric h; we assume that $\operatorname{vol} F = 1$. We define another metric $\tilde{g}_\varepsilon$ on $U_{\varepsilon,j}$ by

$$\tilde{g}_\varepsilon := \mathrm{d}x^2 + \varepsilon^2 h(y)\,;$$

the two metrics coincide up to an $\mathcal{O}(\varepsilon)$ error

This property allows us to treat manifolds embedded in $\mathbb{R}^d$ (with metric $\tilde{g}_\varepsilon$) using product metric g_ε on the edges

Eigenvalue convergence

Let thus $U = I_j \times F$ with metric g_ε, where cross section F is a compact connected Riemannian manifold of dimension $m = d - 1$ with metric h; we assume that $\operatorname{vol} F = 1$. We define another metric $\tilde{g}_\varepsilon$ on $U_{\varepsilon,j}$ by

$$\tilde{g}_\varepsilon := \mathrm{d}x^2 + \varepsilon^2 h(y)\,;$$

the two metrics coincide up to an $\mathcal{O}(\varepsilon)$ error

This property allows us to treat manifolds embedded in $\mathbb{R}^d$ (with metric $\tilde{g}_\varepsilon$) using product metric g_ε on the edges

The sought result now looks as follows.

Theorem [KZ'01, EP'05]: Under the stated assumptions $\lambda_k(M_\varepsilon) \to \lambda_k(M_0)$ as $\varepsilon \to 0$ (giving thus free b.c.!)

The main tool

Our main tool here will be minimax principle. Suppose that $\mathcal{H}$, $\mathcal{H}'$ are separable Hilbert spaces. We want to compare ev's λ_k and λ'_k of nonnegative operators Q and Q' with purely discrete spectra defined via quadratic forms q and q' on $\mathcal{D} \subset \mathcal{H}$ and $\mathcal{D}' \subset \mathcal{H}'$. Set $\|u\|^2_{Q,n} := \|u\|^2 + \|Q^{n/2}u\|^2$.

The main tool

Our main tool here will be minimax principle. Suppose that $\mathcal{H}$, $\mathcal{H}'$ are separable Hilbert spaces. We want to compare ev's λ_k and λ'_k of nonnegative operators Q and Q' with purely discrete spectra defined via quadratic forms q and q' on $\mathcal{D} \subset \mathcal{H}$ and $\mathcal{D}' \subset \mathcal{H}'$. Set $\|u\|^2_{Q,n} := \|u\|^2 + \|Q^{n/2}u\|^2$.

Lemma: Suppose that $\Phi:\ \mathcal{D} \to \mathcal{D}'$ is a linear map such that there are $n_1, n_2 \geq 0$ and $\delta_1, \delta_2 \geq 0$ such that

$$\|u\|^2 \leq \|\Phi u\|'^2 + \delta_1 \|u\|^2_{Q,n_1}\,, \quad q(u) \geq q'(\Phi u) - \delta_2 \|u\|^2_{Q,n_2}$$

for all $u \in \mathcal{D} \subset \mathcal{D}(Q^{\max\{n_1,n_2\}/2})$. Then to each k there is an $\eta_k(\lambda_k, \delta_1, \delta_2) > 0$ which tends to zero as $\delta_1, \delta_2 \to 0$, such that

$$\lambda_k \geq \lambda'_k - \eta_k$$

Idea of the proof

Proposition: $\lambda_k(M_\varepsilon) \leq \lambda_k(M_0) + o(1)$ as $\varepsilon \to 0$

To prove it apply the lemma to $\Phi_\varepsilon : L^2(M_0) \to L^2(M_\varepsilon)$,

$$\Phi_\varepsilon u(z) := \begin{cases} \varepsilon^{-m/2} u(v_k) & \text{if } z \in V_k \\ \varepsilon^{-m/2} u_j(x) & \text{if } z = (x,y) \in U_j \end{cases} \quad \text{for } u \in \mathcal{H}^1(M_0)$$

Idea of the proof

Proposition: $\lambda_k(M_\varepsilon) \le \lambda_k(M_0) + o(1)$ as $\varepsilon \to 0$

To prove it apply the lemma to $\Phi_\varepsilon : L^2(M_0) \to L^2(M_\varepsilon)$,

$$\Phi_\varepsilon u(z) := \begin{cases} \varepsilon^{-m/2} u(v_k) & \text{if } z \in V_k \\ \varepsilon^{-m/2} u_j(x) & \text{if } z = (x,y) \in U_j \end{cases} \quad \text{for } u \in \mathcal{H}^1(M_0)$$

Proposition: $\lambda_k(M_0) \le \lambda_k(M_\varepsilon) + o(1)$ as $\varepsilon \to 0$

Proof again by the lemma. Here one uses *averaging*:

$$N_j u(x) := \int_F u(x,\cdot)\, \mathrm{d}F\,, \quad C_k u := \frac{1}{\mathrm{vol}\, V_k} \int_{V_k} u\, \mathrm{d}V_k$$

to build the comparison map by *interpolation*:

$$(\Psi_\varepsilon)_j(x) := \varepsilon^{m/2}\big(N_j u(x) + \rho(x)(C_k u - N_j u(x))\big)$$

with a smooth ρ interpolating between zero and one

More general b.c.? Recall RS argument

[Ruedenberg-Scher'53] used the heuristic argument:

$$\lambda \int_{V_\varepsilon} \phi\, \overline{u}\, \mathrm{d}V_\varepsilon = \int_{V_\varepsilon} \langle \mathrm{d}\phi, \mathrm{d}u \rangle\, \mathrm{d}V_\varepsilon + \int_{\partial V_\varepsilon} \partial_\mathrm{n}\phi\, \overline{u}\, \mathrm{d}\partial V_\varepsilon$$

The surface term dominates in the limit $\varepsilon \to 0$ giving formally free boundary conditions

More general b.c.? Recall RS argument

[Ruedenberg-Scher'53] used the heuristic argument:

$$\lambda \int_{V_\varepsilon} \phi \, \overline{u} \, \mathrm{d}V_\varepsilon = \int_{V_\varepsilon} \langle \mathrm{d}\phi, \mathrm{d}u \rangle \, \mathrm{d}V_\varepsilon + \int_{\partial V_\varepsilon} \partial_\mathrm{n}\phi \, \overline{u} \, \mathrm{d}\partial V_\varepsilon$$

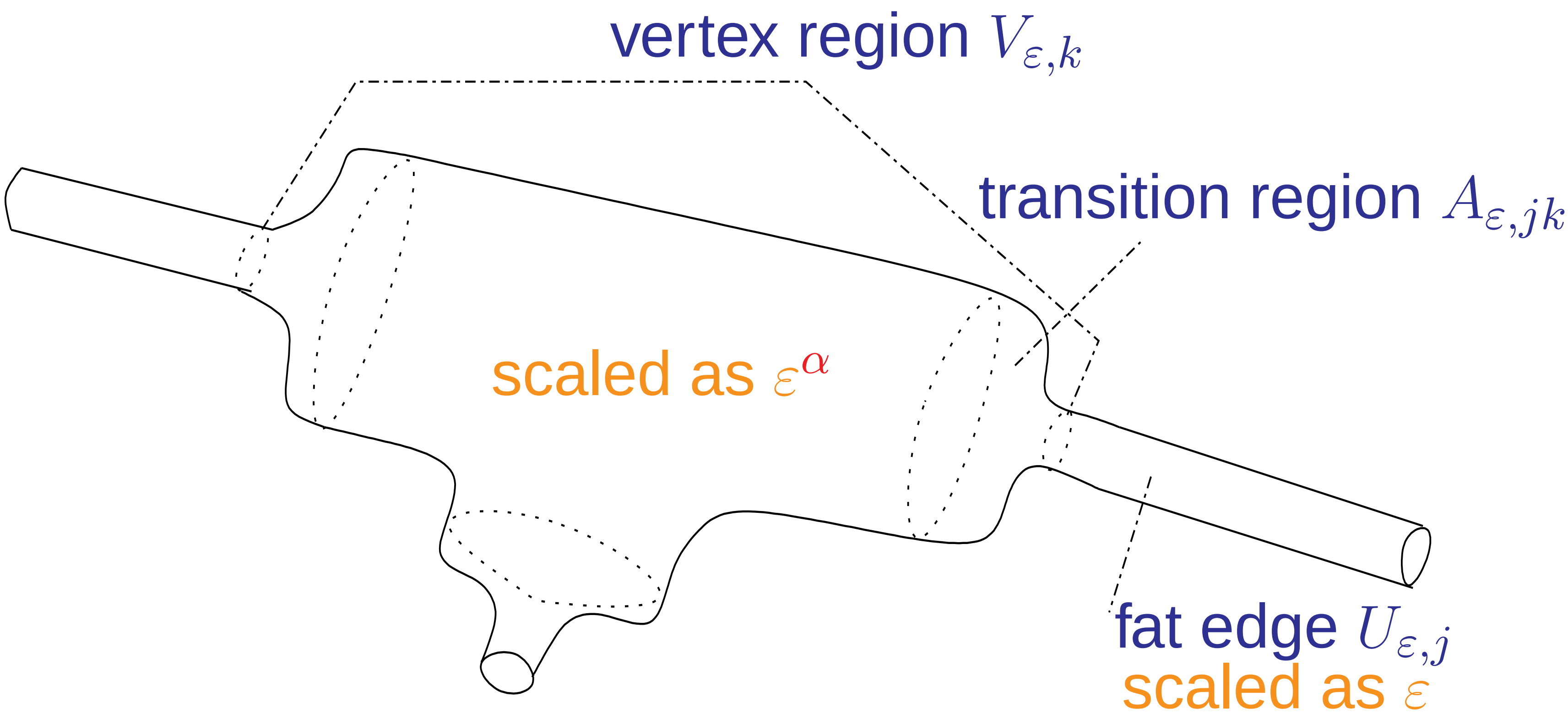
The surface term dominates in the limit $\varepsilon \to 0$ giving formally free boundary conditions

A way out could thus be to use *different* scaling rates of edges and vertices. Of a particular interest is the borderline case, $\mathrm{vol}_d V_\varepsilon \approx \mathrm{vol}_{d-1} \partial V_\varepsilon$, when the integral of $\langle \mathrm{d}\phi, \mathrm{d}u \rangle$ is expected to be negligible and we hope to obtain

$$\lambda_0 \phi_0(v_k) = \sum_{j \in J_k} \phi'_{0,j}(v_k)$$

Scaling with a power α

Let us try to do the same properly using *different scaling* of the *edge* and *vertex* regions. Some technical assumptions needed, e.g., the bottlenecks must be "simple"



Two-speed scaling limit

Let vertices scale as ε^{α}. Using the comparison lemma again (just more in a more complicated way) we find that

- if $\alpha \in (1-d^{-1}, 1]$ the result is as above: the ev's at the spectrum bottom converge the graph Laplacian with *free b.c.*, i.e. continuity and

$$\sum_{\text{edges meeting at } v_k} u_j'(v_k) = 0\,;$$

Two-speed scaling limit

Let vertices scale as ε^{α}. Using the comparison lemma again (just more in a more complicated way) we find that

- if $\alpha \in (1-d^{-1}, 1]$ the result is as above: the ev's at the spectrum bottom converge the graph Laplacian with *free b.c.*, i.e. continuity and

$$\sum_{\text{edges meeting at } v_k} u_j'(v_k) = 0\,;$$

- if $\alpha \in (0, 1-d^{-1})$ the "limiting" Hilbert space is $L^2(M_0) \oplus \mathbb{C}^K$, where K is $\#$ of vertices, and the "limiting" operator acts as *Dirichlet Laplacian* at each edge and as zero on $\mathbb{C}^K$

Two-speed scaling limit

- if $\alpha = 1 - d^{-1}$, Hilbert space is the same but the limiting operator is given by quadratic form $q_0(u) := \sum_j \|u_j'\|^2_{I_j}$, the domain of which consists of $u = \{\{u_j\}_{j\in J}, \{u_k\}_{k\in K}\}$ such that $u \in H^1(M_0) \oplus \mathbb{C}^K$ and the *edge and vertex parts are coupled* by $(\mathrm{vol}\,(V_k^-)^{1/2} u_j(v_k) = u_k$

Two-speed scaling limit

- if $\alpha = 1 - d^{-1}$, Hilbert space is the same but the limiting operator is given by quadratic form $q_0(u) := \sum_j \|u_j'\|^2_{I_j}$, the domain of which consists of $u = \{\{u_j\}_{j\in J}, \{u_k\}_{k\in K}\}$ such that $u \in H^1(M_0) \oplus \mathbb{C}^K$ and the *edge and vertex parts are coupled* by $(\mathrm{vol}\,(V_k^-)^{1/2} u_j(v_k) = u_k$
- finally, if vertex regions do not scale at all, $\alpha = 0$, the manifold components decouple in the limit again,

$$\bigoplus_{j\in J} \Delta^{\mathrm{D}}_{I_j} \oplus \bigoplus_{k\in K} \Delta_{V_{0,k}}$$

Two-speed scaling limit

- if $\alpha = 1 - d^{-1}$, Hilbert space is the same but the limiting operator is given by quadratic form $q_0(u) := \sum_j \|u_j'\|^2_{I_j}$, the domain of which consists of $u = \{\{u_j\}_{j\in J}, \{u_k\}_{k\in K}\}$ such that $u \in H^1(M_0) \oplus \mathbb{C}^K$ and the *edge and vertex parts are coupled* by $(\mathrm{vol}\,(V_k^-))^{1/2} u_j(v_k) = u_k$
- finally, if vertex regions do not scale at all, $\alpha = 0$, the manifold components decouple in the limit again,

$$\bigoplus_{j\in J} \Delta^{\mathrm{D}}_{I_j} \oplus \bigoplus_{k\in K} \Delta_{V_{0,k}}$$

- Hence such a straightforward limiting procedure *does not help* us to justify choice of appropriate s-a extension

Hence the scaling trick does not work: one has to add either *manifold geometry* or *external potentials*

Some newer references

[EP'05] P.E., O. Post: Convergence of spectra of graph-like thin manifolds, *J. Geom. Phys.* **54** (2005), 77-115

[KZ'01] P. Kuchment, H. Zeng: Convergence of spectra of mesoscopic systems collapsing onto a graph, *J. Math. Anal. Appl.* **258** (2001), 671–700

[MV'06] S. Molchanov, B. Vainberg: Scattering solutions in a network of thin fibers: small diameter asymptotics, `math-ph/0609021`

[P'05] O. Post: Branched quantum wave guides with Dirichlet boundary conditions: the decoupling case, *J. Phys. A: Math. Gen.* **38** (2005), 4917-4931

[P'06] O. Post: Spectral convergence of non-compact quasi-one-dimensional spaces, `math-ph/0512081`

[RS'01] J. Rubinstein, M. Schatzmann: Variational problems on multiply connected thin strips, I. Basic estimates and convergence of the Laplacian spectrum, *Arch. Rat. Mech. Anal.* **160** (2001), 271-308

[Sa'01] T. Saito: Convergence of the Neumann Laplacian on shrinking domains, *Analysis* **21** (2001), 171-204

And a few previous millennium ones

[F'96] M. Freidlin, *Markov Processes and Differential Equations: Asymptotic Problems*, Lectures in Mathematics ETH Zürich, Birkhäuser Verlag, Basel 1996

[FW'93] M. Freidlin, A. Wentzell: Diffusion processes on graphs and the averaging principle, *Ann. Prob.* **21** (1993), 2215-2245

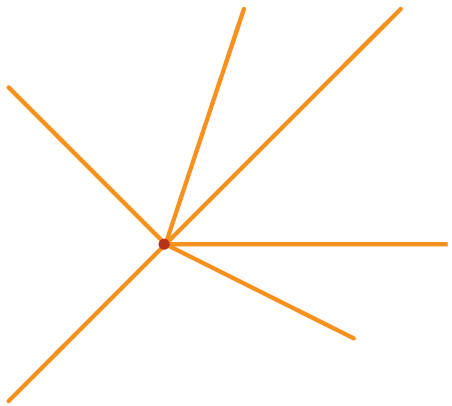
[RuS'53] K. Ruedenberg, C.W. Scherr: Free-electron network model for conjugated systems, I. Theory, *J. Chem. Phys.* **21** (1953), 1565-1581

Potential approximation

A more modest goal: let us look what we can achieve with potential families *on the graph alone*

Potential approximation

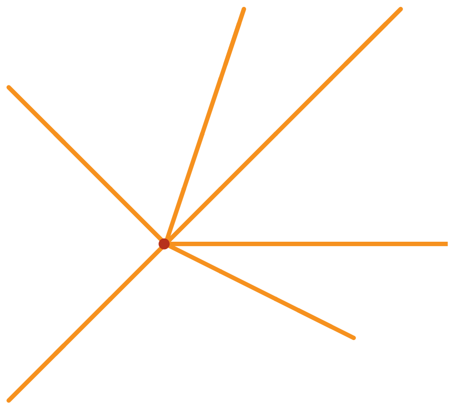
A more modest goal: let us look what we can achieve with potential families *on the graph alone*



Consider once more *star graph* with $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and Schrödinger operator acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j'' + V_j \psi_j$

Potential approximation

A more modest goal: let us look what we can achieve with potential families *on the graph alone*



Consider once more *star graph* with $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and Schrödinger operator acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j'' + V_j\psi_j$

We make the following assumptions:

- $V_j \in L^1_{\mathrm{loc}}(\mathbb{R}_+)\,,\; j = 1, \dots, n$
- δ coupling with a parameter α in the vertex

Then the operator, denoted as $H_\alpha(V)$, is self-adjoint

Potential approximation of δ coupling

Suppose that the potential has a shrinking component,

$$W_{\varepsilon,j} := \frac{1}{\varepsilon} W_j \left(\frac{x}{\varepsilon} \right) , \quad j = 1, \dots, n$$

Potential approximation of δ coupling

Suppose that the potential has a shrinking component,

$$W_{\varepsilon,j} := \frac{1}{\varepsilon} W_j\left(\frac{x}{\varepsilon}\right), \quad j = 1, \dots, n$$

Theorem [E'96]: Suppose that $V_j \in L^1_{\mathrm{loc}}(\mathbb{R}_+)$ are below bounded and $W_j \in L^1(\mathbb{R}_+)$ for $j = 1, \dots, n$. Then

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

as $\varepsilon \to 0+$ in the norm resolvent sense, with the parameter $\alpha := \sum_{j=1}^n \int_0^\infty W_j(x)\, dx$

Potential approximation of δ coupling

Suppose that the potential has a shrinking component,

$$W_{\varepsilon,j} := \frac{1}{\varepsilon} W_j\left(\frac{x}{\varepsilon}\right), \quad j = 1, \dots, n$$

Theorem [E'96]: Suppose that $V_j \in L^1_{\mathrm{loc}}(\mathbb{R}_+)$ are below bounded and $W_j \in L^1(\mathbb{R}_+)$ for $j = 1, \dots, n$. Then

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

as $\varepsilon \to 0+$ in the norm resolvent sense, with the parameter $\alpha := \sum_{j=1}^n \int_0^\infty W_j(x)\, dx$

Proof: Analogous to that for δ interaction on the line. $\square$

Remarks

- Also Birman-Schwinger analysis generalizes easily:

  Theorem [E'96]: Let $V_j \in L^1(\mathbb{R}_+, (1+|x|)\mathrm{d}x)$, $j = 1, \dots, n$. Then $H_0(\lambda V)$ has for all small enough $\lambda > 0$ a single negative ev $\epsilon(\lambda) = -\kappa(\lambda)^2$ *iff*

$$\sum_{j=1}^{n} \int_0^\infty V_j(x)\,\mathrm{d}x \le 0$$

  In that case, its asymptotic behavior is given by

$$\begin{aligned}\kappa(\lambda) \;&=\; -\frac{\lambda}{n}\sum_{j=1}^{n}\int_0^\infty V_j(x)\,\mathrm{d}x - \frac{\lambda^2}{2n}\Bigg\{\sum_{j=1}^{n}\int_0^\infty\!\!\int_0^\infty V_j(x)|x-y|V_j(y)\,\mathrm{d}x\,\mathrm{d}y \\ &+ \sum_{j,\ell=1}^{n}\left(\frac{2}{n}-\delta_{j\ell}\right)\int_0^\infty\!\!\int_0^\infty V_j(x)(x+y)V_\ell(y)\,\mathrm{d}x\,\mathrm{d}y\Bigg\} + \mathcal{O}(\lambda^3)\end{aligned}$$

Remarks

- Also Birman-Schwinger analysis generalizes easily:

  Theorem [E'96]: Let $V_j \in L^1(\mathbb{R}_+, (1+|x|)\mathrm{d}x)$, $j = 1, \dots, n$. Then $H_0(\lambda V)$ has for all small enough $\lambda > 0$ a single negative ev $\epsilon(\lambda) = -\kappa(\lambda)^2$ *iff*

$$\sum_{j=1}^{n} \int_0^\infty V_j(x)\,\mathrm{d}x \le 0$$

  In that case, its asymptotic behavior is given by

$$\begin{aligned}\kappa(\lambda) &= -\frac{\lambda}{n}\sum_{j=1}^{n}\int_0^\infty V_j(x)\,\mathrm{d}x - \frac{\lambda^2}{2n}\left\{\sum_{j=1}^{n}\int_0^\infty\int_0^\infty V_j(x)|x-y|V_j(y)\,\mathrm{d}x\,\mathrm{d}y\right. \\ &\quad + \left.\sum_{j,\ell=1}^{n}\left(\frac{2}{n}-\delta_{j\ell}\right)\int_0^\infty\int_0^\infty V_j(x)(x+y)V_\ell(y)\,\mathrm{d}x\,\mathrm{d}y\right\} + \mathcal{O}(\lambda^3)\end{aligned}$$

- A Seto-Klaus-Newton bound on $\#\sigma_{\mathrm{disc}}(H_0(\lambda V))$ can be obtained in a similar way

More singular couplings

The above scheme does not work for graph Hamiltonians with discontinuous wavefunctions such as δ'_s

More singular couplings

The above scheme does not work for graph Hamiltonians with discontinuous wavefunctions such as δ'_s

Inspiration: Recall that δ' on the line can be approximated by δ's scaled in a *nonlinear* way [Cheon-Shigehara'98]

Moreover, the convergence is *norm resolvent* and gives rise to approximations by *regular potentials* [Albeverio-Nizhnik'00], [E-Neidhardt-Zagrebnov'01]

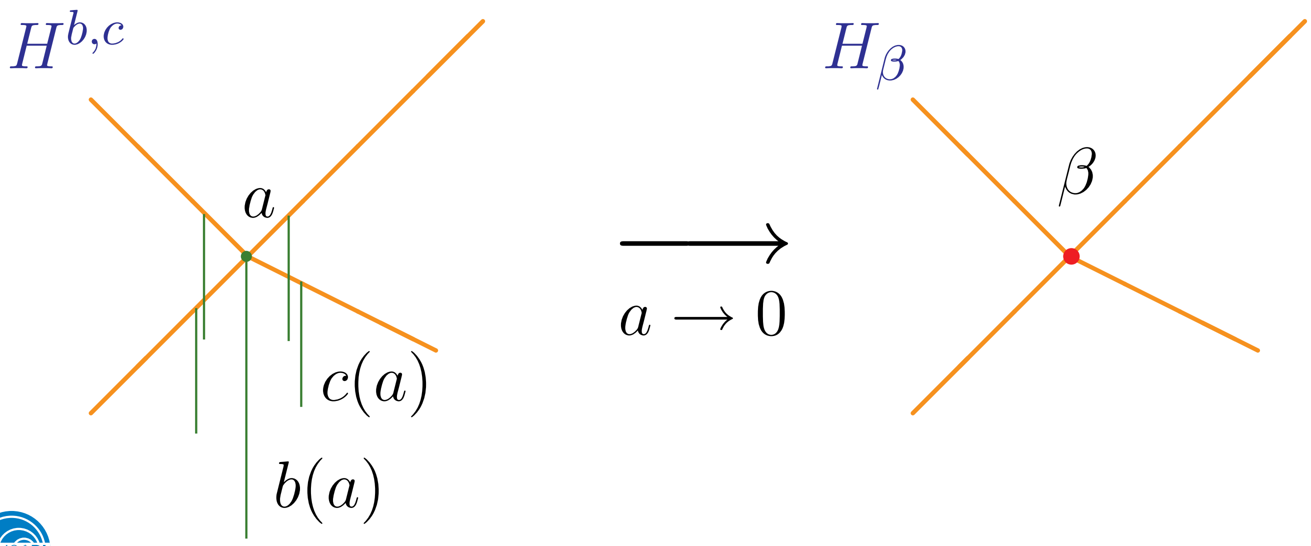
More singular couplings

The above scheme does not work for graph Hamiltonians with discontinuous wavefunctions such as δ'_s

Inspiration: Recall that δ' on the line can be approximated by δ's scaled in a *nonlinear* way [Cheon-Shigehara'98]

Moreover, the convergence is *norm resolvent* and gives rise to approximations by *regular potentials* [Albeverio-Nizhnik'00], [E-Neidhardt-Zagrebnov'01]

This suggests the following scheme:



δ'_s approximation

Theorem [Cheon-E'04]: $H^{b,c}(a) \to H_\beta$ as $a \to 0+$ in the norm-resolvent sense provided b, c are chosen as

$$b(a) := -\frac{\beta}{a^2}, \quad c(a) := -\frac{1}{a}$$

δ'_s approximation

Theorem [Cheon-E'04]: $H^{b,c}(a) \to H_\beta$ as $a \to 0+$ in the norm-resolvent sense provided b, c are chosen as

$$b(a) := -\frac{\beta}{a^2}\,, \quad c(a) := -\frac{1}{a}$$

Proof: Green's functions of both operators are found explicitly be Krein's formula, so the convergence can be established by straightforward computation

δ'_s approximation

Theorem [Cheon-E'04]: $H^{b,c}(a) \to H_\beta$ as $a \to 0+$ in the norm-resolvent sense provided b, c are chosen as

$$b(a) := -\frac{\beta}{a^2}\,, \quad c(a) := -\frac{1}{a}$$

Proof: Green's functions of both operators are found explicitly be Krein's formula, so the convergence can be established by straightforward computation

Remark: Similar approximation can be worked out also for the other couplings mentioned above – cf. [E-Turek'06]. For "most" permutation symmetric ones, e.g., one has

$$b(a) := \frac{in}{a^2}\left(\frac{u-1+nv}{u+1+nv} + \frac{u-1}{u+1}\right)^{-1}, \quad c(a) := -\frac{1}{a} - i\frac{u-1}{u+1}$$

Some references

[AN'00] S. Albeverio, L. Nizhnik: Approximation of general zero-range potentials, *Ukrainian Math. J.* **52** (2000), 582-589

[CS'98] T. Cheon, T. Shigehara: Realizing discontinuous wave functions with renormalized short-range potentials, *Phys. Lett.* **A243** (1998), 111-116

[CE'04] T. Cheon, P.E.: An approximation to δ' couplings on graphs, *J. Phys. A: Math. Gen.* **A37** (2004), L329-335

[E'96] P.E.: Weakly coupled states on branching graphs, *Lett. Math. Phys.* **38** (1996), 313-320

[ENZ'01] P.E., H. Neidhardt, V.A. Zagrebnov: Potential approximations to δ': an inverse Klauder phenomenon with norm-resolvent convergence, *CMP* **224** (2001), 593-612

[ET'06] P.E., O. Turek: Approximations of permutation-symmetric vertex couplings in quantum graphs, Proc. of the Conference "Quantum Graphs and Their Applications" (Snowbird 2005); AMS "Contemporary Math" Series, vol. 415, pp. 109-120

Summarizing Lecture IV

- *Vertex coupling:* to employ the full potential of the graph model, it is vital to understand the physical meaning of the corresponding boundary conditions

Summarizing Lecture IV

- *Vertex coupling:* to employ the full potential of the graph model, it is vital to understand the physical meaning of the corresponding boundary conditions
- *"Fat manifold" approximations:* using the simplest geometry only we get free b.c. in the Neumann-like case, the Dirichlet case investigations are in progress. A little is known about "more geometric" choices of approximating operators

Summarizing Lecture IV

- *Vertex coupling:* to employ the full potential of the graph model, it is vital to understand the physical meaning of the corresponding boundary conditions
- *"Fat manifold" approximations:* using the simplest geometry only we get free b.c. in the Neumann-like case, the Dirichlet case investigations are in progress. A little is known about "more geometric" choices of approximating operators
- *Potential approximation to δ:* well understood as an extension of one-dimensional Schrödinger theory

Summarizing Lecture IV

- *Vertex coupling:* to employ the full potential of the graph model, it is vital to understand the physical meaning of the corresponding boundary conditions
- *"Fat manifold" approximations:* using the simplest geometry only we get free b.c. in the Neumann-like case, the Dirichlet case investigations are in progress. A little is known about "more geometric" choices of approximating operators
- *Potential approximation to δ:* well understood as an extension of one-dimensional Schrödinger theory
- *Potential approximation to more singular coupling:* there are particular results showing the way, a deeper analysis needed

Lecture V

Leaky graphs – what they are, and can one say about their spectral and scattering properties

Lecture overview

- Why we might want *something better* than the ideal graph model of the previous lecture

Lecture overview

- Why we might want *something better* than the ideal graph model of the previous lecture
- A model of *“leaky” quantum wires and graphs*, with Hamiltonians of the type $H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)$

Lecture overview

- Why we might want *something better* than the ideal graph model of the previous lecture
- A model of *"leaky" quantum wires and graphs*, with Hamiltonians of the type $H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)$
- *Geometrically induced spectral properties* of leaky wires and graphs

Lecture overview

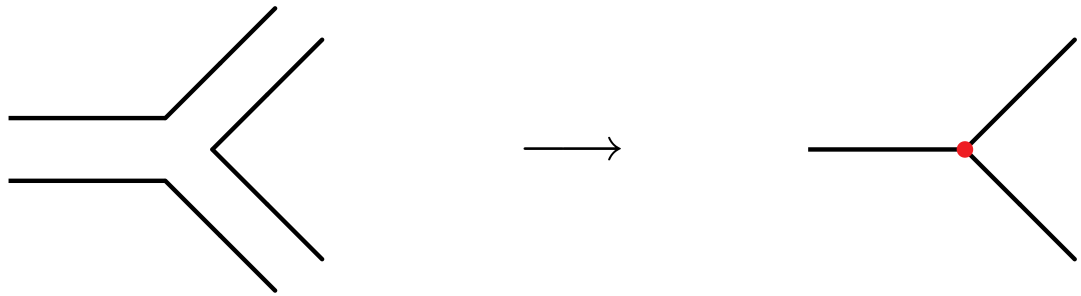
- Why we might want *something better* than the ideal graph model of the previous lecture
- A model of *“leaky” quantum wires and graphs*, with Hamiltonians of the type $H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x-\Gamma)$
- *Geometrically induced spectral properties* of leaky wires and graphs
- *Scattering on leaky wires:* existence and properties

Lecture overview

- Why we might want *something better* than the ideal graph model of the previous lecture
- A model of *“leaky” quantum wires and graphs*, with Hamiltonians of the type $H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)$
- *Geometrically induced spectral properties* of leaky wires and graphs
- *Scattering on leaky wires:* existence and properties
- *How to find spectrum numerically:* an approximation by point interaction Hamiltonians with application to resonances

Drawbacks of "ideal" graphs

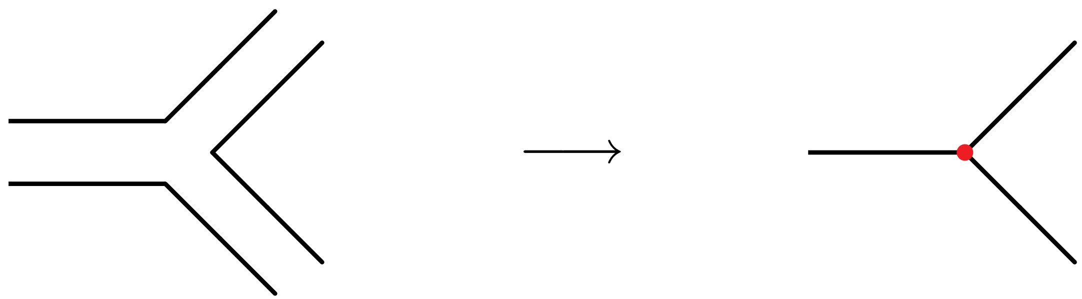
- Presence of *ad hoc parameters* in the b.c. describing branchings. A natural remedy: fit these using an approximation procedure, e.g.



As we have seen in *Lecture IV* it is possible but not quite easy and a lot of work remains to be done

Drawbacks of “ideal” graphs

- Presence of *ad hoc parameters* in the b.c. describing branchings. A natural remedy: fit these using an approximation procedure, e.g.



As we have seen in *Lecture IV* it is possible but not quite easy and a lot of work remains to be done

- More important, *quantum tunneling is neglected* in “ideal” graph models – recall that a true quantum-wire boundary is a *finite potential jump* – hence topology is taken into account but *geometric effects may not be*

Leaky quantum graphs

The last observation motivates us to consider *"leaky"* graphs, i.e. motion in *the whole space* with an *attractive interaction* supported by graph edges. Formally we have

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

in $L^2(\mathbb{R}^2)$, where Γ is the graph in question.

Leaky quantum graphs

The last observation motivates us to consider *"leaky"* graphs, i.e. motion in *the whole space* with an *attractive interaction* supported by graph edges. Formally we have

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

in $L^2(\mathbb{R}^2)$, where Γ is the graph in question.

A proper definition of $H_{\alpha,\Gamma}$: it can be associated naturally with the quadratic form,

$$\psi \mapsto \|\nabla\psi\|^2_{L^2(\mathbb{R}^n)} - \alpha \int_\Gamma |\psi(x)|^2 \mathrm{d}x\,,$$

which is closed and below bounded in $W^{2,1}(\mathbb{R}^n)$; the second term makes sense in view of Sobolev embedding. This definition also works for various "wilder" sets Γ

Leaky graph Hamiltonians

For Γ with locally finite number of smooth edges and *no cusps* we can use an *alternative definition* by boundary conditions: $H_{\alpha,\Gamma}$ acts as $-\Delta$ on functions from $W^{2,1}_{\mathrm{loc}}(\mathbb{R}^2 \setminus \Gamma)$, which are continuous and exhibit a normal-derivative jump,

$$\frac{\partial\psi}{\partial n}(x)\Big|_{+} - \frac{\partial\psi}{\partial n}(x)\Big|_{-} = -\alpha\psi(x)$$

Leaky graph Hamiltonians

For Γ with locally finite number of smooth edges and *no cusps* we can use an *alternative definition* by boundary conditions: $H_{\alpha,\Gamma}$ acts as $-\Delta$ on functions from $W^{2,1}_{\mathrm{loc}}(\mathbb{R}^2 \setminus \Gamma)$, which are continuous and exhibit a normal-derivative jump,

$$\frac{\partial\psi}{\partial n}(x)\Big|_+ - \frac{\partial\psi}{\partial n}(x)\Big|_- = -\alpha\psi(x)$$

Remarks:

- *for graphs in* $\mathbb{R}^3$ we use generalized b.c. which define a two-dimensional point interaction in normal plane
- one can combine *"edges" of different dimensions* as long as $\operatorname{codim}\Gamma$ does not exceed three

A remark on photonic crystals

On the physical side, description of semiconductor wires is not the only situation when one can meet similar objects

An example is given by *photonic crystals*, i.e. devices in which light travels space structured by changes of the refraction index – typically formed by a glass with a variety of holes filled by the air

A remark on photonic crystals

On the physical side, description of semiconductor wires is not the only situation when one can meet similar objects

An example is given by *photonic crystals*, i.e. devices in which light travels space structured by changes of the refraction index – typically formed by a glass with a variety of holes filled by the air

The dynamics is now naturally governed by the *Maxwell equations* with varying coefficients corresponding to the material properties

It appears, however, that if the structure is thin and optical contrast high one can reduce *approximatively* the problem to an operator of the above described type, just the physical meaning of the quantities is different – see, for instance, [Figotin-Kuchment'98], [Kuchment-Kunyansky'99, '02]

Geometrically induced spectrum

(a) *Bending* means *binding*, i.e. it may create isolated eigenvalues of $H_{\alpha,\Gamma}$. Consider a *piecewise* C^1*-smooth* $\Gamma : \mathbb{R} \to \mathbb{R}^2$ parameterized by its arc length, and assume:

Geometrically induced spectrum

(a) *Bending* means *binding*, i.e. it may create isolated eigenvalues of $H_{\alpha,\Gamma}$. Consider a *piecewise* C^1*-smooth* $\Gamma:\,\mathbb{R}\to\mathbb{R}^2$ parameterized by its arc length, and assume:

- $|\Gamma(s)-\Gamma(s')|\ge c|s-s'|$ holds for some $c\in(0,1)$
- Γ is *asymptotically straight*: there are $d>0,\;\; \mu>\frac{1}{2}$ and $\omega\in(0,1)$ such that

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

  in the sector $S_\omega := \left\{(s,s'):\;\omega<\frac{s}{s'}<\omega^{-1}\right\}$

- *straight line is excluded*, i.e. $|\Gamma(s)-\Gamma(s')|<|s-s'|$ holds for some $s,s'\in\mathbb{R}$

Bending means binding

Theorem [E-Ichinose'01]: Under these assumptions, $\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}) = [-\frac{1}{4}\alpha^2, \infty)$ and $H_{\alpha,\Gamma}$ has *at least one eigenvalue* below the threshold $-\frac{1}{4}\alpha^2$

Bending means binding

Theorem [E-Ichinose'01]: Under these assumptions, $\sigma_{\rm ess}(H_{\alpha,\Gamma}) = [-\frac14\alpha^2,\infty)$ and $H_{\alpha,\Gamma}$ has *at least one eigenvalue* below the threshold $-\frac14\alpha^2$

- Naturally, this has *no analogy in "ideal" graphs!*
- The same for *curves in* $\mathbb{R}^3$, under stronger regularity, with $-\frac14\alpha^2$ is replaced by the corresponding 2D p.i. ev
- For *curved surfaces* $\Gamma\subset\mathbb{R}^3$ such a result is proved in the strong coupling asymptotic regime only
- *Implications for graphs:* let $\tilde\Gamma\supset\Gamma$ in the set sense, then $H_{\alpha,\tilde\Gamma}\le H_{\alpha,\Gamma}$. If the essential spectrum threshold is the same for both graphs and Γ fits the above assumptions, we have $\sigma_{\rm disc}(H_{\alpha,\Gamma})\ne\emptyset$ by minimax principle

Proof: generalized BS principle

Classical Birman-Schwinger principle based on the identity

$$(H_0 - V - z)^{-1} = (H_0 - z)^{-1} + (H_0 - z)^{-1} V^{1/2}$$
$$\times \left\{ I - |V|^{1/2} (H_0 - z)^{-1} V^{1/2} \right\}^{-1} |V|^{1/2} (H_0 - z)^{-1}$$

can be extended to generalized Schrödinger operators $H_{\alpha,\Gamma}$ [BEKŠ'94]: the multiplication by $(H_0 - z)^{-1} V^{1/2}$ etc. is replaced by suitable trace maps. In this way we find that $-\kappa^2$ is an eigenvalue of $H_{\alpha,\Gamma}$ *iff* the integral operator $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ on $L^2(\mathbb{R})$ with the kernel

$$(s, s') \mapsto \frac{\alpha}{2\pi} K_0 \left(\kappa |\Gamma(s) - \Gamma(s')| \right)$$

has an eigenvalue equal to one

Sketch of the proof

We treat $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ as a *perturbation* of the operator $\mathcal{R}^{\kappa}_{\alpha,\Gamma_0}$ referring to a *straight line*. The spectrum of the latter is found easily: it is *purely ac* and equal to $[0, \alpha/2\kappa)$

Sketch of the proof

We treat $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ as a *perturbation* of the operator $\mathcal{R}^{\kappa}_{\alpha,\Gamma_0}$ referring to a *straight line*. The spectrum of the latter is found easily: it is *purely ac* and equal to $[0, \alpha/2\kappa)$

The curvature-induced perturbation is *sign-definite*: we have $\left(\mathcal{R}^{\kappa}_{\alpha,\Gamma} - \mathcal{R}^{\kappa}_{\alpha,\Gamma_0}\right)(s,s') \geq 0$, and the inequality is sharp somewhere unless Γ is a straight line. Using a *variational argument* with a suitable trial function we can check the inequality $\sup \sigma(\mathcal{R}^{\kappa}_{\alpha,\Gamma}) > \frac{\alpha}{2\kappa}$

Sketch of the proof

We treat $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ as a *perturbation* of the operator $\mathcal{R}^{\kappa}_{\alpha,\Gamma_0}$ referring to a *straight line*. The spectrum of the latter is found easily: it is *purely ac* and equal to $[0, \alpha/2\kappa)$

The curvature-induced perturbation is *sign-definite*: we have $\left(\mathcal{R}^{\kappa}_{\alpha,\Gamma} - \mathcal{R}^{\kappa}_{\alpha,\Gamma_0}\right)(s,s') \geq 0$, and the inequality is sharp somewhere unless Γ is a straight line. Using a *variational argument* with a suitable trial function we can check the inequality $\sup \sigma(\mathcal{R}^{\kappa}_{\alpha,\Gamma}) > \frac{\alpha}{2\kappa}$

Due to the assumed asymptotic straightness of Γ the perturbation $\mathcal{R}^{\kappa}_{\alpha,\Gamma} - \mathcal{R}^{\kappa}_{\alpha,\Gamma_0}$ is *Hilbert-Schmidt*, hence the spectrum of $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ in the interval $(\alpha/2\kappa, \infty)$ is discrete

Sketch of the proof

We treat $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ as a *perturbation* of the operator $\mathcal{R}^{\kappa}_{\alpha,\Gamma_0}$ referring to a *straight line*. The spectrum of the latter is found easily: it is *purely ac* and equal to $[0, \alpha/2\kappa)$

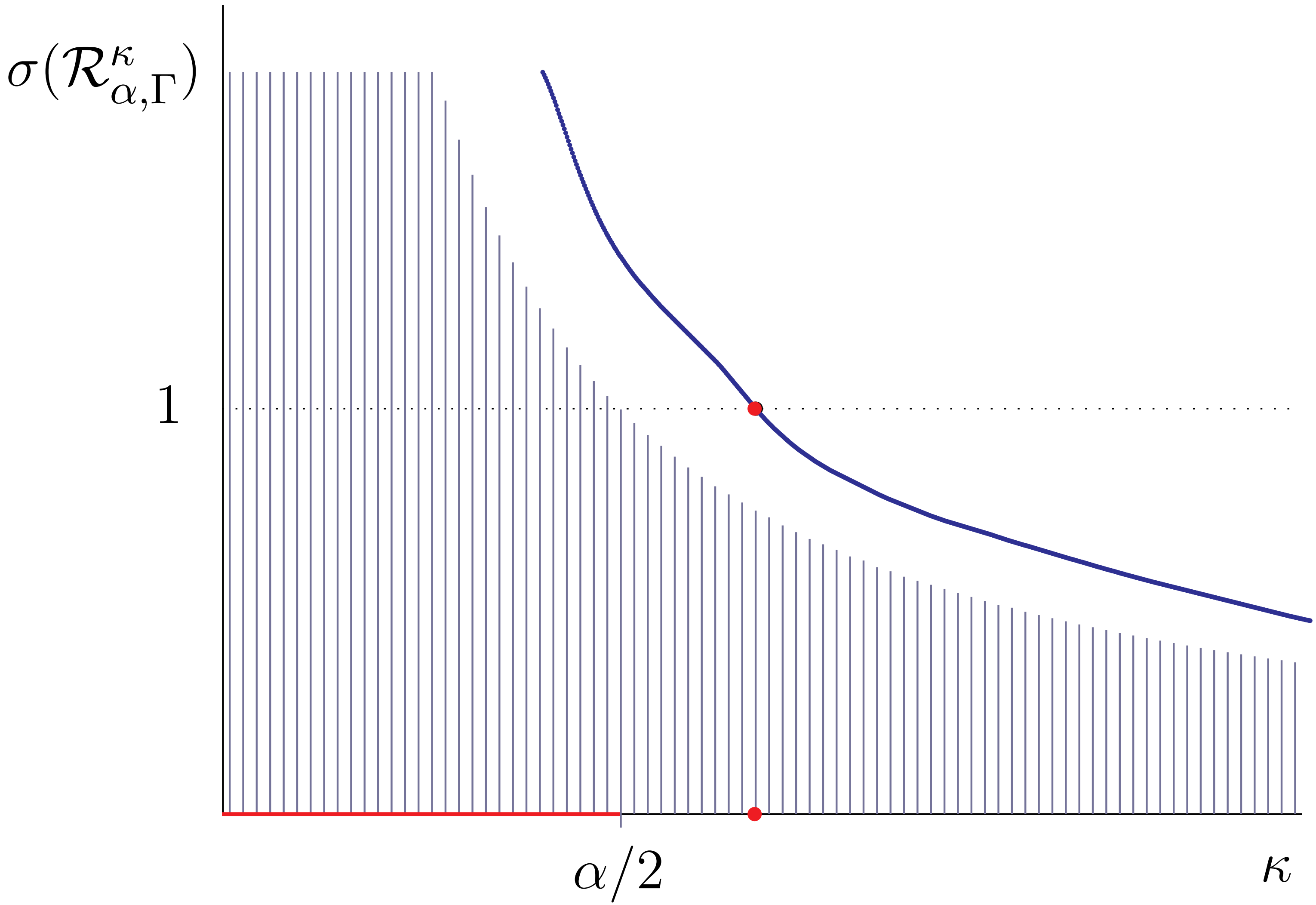
The curvature-induced perturbation is *sign-definite*: we have $\left(\mathcal{R}^{\kappa}_{\alpha,\Gamma} - \mathcal{R}^{\kappa}_{\alpha,\Gamma_0}\right)(s,s') \geq 0$, and the inequality is sharp somewhere unless Γ is a straight line. Using a *variational argument* with a suitable trial function we can check the inequality $\sup \sigma(\mathcal{R}^{\kappa}_{\alpha,\Gamma}) > \frac{\alpha}{2\kappa}$

Due to the assumed asymptotic straightness of Γ the perturbation $\mathcal{R}^{\kappa}_{\alpha,\Gamma} - \mathcal{R}^{\kappa}_{\alpha,\Gamma_0}$ is *Hilbert-Schmidt*, hence the spectrum of $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ in the interval $(\alpha/2\kappa, \infty)$ is discrete

To conclude we employ continuity and $\lim_{\kappa\to\infty} \|\mathcal{R}^{\kappa}_{\alpha,\Gamma}\| = 0$.

The argument can be pictorially expressed as follows:

Pictorial sketch of the proof

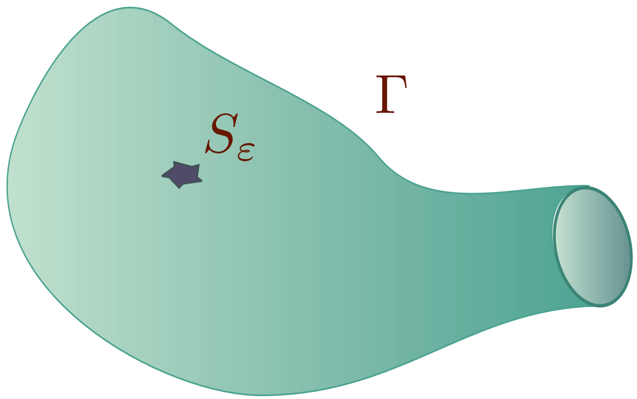


Punctured manifolds

(b) A natural question is what happens with $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma})$ if Γ has a small *"hole"*. We will give the answer for a compact, $(n-1)$-dimensional, $C^{1+[n/2]}$-smooth manifold in $\mathbb{R}^n$

Punctured manifolds

(b) A natural question is what happens with $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma})$ if Γ has a small *"hole"*. We will give the answer for a compact, $(n-1)$-dimensional, $C^{1+[n/2]}$-smooth manifold in $\mathbb{R}^n$



Consider a family $\{S_\varepsilon\}_{0\le\varepsilon<\eta}$ of subsets of Γ such that

- each S_ε is *Lebesgue measurable* on Γ
- they shrink to origin, $\sup_{x\in S_\varepsilon} |x| = \mathcal{O}(\varepsilon)$ as $\varepsilon \to 0$
- $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \ne \emptyset$, nontrivial for $n \ge 3$

Punctured manifolds: ev asymptotics

Call $H_\varepsilon := H_{\alpha,\Gamma\setminus S_\varepsilon}$. For small enough ε these operators have the same finite number of eigenvalues, naturally ordered, which satisfy $\lambda_j(\varepsilon) \to \lambda_j(0)$ as $\varepsilon \to 0$

Punctured manifolds: ev asymptotics

Call $H_\varepsilon := H_{\alpha,\Gamma\setminus S_\varepsilon}$. For small enough ε these operators have the same finite number of eigenvalues, naturally ordered, which satisfy $\lambda_j(\varepsilon) \to \lambda_j(0)$ as $\varepsilon \to 0$

Let φ_j be the eigenfunctions of H_0. By Sobolev trace thm $\varphi_j(0)$ makes sense. Put $s_j := |\varphi_j(0)|^2$ if $\lambda_j(0)$ is simple, otherwise they are ev's of $C := \left(\overline{\varphi_i(0)}\varphi_j(0)\right)$ corresponding to a degenerate eigenvalue

Punctured manifolds: ev asymptotics

Call $H_\varepsilon := H_{\alpha,\Gamma\setminus S_\varepsilon}$. For small enough ε these operators have the same finite number of eigenvalues, naturally ordered, which satisfy $\lambda_j(\varepsilon) \to \lambda_j(0)$ as $\varepsilon \to 0$

Let φ_j be the eigenfunctions of H_0. By Sobolev trace thm $\varphi_j(0)$ makes sense. Put $s_j := |\varphi_j(0)|^2$ if $\lambda_j(0)$ is simple, otherwise they are ev's of $C := \left(\overline{\varphi_i(0)}\varphi_j(0)\right)$ corresponding to a degenerate eigenvalue

Theorem [E-Yoshitomi'03]: Under the assumptions made about the family $\{S_\varepsilon\}$, we have

$$\lambda_j(\varepsilon) = \lambda_j(0) + \alpha s_j m_\Gamma(S_\varepsilon) + o(\varepsilon^{n-1}) \quad \text{as} \quad \varepsilon \to 0$$

Remarks

- Formally a small-hole perturbation acts as a *repulsive δ interaction* with the coupling $\alpha m_\Gamma(S_\varepsilon)$

Remarks

- Formally a small-hole perturbation acts as a *repulsive δ interaction* with the coupling $\alpha m_\Gamma(S_\varepsilon)$
- No self-similarity of S_ε required

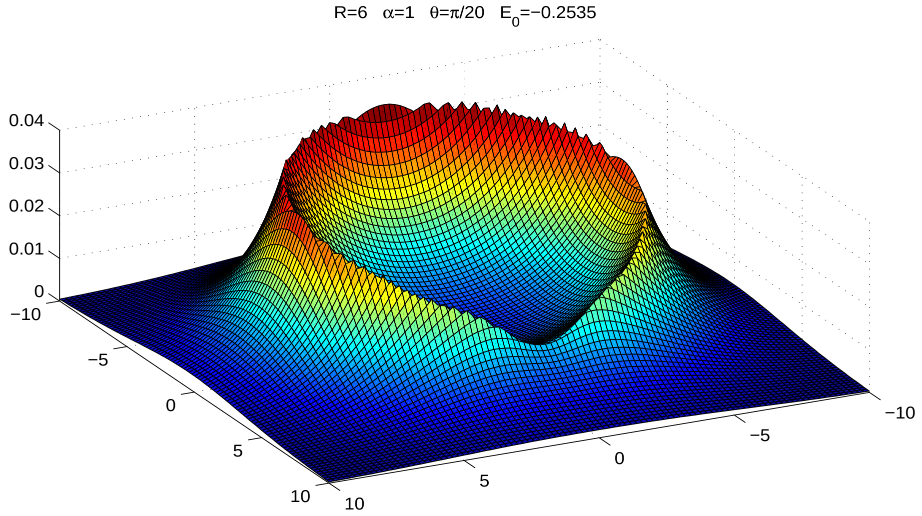
Remarks

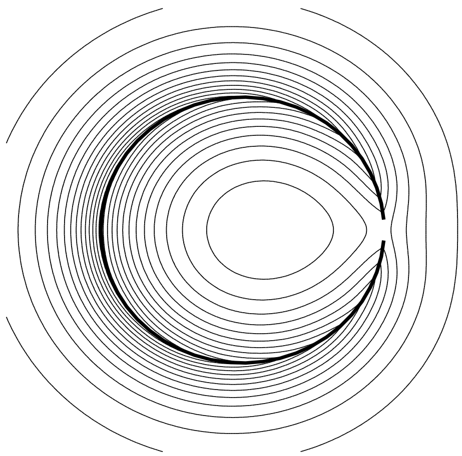
- Formally a small-hole perturbation acts as a *repulsive δ interaction* with the coupling $\alpha m_\Gamma(S_\varepsilon)$
- No self-similarity of S_ε required
- If $n = 2$, i.e. Γ is a curve, $m_\Gamma(S_\varepsilon)$ is the length of the hiatus. In this case the same asymptotic formula holds for bound states of an infinite curved Γ

Remarks

- Formally a small-hole perturbation acts as a *repulsive δ interaction* with the coupling $\alpha m_\Gamma(S_\varepsilon)$
- No self-similarity of S_ε required
- If $n=2$, i.e. Γ is a curve, $m_\Gamma(S_\varepsilon)$ is the length of the hiatus. In this case the same asymptotic formula holds for bound states of an infinite curved Γ
- Asymptotic perturbation theory for quadratic forms does not apply, because $C_0^\infty(\mathbb{R}^n) \ni u \mapsto |u(0)|^2 \in \mathbb{R}$ does not extend to a bounded form in $W^{1,2}(\mathbb{R}^n)$

Illustration: a ring with $\frac{\pi}{20}$ cut





Strongly attractive curves

(c) *Strong coupling asymptotics:* let $\Gamma : \mathbb{R} \to \mathbb{R}^2$ be as above, now supposed to be C^4*-smooth*

Theorem [E-Yoshitomi'01]: The j-th ev of $H_{\alpha,\Gamma}$ is

$$\lambda_j(\alpha) = -\frac{1}{4}\alpha^2 + \mu_j + \mathcal{O}(\alpha^{-1}\ln\alpha) \quad \text{as} \quad \alpha \to \infty\,,$$

where μ_j is the j-th ev of $S_\Gamma := -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}\gamma(s)^2$ on $L^2((\mathbb{R})$ and γ is the curvature of Γ.

Strongly attractive curves

(c) *Strong coupling asymptotics:* let $\Gamma:\ \mathbb{R}\to\mathbb{R}^2$ be as above, now supposed to be C^4*-smooth*

Theorem [E-Yoshitomi'01]: The j-th ev of $H_{\alpha,\Gamma}$ is

$$\lambda_j(\alpha) = -\frac{1}{4}\alpha^2 + \mu_j + \mathcal{O}(\alpha^{-1}\ln\alpha) \quad \text{as} \quad \alpha\to\infty\,,$$

where μ_j is the j-th ev of $S_\Gamma := -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}\gamma(s)^2$ on $L^2((\mathbb{R})$ and γ is the curvature of Γ. The same holds if Γ is a loop; then we also have

$$\#\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) = \frac{|\Gamma|\alpha}{2\pi} + \mathcal{O}(\ln\alpha) \quad \text{as} \quad \alpha\to\infty$$

Sketch of the proof

For definiteness consider the loop case: take a closed Γ and call $L = |\Gamma|$. We start from a *tubular neighborhood* of Γ

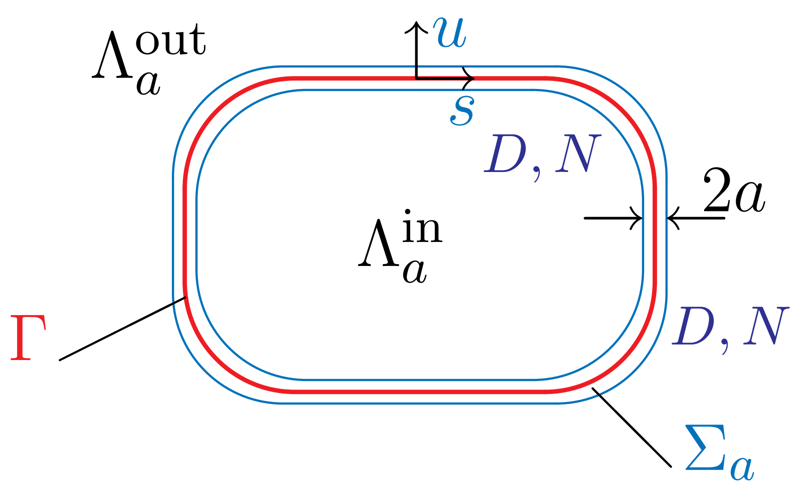
Sketch of the proof

For definiteness consider the loop case: take a closed Γ and call $L = |\Gamma|$. We start from a *tubular neighborhood* of Γ

Lemma: $\Phi_a : [0, L) \times (-a, a) \to \mathbb{R}^2$ defined by

$$(s, u) \mapsto (\gamma_1(s) - u\gamma_2'(s), \gamma_2(s) + u\gamma_1'(s)).$$

is a diffeomorphism for all $a > 0$ small enough



constant-width strip, do not take the LaTeX drawing too literary!

DN bracketing

The idea is to apply to the operator $H_{\alpha,\Gamma}$ in question *Dirichlet-Neumann bracketing* at the boundary of $\Sigma_a := \Phi([0,L)\times(-a,a))$. This yields

$$(-\Delta_{\Lambda_a}^{\mathrm{N}}) \oplus L_{a,\alpha}^{-} \le H_{\alpha,\Gamma} \le (-\Delta_{\Lambda_a}^{\mathrm{D}}) \oplus L_{a,\alpha}^{+},$$

where $\Lambda_a = \Lambda_a^{\mathrm{in}} \cup \Lambda_a^{\mathrm{out}}$ is the exterior domain, and $L_{a,\alpha}^{\pm}$ are self-adjoint operators associated with the forms

$$q_{a,\alpha}^{\pm}[f] = \|\nabla f\|_{L^2(\Sigma_a)}^2 - \alpha \int_\Gamma |f(x)|^2 \,\mathrm{d}S$$

where $f \in W_0^{1,2}(\Sigma_a)$ and $W^{1,2}(\Sigma_a)$ for $\pm$, respectively

DN bracketing

The idea is to apply to the operator $H_{\alpha,\Gamma}$ in question *Dirichlet-Neumann bracketing* at the boundary of $\Sigma_a := \Phi([0,L)\times(-a,a))$. This yields

$$(-\Delta^{\mathrm{N}}_{\Lambda_a}) \oplus L^-_{a,\alpha} \le H_{\alpha,\Gamma} \le (-\Delta^{\mathrm{D}}_{\Lambda_a}) \oplus L^+_{a,\alpha},$$

where $\Lambda_a = \Lambda_a^{\mathrm{in}} \cup \Lambda_a^{\mathrm{out}}$ is the exterior domain, and $L^\pm_{a,\alpha}$ are self-adjoint operators associated with the forms

$$q^\pm_{a,\alpha}[f] = \|\nabla f\|^2_{L^2(\Sigma_a)} - \alpha \int_\Gamma |f(x)|^2 \,\mathrm{d}S$$

where $f \in W^{1,2}_0(\Sigma_a)$ and $W^{1,2}(\Sigma_a)$ for $\pm$, respectively

Important: The exterior part does not contribute to the negative spectrum, so we may consider $L^\pm_{a,\alpha}$ only

Transformed interior operator

We use the curvilinear coordinates passing from $L^{\pm}_{a,\alpha}$ to unitarily equivalent operators given by quadratic forms

$$b^{+}_{a,\alpha}[f] = \int_0^L \int_{-a}^{a} (1+uk(s))^{-2} \left|\frac{\partial f}{\partial s}\right|^2 \mathrm{d}u\,\mathrm{d}s + \int_0^L \int_{-a}^{a} \left|\frac{\partial f}{\partial u}\right|^2 \mathrm{d}u\,\mathrm{d}s$$

$$+ \int_0^L \int_{-a}^{a} V(s,u)|f|^2\,\mathrm{d}s\,\mathrm{d}u - \alpha \int_0^L |f(s,0)|^2\,\mathrm{d}s$$

with $f \in W^{1,2}((0,L)\times(-a,a))$ satisfying periodic b.c. in the variable s and Dirichlet b.c. at $u=\pm a$, and

$$b^{-}_{a,\alpha}[f] = b^{+}_{a,\alpha}[f] - \sum_{j=0}^{1} \frac{1}{2}(-1)^j \int_0^L \frac{k(s)}{1+(-1)^j a k(s)} |f(s,(-1)^j a)|^2\,\mathrm{d}s$$

where V is the curvature induced potential,

$$V(s,u) = -\frac{k(s)^2}{4(1+uk(s))^2} + \frac{uk''(s)}{2(1+uk(s))^3} - \frac{5u^2 k'(s)^2}{4(1+uk(s))^4}$$

Estimates with separated variables

We pass to rougher bounds squeezing $H_{\alpha,\Gamma}$ between

$$\tilde{H}^{\pm}_{a,\alpha} = U^{\pm}_{a} \otimes 1 + 1 \otimes T^{\pm}_{a,\alpha}$$

Estimates with separated variables

We pass to rougher bounds squeezing $H_{\alpha,\Gamma}$ between

$$\tilde{H}^{\pm}_{a,\alpha} = U^{\pm}_{a} \otimes 1 + 1 \otimes T^{\pm}_{a,\alpha}$$

Here $U^{\pm}_{a}$ are s-a operators on $L^2(0,L)$

$$U^{\pm}_{a} = -(1 \mp a\|k\|_{\infty})^{-2} \frac{\mathrm{d}^2}{\mathrm{d}s^2} + V_{\pm}(s)$$

with PBC, where $V_{-}(s) \le V(s,u) \le V_{+}(s)$ with an $\mathcal{O}(a)$ error, and the transverse operators are associated with the forms

$$t^{+}_{a,\alpha}[f] = \int_{-a}^{a} |f'(u)|^2 \,\mathrm{d}u - \alpha|f(0)|^2$$

and

$$t^{-}_{a,\alpha}[f] = t^{-}_{a,\alpha}[f] - \|k\|_{\infty}(|f(a)|^2 + |f(-a)|^2)$$

with $f \in W^{1,2}_{0}(-a,a)$ and $W^{1,2}(-a,a)$, respectively

Concluding the argument

Lemma: There are positive $c,\ c_N$ such that $T^{\pm}_{\alpha,a}$ has for α large enough a single negative eigenvalue $\kappa^{\pm}_{\alpha,a}$ satisfying

$$-\frac{\alpha^2}{4}\left(1+c_N \mathrm{e}^{-\alpha a/2}\right) < \kappa^{-}_{\alpha,a} < -\frac{\alpha^2}{4} < \kappa^{+}_{\alpha,a} < -\frac{\alpha^2}{4}\left(1-8\mathrm{e}^{-\alpha a/2}\right)$$

Concluding the argument

Lemma: There are positive c, c_N such that $T^{\pm}_{\alpha,a}$ has for α large enough a single negative eigenvalue $\kappa^{\pm}_{\alpha,a}$ satisfying

$$-\frac{\alpha^2}{4}\left(1+c_N \mathrm{e}^{-\alpha a/2}\right) < \kappa^{-}_{\alpha,a} < -\frac{\alpha^2}{4} < \kappa^{+}_{\alpha,a} < -\frac{\alpha^2}{4}\left(1-8\mathrm{e}^{-\alpha a/2}\right)$$

Finishing the proof:

- the eigenvalues of $U^{\pm}_a$ differ by $\mathcal{O}(a)$ from those of the comparison operator
- we choose $a = 6\alpha^{-1}\ln\alpha$ as the neighbourhood width
- putting the estimates together we get the eigenvalue asymptotics for a planar loop, i.e. the claim *(ii)*
- if Γ is not closed, the same can be done with the comparison operators $S^{\mathrm{D,N}}_{\Gamma}$ having appropriate b.c. at the endpoints of Γ. This yields the claim *(i)*

Further extensions

- $H_{\alpha,\Gamma}$ with a *periodic* Γ has a band-type spectrum, but analogous asymptotics is valid for its *Floquet components* $H_{\alpha,\Gamma}(\theta)$, with the comparison operator $S_\Gamma(\theta)$ satisfying the appropriate b.c. over the period cell. It is important that the error term is uniform w.r.t. θ

Further extensions

- $H_{\alpha,\Gamma}$ with a *periodic* Γ has a band-type spectrum, but analogous asymptotics is valid for its *Floquet components* $H_{\alpha,\Gamma}(\theta)$, with the comparison operator $S_\Gamma(\theta)$ satisfying the appropriate b.c. over the period cell. It is important that the error term is uniform w.r.t. θ
- Similar result holds for planar loops *threaded by mg field*, homogeneous, AB flux line, etc.

Further extensions

- $H_{\alpha,\Gamma}$ with a *periodic* Γ has a band-type spectrum, but analogous asymptotics is valid for its *Floquet components* $H_{\alpha,\Gamma}(\theta)$, with the comparison operator $S_\Gamma(\theta)$ satisfying the appropriate b.c. over the period cell. It is important that the error term is uniform w.r.t. θ
- Similar result holds for planar loops *threaded by mg field*, homogeneous, AB flux line, etc.
- *Higher dimensions:* the results extend to loops, infinite and periodic curves in $\mathbb{R}^3$

Further extensions

- $H_{\alpha,\Gamma}$ with a *periodic* Γ has a band-type spectrum, but analogous asymptotics is valid for its *Floquet components* $H_{\alpha,\Gamma}(\theta)$, with the comparison operator $S_\Gamma(\theta)$ satisfying the appropriate b.c. over the period cell. It is important that the error term is uniform w.r.t. θ
- Similar result holds for planar loops *threaded by mg field*, homogeneous, AB flux line, etc.
- *Higher dimensions:* the results extend to loops, infinite and periodic curves in $\mathbb{R}^3$
- and to *curved surfaces* in $\mathbb{R}^3$; then the comparison operator is $-\Delta_{\mathrm{LB}} + K - M^2$, where K, M, respectively, are the corresponding Gauss and mean curvatures

Some references

[BEKŠ'04] J.F. Brasche, P. Exner, Yu.A. Kuperin, P. Šeba: Schrödinger operators with singular interactions, *J. Math. Anal. Appl.* **184** (1994), 112-139

[BT'92] J.F. Brasche, A. Teta: Spectral analysis and scattering theory for Schrödinger operators with an interaction supported by a regular curve, in *Ideas and Methods in Quantum and Statistical Physics*, ed. S. Albeverio, et al., CUP 1992, pp. 197-211

[EI'01] P.E., T. Ichinose: Geometrically induced spectrum in curved leaky wires, *J. Phys.* **A34** (2001), 1439-1450

[EK'02] P.E., S. Kondej: Curvature-induced bound states for a δ interaction supported by a curve in $\mathbb{R}^3$, *Ann. H. Poincaré* **3** (2002), 967-981

[EK'03] P.E., S. Kondej: Bound states due to a strong δ interaction supported by a curved surface, *J. Phys.* **A36** (2003), 443-457

[EY'01] P.E., K. Yoshitomi: Band gap of the Schrödinger operator with a strong δ-interaction on a periodic curve, *Ann. H. Poincaré* **2** (2001), 1139-1158

[EY'02a] P.E., K. Yoshitomi: Asymptotics of eigenvalues of the Schrödinger operator with a strong δ-interaction on a loop, *J. Geom. Phys.* **41** (2002), 344-358

[EY'02b] P.E., K. Yoshitomi: Persistent currents for 2D Schrödinger operator with a strong δ-interaction on a loop, *J. Phys.* **A35** (2002), 3479-3487

[EY'03] P.E., K. Yoshitomi: Eigenvalue asymptotics for the Schrödinger operator with a δ-interaction on a punctured surface, *Lett. Math. Phys.* **65** (2003), 19-26

And on photonic crystals

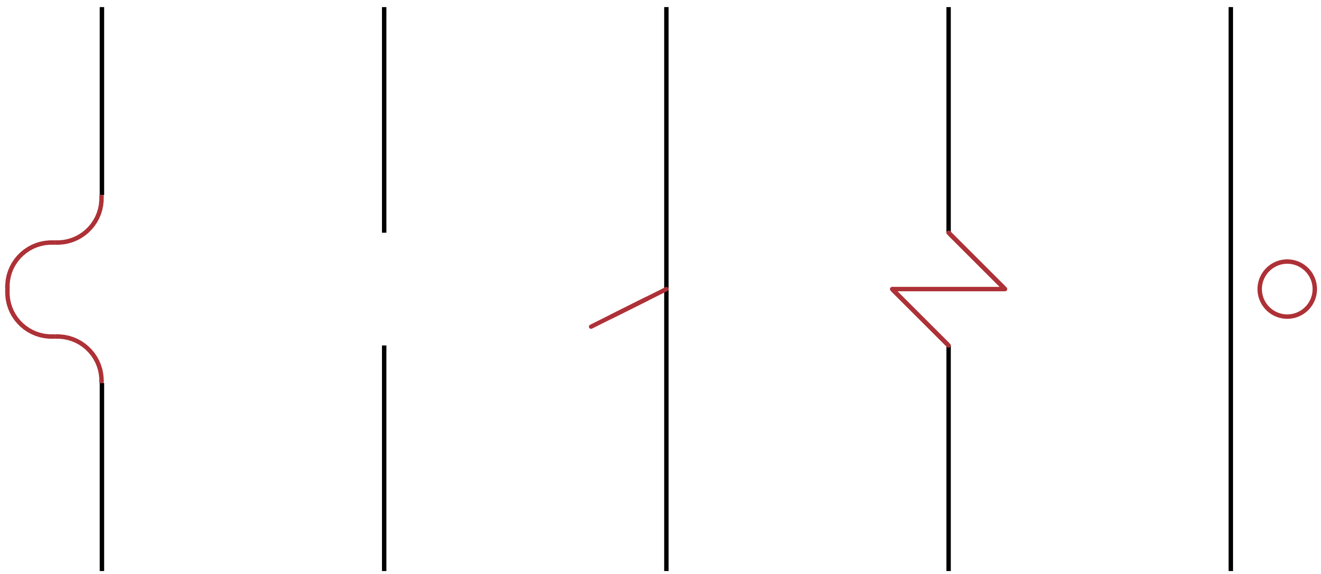
[FK'98] A. Figotin, P. Kuchment: Spectral properties of classical waves in high contrast periodic media, *SIAM J. Appl. Math.* **58** (1998), 683-702

[KK'99] P. Kuchment, L. Kunyansky: Spectral properties of high-contrast band-gap materials and operators on graphs, *Experimental Mathematics* **8** (1999), 1-28

[KK'02] P. Kuchment, L. Kunyansky: Differential operators on graphs and photonic crystals, *Adv. Comput. Math.* **16** (2002), 263-290

Scattering on a locally deformed line

Scattering requires to specify a *free dynamics*. Here we will suppose that the latter is described by $H_{\alpha,\Sigma}$, where Σ is a *straight line*, $\Sigma = \{(x_1, 0) : x_1 \in\}$, and that the graph Γ in question differs from Σ by a *local deformation* only



Assumptions

We will consider the following class of local deformations:

- there exists a *compact* $M \subset \mathbb{R}^2$ such that $\Gamma \setminus M = \Sigma \setminus M$,
- the set $\Gamma \setminus \Sigma$ admits a finite decomposition,

$$\Gamma \setminus \Sigma = \bigcup_{i=1}^{N} \Gamma_i\,, \quad N < \infty\,,$$

where the Γ_i's are finite C^1 curves such that *no pair* of components of Γ *crosses* at their interior points, neither a component has a *self-intersection*; we allow the components to touch at their endpoints but assume they do not form a *cusp* there

As we have said, $H_{\alpha,\Gamma}$ is then well defined

Krein's formula

Our main tool will be a formula comparing the resolvents of $H_{\alpha,\Gamma}$ and $H_{\alpha,\Sigma}$. We will use the decomposition

$$\Lambda = \Lambda_0 \cup \Lambda_1 \quad \text{with} \quad \Lambda_0 := \Sigma \setminus \Gamma\,, \;\; \Lambda_1 := \Gamma \setminus \Sigma = \bigcup_{i=1}^{N} \Gamma_i\,;$$

the coupling constant of the perturbation will be naturally equal to α on the "subtracted" set Λ_0 and $-\alpha$ on Λ_1

Krein's formula

Our main tool will be a formula comparing the resolvents of $H_{\alpha,\Gamma}$ and $H_{\alpha,\Sigma}$. We will use the decomposition

$$\Lambda = \Lambda_0 \cup \Lambda_1 \quad \text{with} \quad \Lambda_0 := \Sigma \setminus \Gamma\,, \;\; \Lambda_1 := \Gamma \setminus \Sigma = \bigcup_{i=1}^{N} \Gamma_i\,;$$

the coupling constant of the perturbation will be naturally equal to α on the "subtracted" set Λ_0 and $-\alpha$ on Λ_1
To construct resolvent of $H_{\alpha,\Sigma}$ we use R^k, the one of $-\Delta$, which is for $k^2 \in \rho(-\Delta)$ an integral operator with the kernel

$$G^k(x-y) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\mathrm{e}^{ip(x-y)}}{p^2 - k^2}\, \mathrm{d}p = \frac{1}{2\pi} K_0(ik|x-y|)\,,$$

where $K_0(\cdot)$ stands for the Macdonald function

Krein's formula, continued

A straightforward computation shows that the resolvent R^k_Σ of $H_{\alpha,\Sigma}$ has the kernel $G^k_\Sigma(x-y)$ given by

$$G^k(x-y) + \frac{\alpha}{4\pi^3}\int_{\mathbb{R}^3} \frac{e^{ipx-ip'y}}{(p^2-k^2)(p'^2-k^2)}\,\frac{\tau_k(p_1)}{2\tau_k(p_1)-\alpha}\,dp\,dp_2',$$

where $\tau_k(p_1) := (p_1^2 - k^2)^{1/2}$ and $p = (p_1, p_2)$, $p' = (p_1, p_2')$

Krein's formula, continued

A straightforward computation shows that the resolvent R^k_Σ of $H_{\alpha,\Sigma}$ has the kernel $G^k_\Sigma(x-y)$ given by

$$G^k(x-y) + \frac{\alpha}{4\pi^3} \int_{3} \frac{\mathrm{e}^{ipx-ip'y}}{(p^2-k^2)(p'^2-k^2)} \frac{\tau_k(p_1)}{2\tau_k(p_1)-\alpha} \,\mathrm{d}p\, \mathrm{d}p'_2 \,,$$

where $\tau_k(p_1) := (p_1^2 - k^2)^{1/2}$ and $p = (p_1, p_2)$, $p' = (p_1, p'_2)$

We need embeddings of R^k_Σ to $L^2(\nu)$, where $\nu \equiv \nu_\Lambda$ is the Dirac measure on Λ. It can be written as $\nu_\Lambda = \nu_0 + \sum_{i=1}^N \nu_i$, where ν_0 is the Dirac measure on Λ_0. It convenient also to introduce the space $\mathrm{h} \equiv L^2(\nu)$ which decomposes into

$$\mathrm{h} = \mathrm{h}_0 \oplus \mathrm{h}_1 \quad \text{with} \quad \mathrm{h}_0 \equiv L^2(\nu_0) \quad \text{and} \quad \mathrm{h}_1 \equiv \bigoplus_{i=1}^N L^2(\nu_i)$$

Embeddings

Now we are able to introduce the operator

$$\mathrm{R}^k_{\Sigma,\nu} : \mathrm{h} \to L^2\,, \quad \mathrm{R}^k_{\Sigma,\nu} f = G^k_\Sigma * f\nu \quad \text{for} \quad f \in \mathrm{h}$$

defined for suitable values of k. Similarly, $(\mathrm{R}^k_{\Sigma,\nu})^* : L^2 \to \mathrm{h}$ is its adjoint and $\mathrm{R}^k_{\Sigma,\nu\nu}$ denotes the operator-valued matrix in h with the “block elements” $G^k_{\Sigma,ij} \equiv G^k_{\Sigma,\nu_i\nu_j} : L^2(\nu_j) \to L^2(\nu_i)$

Embeddings

Now we are able to introduce the operator

$$\mathrm{R}^k_{\Sigma,\nu} : \mathrm{h} \to L^2\,, \quad \mathrm{R}^k_{\Sigma,\nu} f = G^k_\Sigma * f\nu \quad \text{for} \quad f \in \mathrm{h}$$

defined for suitable values of k. Similarly, $(\mathrm{R}^k_{\Sigma,\nu})^* : L^2 \to \mathrm{h}$ is its adjoint and $\mathrm{R}^k_{\Sigma,\nu\nu}$ denotes the operator-valued matrix in h with the “block elements” $G^k_{\Sigma,ij} \equiv G^k_{\Sigma,\nu_i\nu_j} : L^2(\nu_j) \to L^2(\nu_i)$

They have the following properties:

- For any $\kappa \in (\alpha/2, \infty)$ the operator $\mathrm{R}^{i\kappa}_{\Sigma,\nu}$ is bounded. In fact, $\mathrm{R}^{i\kappa}_{\Sigma,\nu}$ is a continuous embedding into $W^{1,2}$
- For any $\sigma > 0$ there exists κ_σ such that for $\kappa > \kappa_\sigma$ the operator $\mathrm{R}^{i\kappa}_{\Sigma,\nu\nu}$ is bounded with the norm less than σ

Krein's formula, continued

Introduce an operator-valued matrix in $\mathrm{h} = \mathrm{h}_0 \oplus \mathrm{h}_1$ as

$$\Theta^k = -(\alpha^{-1}\check{\mathbb{I}} + \mathrm{R}^k_{\Sigma,\nu\nu}) \quad \text{with} \quad \check{\mathbb{I}} = \begin{pmatrix} \mathbb{I}_0 & 0 \\ 0 & -\mathbb{I}_1 \end{pmatrix},$$

where $\mathbb{I}_i$ are the unit operators in h_i. Using the properties of the embeddings we prove the following claim:

Krein's formula, continued

Introduce an operator-valued matrix in $\mathrm{h} = \mathrm{h}_0 \oplus \mathrm{h}_1$ as

$$\Theta^k = -(\alpha^{-1}\check{\mathbb{I}} + \mathrm{R}^k_{\Sigma,\nu\nu}) \quad \text{with} \quad \check{\mathbb{I}} = \begin{pmatrix} \mathbb{I}_0 & 0 \\ 0 & -\mathbb{I}_1 \end{pmatrix},$$

where $\mathbb{I}_i$ are the unit operators in h_i. Using the properties of the embeddings we prove the following claim:

Proposition: Let Θ^k have inverse in $\mathcal{B}(\mathrm{h})$ for $k \in \mathbb{C}^+$ and suppose that the operator

$$R^k_\Gamma = R^k_\Sigma + \mathrm{R}^k_{\Sigma,\nu}(\Theta^k)^{-1}(\mathrm{R}^k_{\Sigma,\nu})^*$$

is defined everywhere on L^2. Then k^2 belongs to $\rho(H_{\alpha,\Gamma})$ and the resolvent $(H_{\alpha,\Gamma} - k^2)^{-1}$ is given by R^k_Γ

Wave operators

The existence and completeness of wave operators for the pair $(H_{\alpha,\Gamma}, H_{\alpha,\Sigma})$ follows from the standard trace-class criterion, conventionally called Birman-Kuroda theorem. Specifically, we have

Theorem [E-Kondej'05]: $B^{i\kappa}$ is a trace class operator for κ sufficiently large

Wave operators

The existence and completeness of wave operators for the pair $(H_{\alpha,\Gamma}, H_{\alpha,\Sigma})$ follows from the standard trace-class criterion, conventionally called Birman-Kuroda theorem. Specifically, we have

Theorem [E-Kondej'05]: $B^{i\kappa}$ is a trace class operator for κ sufficiently large

Proof is inspired by [Brasche-Teta'92]. We use the estimate $(\Theta^{i\kappa})^{-1} \le C'(\Theta^{i\kappa,+})^{-1}$, where $\Theta^{i\kappa,+} := \alpha^{-1}\mathbb{I} + \mathrm{R}^{i\kappa}_{\Sigma,\nu\nu}$ and $\mathbb{I}$ is the $(N+1)\times(N+1)$ unit matrix, for some $C'>0$ and all κ sufficiently large; it is clear that $(\Theta^{i\kappa,+})^{-1}$ is positive and bounded. This gives

$$B^{i\kappa} \le C' B^{i\kappa,+}\,, \qquad B^{i\kappa,+} := \mathrm{R}^{i\kappa}_{\Sigma,\nu}(\Theta^{i\kappa,+})^{-1}(\mathrm{R}^{i\kappa}_{\Sigma,\nu})^*$$

Proof, continued

Define $B_\delta^{i\kappa,+}$ as integral operator with the kernel

$$B_\delta^{i\kappa,+}(x,y) = \chi_\delta(x) B^{i\kappa,+}(x,y) \chi_\delta(y)\,,$$

where χ_δ stands for the indicator function of the ball $\mathcal{B}(0,\delta)$; one has $B_\delta^{i\kappa,+} \to B^{i\kappa,+}$ as $\delta \to \infty$ in the weak sense.

Proof, continued

Define $B_\delta^{i\kappa,+}$ as integral operator with the kernel

$$B_\delta^{i\kappa,+}(x,y) = \chi_\delta(x) B^{i\kappa,+}(x,y)\chi_\delta(y)\,,$$

where χ_δ stands for the indicator function of the ball $\mathcal{B}(0,\delta)$; one has $B_\delta^{i\kappa,+} \to B^{i\kappa,+}$ as $\delta \to \infty$ in the weak sense. Then

$$\int_{\mathbb{R}^2} B_\delta^{i\kappa,+}(x,x)\mathrm{d}x = \int_{\mathbb{R}^2} (G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x), (\Theta^{i\kappa,+})^{-1} G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x))_{\mathrm{h}}\,\mathrm{d}x$$

$$\le \|(\Theta^{i\kappa,+})^{-1}\| \int_{\mathbb{R}^2} \|G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x)\|_{\mathrm{h}}^2\,\mathrm{d}x \le C\|(\Theta^{i\kappa,+})^{-1}\|\,,$$

hence $B_\delta^{i\kappa,+}$ is trace class for any $\delta > 0$, and the same is true for the limiting operator.

Proof, continued

Define $B_\delta^{i\kappa,+}$ as integral operator with the kernel

$$B_\delta^{i\kappa,+}(x,y) = \chi_\delta(x) B^{i\kappa,+}(x,y)\chi_\delta(y)\,,$$

where χ_δ stands for the indicator function of the ball $\mathcal{B}(0,\delta)$; one has $B_\delta^{i\kappa,+} \to B^{i\kappa,+}$ as $\delta \to \infty$ in the weak sense. Then

$$\int_{\mathbb{R}^2} B_\delta^{i\kappa,+}(x,x)\mathrm{d}x = \int_{\mathbb{R}^2} (G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x), (\Theta^{i\kappa,+})^{-1} G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x))_{\mathrm{h}}\,\mathrm{d}x$$

$$\le \|(\Theta^{i\kappa,+})^{-1}\| \int_{\mathbb{R}^2} \|G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x)\|_{\mathrm{h}}^2\,\mathrm{d}x \le C\|(\Theta^{i\kappa,+})^{-1}\|\,,$$

hence $B_\delta^{i\kappa,+}$ is trace class for any $\delta>0$, and the same is true for the limiting operator.

Similarly one finds a Hermitian trace class operator $B^{i\kappa,-}$ which provides an estimate from below, $B^{i\kappa,-} \le B^{i\kappa}$; this means that $B^{i\kappa}$ is a trace class operator too. $\square$

Generalized eigenfunctions

We want to find the S-matrix, $S\psi_\lambda^- = \psi_\lambda^+$, for scattering in the *negative part of the spectrum* with a fixed energy $\lambda \in (-\frac{1}{4}\alpha^2, 0)$ corresponding to the effective momentum $k_\alpha(\lambda) := (\lambda + \alpha^2/4)^{1/2}$. We employ generalized ef's of $H_{\alpha,\Sigma}$,

$$\omega_\lambda(x_1, x_2) = \mathrm{e}^{i(\lambda+\alpha^2/4)^{1/2}x_1} \mathrm{e}^{-\alpha|x_2|/2},$$

their analogues ω_z for complex energies and regularizations $\omega_z^\delta(x) = \mathrm{e}^{-\delta x_1^2}\omega_z(x)$ for $z \in \rho(H_{\alpha,\Sigma})$, belonging to $D(H_{\alpha,\Sigma})$.

Generalized eigenfunctions

We want to find the S-matrix, $S\psi_\lambda^- = \psi_\lambda^+$, for scattering in the *negative part of the spectrum* with a fixed energy $\lambda \in (-\frac{1}{4}\alpha^2, 0)$ corresponding to the effective momentum $k_\alpha(\lambda) := (\lambda + \alpha^2/4)^{1/2}$. We employ generalized ef's of $H_{\alpha,\Sigma}$,

$$\omega_\lambda(x_1, x_2) = \mathrm{e}^{i(\lambda+\alpha^2/4)^{1/2}x_1}\mathrm{e}^{-\alpha|x_2|/2},$$

their analogues ω_z for complex energies and regularizations $\omega_z^\delta(x) = \mathrm{e}^{-\delta x_1^2}\omega_z(x)$ for $z \in \rho(H_{\alpha,\Sigma})$, belonging to $D(H_{\alpha,\Sigma})$. Consider now ψ_z^δ such that $(H_{\alpha,\Gamma} - z)\psi_z^\delta = (H_{\alpha,\Sigma} - z)\omega_z^\delta$. After taking the limit $\lim_{\epsilon\to 0}\psi_{\lambda+i\epsilon}^\delta = \psi_\lambda^\delta$ in the topology of L^2 the function ψ_λ^δ still belongs to $D(H_{\alpha,\Sigma})$ and we have

$$\psi_\lambda^\delta = \omega_\lambda^\delta + \mathrm{R}_{\Sigma,\nu}^{k_\alpha(\lambda)}(\Theta^{k_\alpha(\lambda)})^{-1}I_\Lambda\omega_\lambda^\delta$$

Generalized eigenfunctions, continued

Here $\mathrm{R}_{\Sigma,\nu}^{k_\alpha(\lambda)}$ is integral operator on the Hilbert space h with the kernel $G_\Sigma^{k_\alpha(\lambda)}(x-y) := \lim_{\varepsilon\to 0} G_\Sigma^{k_\alpha(\lambda+i\varepsilon)}(x-y)$ and $\Theta^{k_\alpha(\lambda)} := -\alpha^{-1}\check{\mathbb{I}} - \mathrm{R}_{\Sigma,\nu\nu}^{k_\alpha(\lambda)}$ are the operators on h with $\mathrm{R}_{\Sigma,\nu\nu}^{k_\alpha(\lambda)}$ being the natural embedding . By a direct computation, the kernel is found to be

$$G_\Sigma^{k_\alpha(\lambda)}(x-y) = K_0(i\sqrt{\lambda}|x-y|) + \mathcal{P}\int_0^\infty \frac{\mu_0(t;x,y)}{t-\lambda-\alpha^2/4}\,\mathrm{d}t + s_\alpha(\lambda)\,\mathrm{e}^{ik_\alpha(\lambda)|x_1-y_1|}\,\mathrm{e}^{-\alpha/2(|x_2|+|y_2|)},$$

where $s_\alpha(\lambda) := i\alpha(2^3 k_\alpha(\lambda))^{-1}$ and

$$\mu_0(t;x,y) := -\frac{i\alpha}{2^5\pi}\,\frac{\mathrm{e}^{it^{1/2}(x_1-y_1)}\,\mathrm{e}^{-(t-\lambda)^{1/2}(|x_2|+|y_2|)^{1/2}}}{t^{1/2}((t-\lambda)^{1/2})}\,.$$

Generalized eigenfunctions, continued

Of course, the pointwise limits $\psi_\lambda = \lim_{\delta\to 0}\psi_\lambda^\delta$ cease to L^2, however, they still belong to L^2 locally and provide us with the generalized eigenfunction of $H_{\alpha,\Gamma}$ in the form

$$\psi_\lambda = \omega_\lambda + \mathrm{R}_{\Sigma,\nu}^{k_\alpha(\lambda)}(\Theta^{k_\alpha(\lambda)})^{-1} J_\Lambda \omega_\lambda\,,$$

where $J_\Lambda\omega_\lambda$ is an embedding of ω_λ to $L^2(\nu_\Lambda)$

Generalized eigenfunctions, continued

Of course, the pointwise limits $\psi_\lambda = \lim_{\delta\to 0} \psi_\lambda^\delta$ cease to L^2, however, they still belong to L^2 locally and provide us with the generalized eigenfunction of $H_{\alpha,\Gamma}$ in the form

$$\psi_\lambda = \omega_\lambda + \mathrm{R}_{\Sigma,\nu}^{k_\alpha(\lambda)} (\Theta^{k_\alpha(\lambda)})^{-1} J_\Lambda \omega_\lambda \,,$$

where $J_\Lambda \omega_\lambda$ is an embedding of ω_λ to $L^2(\nu_\Lambda)$

To find the S-matrix we have to investigate the behavior of ψ_λ for $|x_1| \to \infty$. By a direct computation, we find that for y of a compact $M \subset \mathbb{R}^2$ and $|x_1| \to \infty$ we have

$$G_\Sigma^{k_\alpha(\lambda)}(x-y) \approx s_\alpha(\lambda)\, \mathrm{e}^{ik_\alpha(\lambda)|x_1-y_1|}\, e^{-\alpha/2(|x_2|+|y_2|)}$$

S-matrix at negative energy

Using this asymptotics we find the sought on-shell S-matrix:

Theorem [E-Kondej'05]: For a fixed $\lambda \in (-\frac{1}{4}\alpha^2, 0)$ the generalized eigenfunctions behave asymptotically as

$$\psi_\lambda(x) \approx \begin{cases} \mathcal{T}(\lambda)\, \mathrm{e}^{ik_\alpha(\lambda)x_1}\, \mathrm{e}^{-\alpha|x_2|/2} & \text{for} \quad x_1 \to \infty \\ \mathrm{e}^{ik_\alpha(\lambda)x_1} \mathrm{e}^{-\alpha|x_2|/2} + \mathcal{R}(\lambda)\, \mathrm{e}^{-ik_\alpha(\lambda)x_1} \mathrm{e}^{-\alpha|x_2|/2} & \text{for} \quad x_1 \to -\infty \end{cases}$$

where $k_\alpha(\lambda) := (\lambda + \alpha^2/4)^{1/2}$ and the *transmission and reflection amplitudes* $\mathcal{T}(\lambda)\,, \mathcal{R}(\lambda)$ are given respectively by

$$\mathcal{T}(\lambda) = 1 - s_\alpha(\lambda) \left((\Theta^{k_\alpha(\lambda)})^{-1} J_\Lambda \omega_\lambda, J_\Lambda \omega_\lambda \right)_{\mathrm{h}}$$

and

$$\mathcal{R}(\lambda) = s_\alpha(\lambda) \left((\Theta^{k_\alpha(\lambda)})^{-1} J_\Lambda \omega_\lambda, J_\Lambda \bar{\omega}_\lambda \right)_{\mathrm{h}}$$

Strong coupling: a conjecture

Consider Γ which is a C^4-*smooth* local deformation of a line. In analogy with the spectral result of [E-Yoshitomi'01] quoted above one expects that in *strong coupling* case the scattering will be determined in the leading order by the *local geometry* of Γ through the same comparison operator, namely $K_\Gamma := -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}\gamma(s)^2$ on $L^2(\mathbb{R})$.

Strong coupling: a conjecture

Consider Γ which is a C^4-*smooth* local deformation of a line. In analogy with the spectral result of [E-Yoshitomi'01] quoted above one expects that in *strong coupling* case the scattering will be determined in the leading order by the *local geometry* of Γ through the same comparison operator, namely $K_\Gamma := -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}\gamma(s)^2$ on $L^2(\mathbb{R})$.

Let $\mathcal{T}_K(k)$, $\mathcal{R}_K(k)$ be the corresponding transmission and reflection amplitudes at a fixed momentum k. Denote by $\mathbf{S}_{\Gamma,\alpha}(\lambda)$ and $\mathbf{S}_K(\lambda)$ the on-shell $S-$matrixes of $H_{\alpha,\Gamma}$ and K at energy λ, respectively.

Conjecture: For a fixed $k \neq 0$ and $\alpha \to \infty$ we have the relation

$$\mathbf{S}_{\Gamma,\alpha}\left(k^2 - \frac{1}{4}\alpha^2\right) \to \mathbf{S}_K(k^2)$$

How can one find the spectrum?

The above general results do not tell us how to find the spectrum for a particular Γ. There are various possibilities:

- *Direct solution* of the PDE problem $H_{\alpha,\Gamma}\psi = \lambda\psi$ is feasible in a few simple examples only

How can one find the spectrum?

The above general results do not tell us how to find the spectrum for a particular Γ. There are various possibilities:

- *Direct solution* of the PDE problem $H_{\alpha,\Gamma}\psi = \lambda\psi$ is feasible in a few simple examples only
- Using trace maps of $R^k \equiv (-\Delta - k^2)^{-1}$ and the *generalized BS principle*

$$R^k := R_0^k + \alpha R_{\mathrm{d}x,m}^k [I - \alpha R_{m,m}^k]^{-1} R_{m,\mathrm{d}x}^k \,,$$

where m is δ measure on Γ, we pass to a 1D integral operator problem, $\alpha R_{m,m}^k \psi = \psi$

How can one find the spectrum?

The above general results do not tell us how to find the spectrum for a particular Γ. There are various possibilities:

- *Direct solution* of the PDE problem $H_{\alpha,\Gamma}\psi = \lambda\psi$ is feasible in a few simple examples only
- Using trace maps of $R^k \equiv (-\Delta - k^2)^{-1}$ and the *generalized BS principle*

$$R^k := R_0^k + \alpha R_{\mathrm{d}x,m}^k [I - \alpha R_{m,m}^k]^{-1} R_{m,\mathrm{d}x}^k \,,$$

  where m is δ measure on Γ, we pass to a 1D integral operator problem, $\alpha R_{m,m}^k \psi = \psi$
- *discretization* of the latter which amounts to a point-interaction approximations to $H_{\alpha,\Gamma}$

2D point interactions

Such an interaction at the point a with the "coupling constant" α is defined by b.c. which change *locally* the domain of $-\Delta$: the functions behave as

$$\psi(x) = -\frac{1}{2\pi} \log|x-a|\, L_0(\psi,a) + L_1(\psi,a) + \mathcal{O}(|x-a|)\,,$$

where the generalized b.v. $L_0(\psi,a)$ and $L_1(\psi,a)$ satisfy

$$L_1(\psi,a) + 2\pi\alpha L_0(\psi,a) = 0\,, \qquad \alpha \in \mathbb{R}$$

2D point interactions

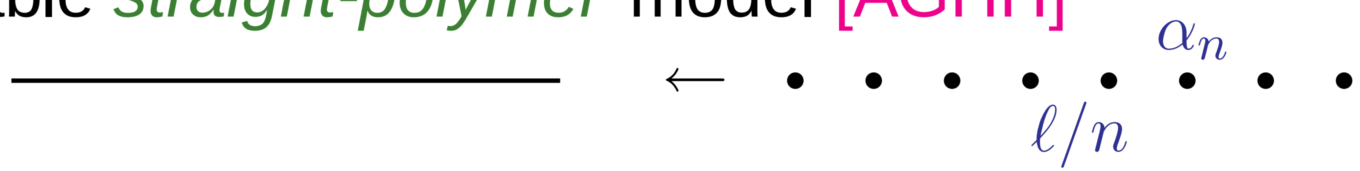
Such an interaction at the point a with the "coupling constant" α is defined by b.c. which change *locally* the domain of $-\Delta$: the functions behave as

$$\psi(x) = -\frac{1}{2\pi} \log|x-a|\, L_0(\psi,a) + L_1(\psi,a) + \mathcal{O}(|x-a|)\,,$$

where the generalized b.v. $L_0(\psi,a)$ and $L_1(\psi,a)$ satisfy

$$L_1(\psi,a) + 2\pi\alpha L_0(\psi,a) = 0\,, \qquad \alpha \in \mathbb{R}$$

For our purpose, the coupling should depend on the set Y approximating Γ. To see how compare a line Γ with the solvable *straight-polymer* model [AGHH]



2D point-interaction approximation

Spectral threshold convergence requires $\alpha_n = \alpha n$ which means that individual point interactions get *weaker*. Hence we approximate $H_{\alpha,\Gamma}$ by point-interaction Hamiltonians H_{α_n,Y_n} with $\alpha_n = \alpha|Y_n|$, where $|Y_n| := \sharp Y_n$.

2D point-interaction approximation

Spectral threshold convergence requires $\alpha_n = \alpha n$ which means that individual point interactions get *weaker*. Hence we approximate $H_{\alpha,\Gamma}$ by point-interaction Hamiltonians H_{α_n,Y_n} with $\alpha_n = \alpha|Y_n|$, where $|Y_n| := \sharp Y_n$.

Theorem [E-Němcová'03]: Let a family $\{Y_n\}$ of finite sets $Y_n \subset \Gamma \subset \mathbb{R}^2$ be such that

$$\frac{1}{|Y_n|} \sum_{y \in Y_n} f(y) \;\to\; \int_\Gamma f \, \mathrm{d}m$$

holds for any bounded continuous function $f : \Gamma \to \mathbb{C}$, *together with technical conditions*, then $H_{\alpha_n,Y_n} \to H_{\alpha,\Gamma}$ in the strong resolvent sense as $n \to \infty$.

Comments on the approximation

- A more general result is valid: Γ need not be a graph and the coupling may be non-constant; also a magnetic field can be added [Ožanová'06] *(=Němcová)*

Comments on the approximation

- A more general result is valid: Γ need not be a graph and the coupling may be non-constant; also a magnetic field can be added [Ožanová'06] *(=Němcová)*
- The result applies to finite graphs, however, an infinite Γ can be approximated in strong resolvent sense by a *family of cut-off graphs*

Comments on the approximation

- A more general result is valid: Γ need not be a graph and the coupling may be non-constant; also a magnetic field can be added [Ožanová'06] *(=Němcová)*
- The result applies to finite graphs, however, an infinite Γ can be approximated in strong resolvent sense by a *family of cut-off graphs*
- The idea is due to [Brasche-Figari-Teta'98], who analyzed point-interaction approximations of measure perturbations with $\operatorname{codim} \Gamma = 1$ in $\mathbb{R}^3$. There are differences, however, for instance in the 2D case we can approximate *attractive* interactions only

Comments on the approximation

- A more general result is valid: Γ need not be a graph and the coupling may be non-constant; also a magnetic field can be added [Ožanová'06] *(=Němcová)*
- The result applies to finite graphs, however, an infinite Γ can be approximated in strong resolvent sense by a *family of cut-off graphs*
- The idea is due to [Brasche-Figari-Teta'98], who analyzed point-interaction approximations of measure perturbations with $\operatorname{codim}\Gamma = 1$ in $\mathbb{R}^3$. There are differences, however, for instance in the 2D case we can approximate *attractive* interactions only
- *A uniform resolvent convergence* can be achieved in this scheme if the term $-\varepsilon^2\Delta^2$ is added to the Hamiltonian [Brasche-Ožanová'06]

Scheme of the proof

Resolvent of H_{α_n,Y_n} is given *Krein's formula*. Given $k^2 \in \rho(H_{\alpha_n,Y_n})$ define $|Y_n| \times |Y_n|$ matrix by

$$\Lambda_{\alpha_n,Y_n}(k^2;x,y) = \frac{1}{2\pi}\left[2\pi|Y_n|\alpha + \ln\left(\frac{ik}{2}\right) + \gamma_E\right]\delta_{xy} - G_k(x-y)\,(1-\delta_{xy})$$

for $x, y \in Y_n$, where γ_E is *Euler' constant*.

Scheme of the proof

Resolvent of H_{α_n,Y_n} is given *Krein's formula*. Given $k^2 \in \rho(H_{\alpha_n,Y_n})$ define $|Y_n| \times |Y_n|$ matrix by

$$\Lambda_{\alpha_n,Y_n}(k^2;x,y) = \frac{1}{2\pi}\left[2\pi|Y_n|\alpha + \ln\left(\frac{ik}{2}\right) + \gamma_E\right]\delta_{xy} - G_k(x-y)\,(1-\delta_{xy})$$

for $x,y \in Y_n$, where γ_E is *Euler' constant*. Then

$$(H_{\alpha_n,Y_n} - k^2)^{-1}(x,y) = G_k(x-y) + \sum_{x',y' \in Y_n} \left[\Lambda_{\alpha_n,Y_n}(k^2)\right]^{-1}(x',y')G_k(x-x')\,G_k(y-y')$$

Scheme of the proof

Resolvent of $H_{\alpha,\Gamma}$ is given by the *generalized BS formula* given above; one has to check directly that the difference of the two vanishes as $n \to \infty$ $\square$

Scheme of the proof

Resolvent of $H_{\alpha,\Gamma}$ is given by the *generalized BS formula* given above; one has to check directly that the difference of the two vanishes as $n \to \infty$ $\square$

Remarks:

- Spectral condition in the n-th approximation, i.e. $\det \Lambda_{\alpha_n,Y_n}(k^2) = 0$, is a discretization of the integral equation coming from the generalized BS principle
- A solution to $\Lambda_{\alpha_n,Y_n}(k^2)\eta = 0$ determines the approximating ef by $\psi(x) = \sum_{y_j \in Y_n} \eta_j G_k(x - y_j)$
- A *match with solvable models* illustrates the convergence and shows that it is *not fast,* slower than n^{-1} in the eigenvalues. This comes from singular “spikes” in the approximating functions

Something more on resonances

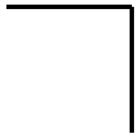
Consider infinite curves Γ, straight outside a compact, and ask for examples of resonances. Recall the L^2-approach: in 1D potential scattering one explores *spectral properties* of the problem cut to a finite length L. It is time-honored trick that scattering resonances are manifested as avoided crossings in L dependence of the spectrum – for a recent proof see [Hagedorn-Meller'00]. Try the same here:

Something more on resonances

Consider infinite curves Γ, straight outside a compact, and ask for examples of resonances. Recall the L^2-approach: in 1D potential scattering one explores *spectral properties* of the problem cut to a finite length L. It is time-honored trick that scattering resonances are manifested as avoided crossings in L dependence of the spectrum – for a recent proof see [Hagedorn-Meller'00]. Try the same here:

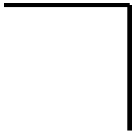
- *Broken line:* absence of "intrinsic" resonances due lack of higher transverse thresholds
- *Z-shaped Γ:* if a single bend has a significant reflection, a double band should exhibit resonances
- *Bottleneck curve:* a good candidate to demonstrate tunneling resonances

Broken line

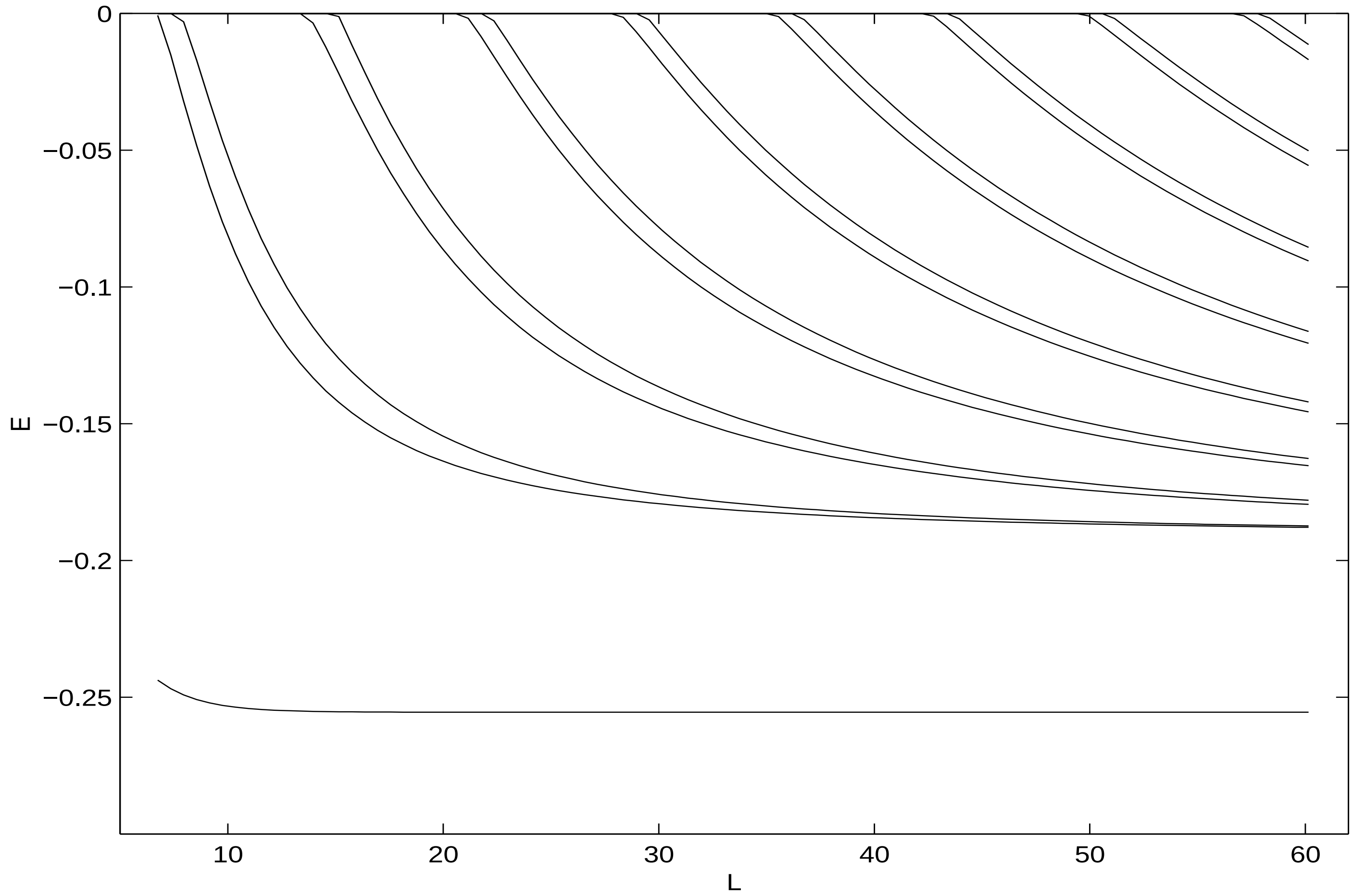


$\alpha = 1$

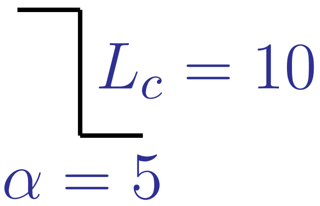
Broken line



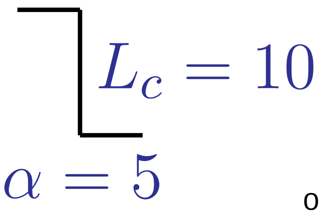
$\alpha = 1$

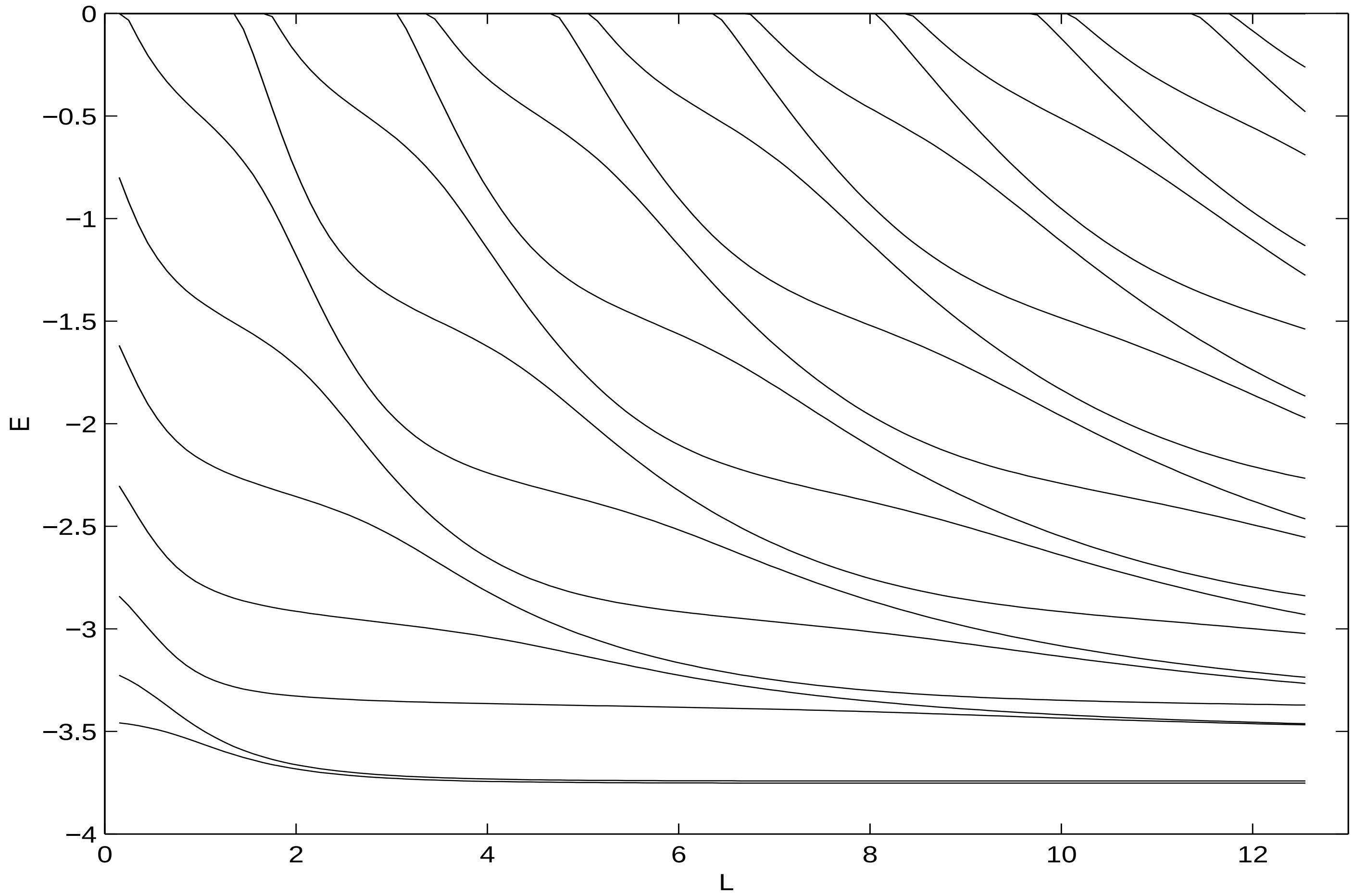


Z shape with $\theta = \frac{\pi}{2}$

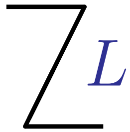


Z shape with $\theta = \frac{\pi}{2}$





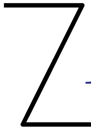
Z shape with $\theta = 0.32\pi$



$L_c = 10$

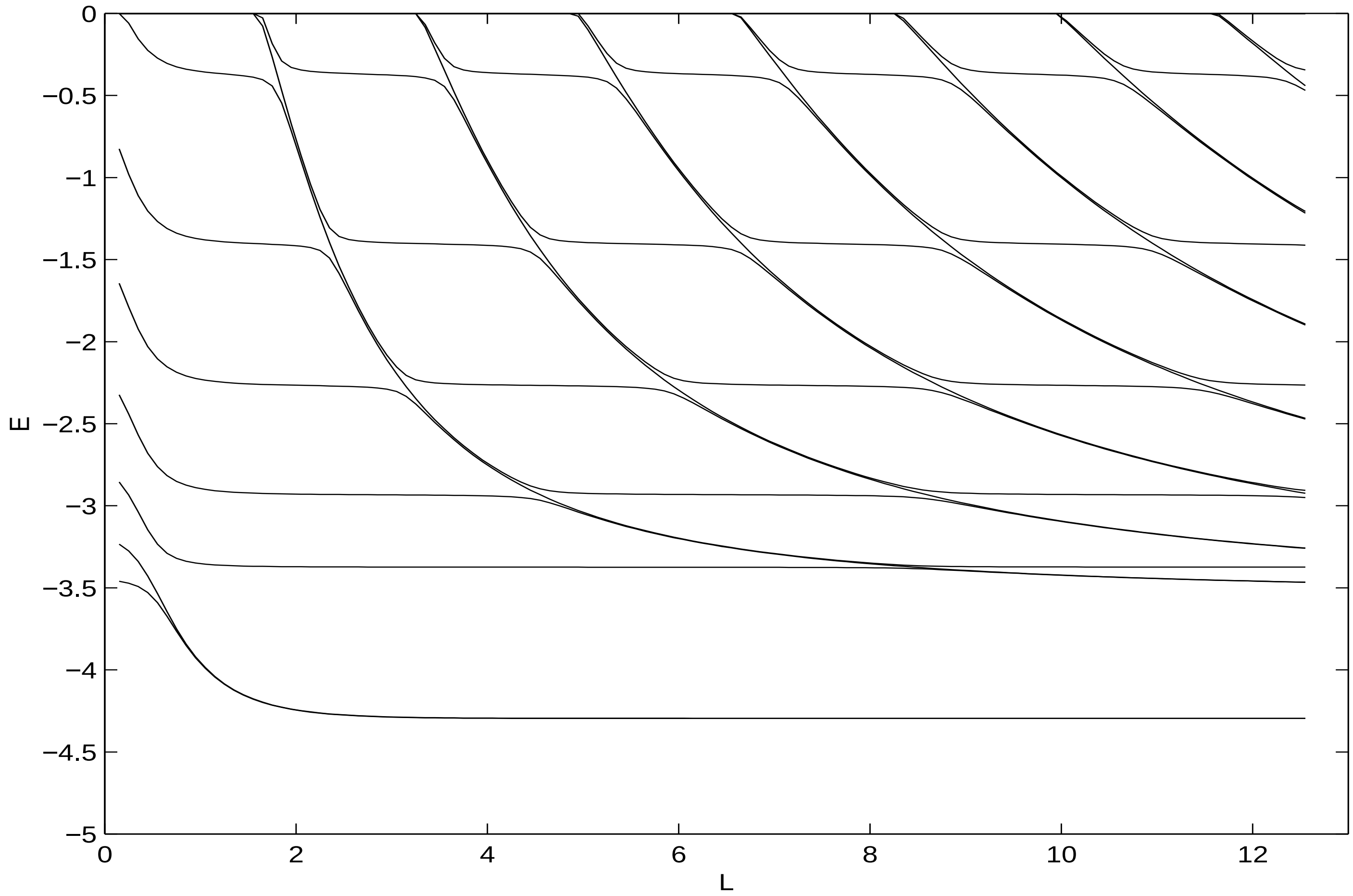
$\alpha = 5$

Z shape with $\theta = 0.32\pi$



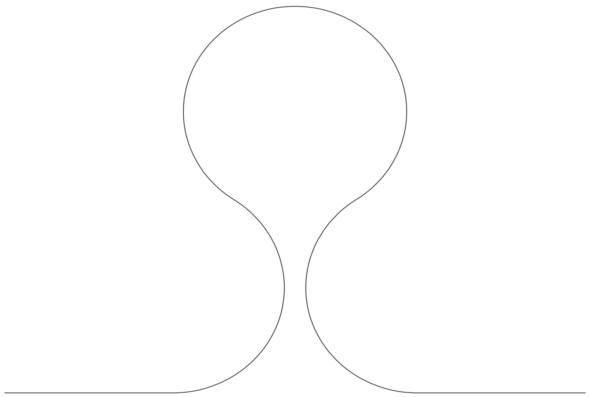
$L_c = 10$

$\alpha = 5$



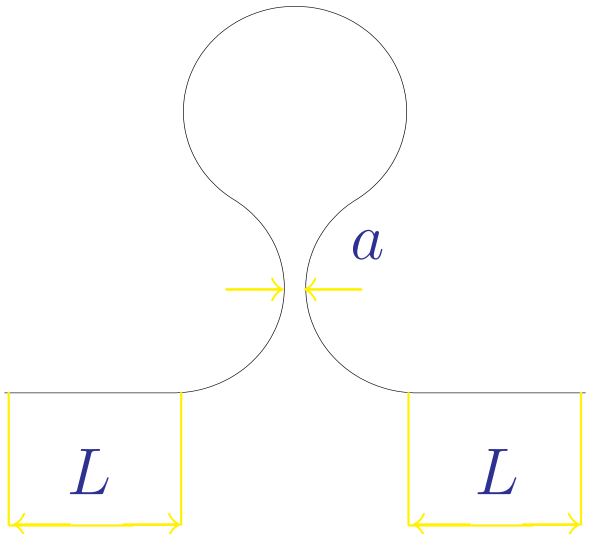
A bottleneck curve

Consider a straight line deformation which shaped as an open loop with a bottleneck the width a of which we will vary



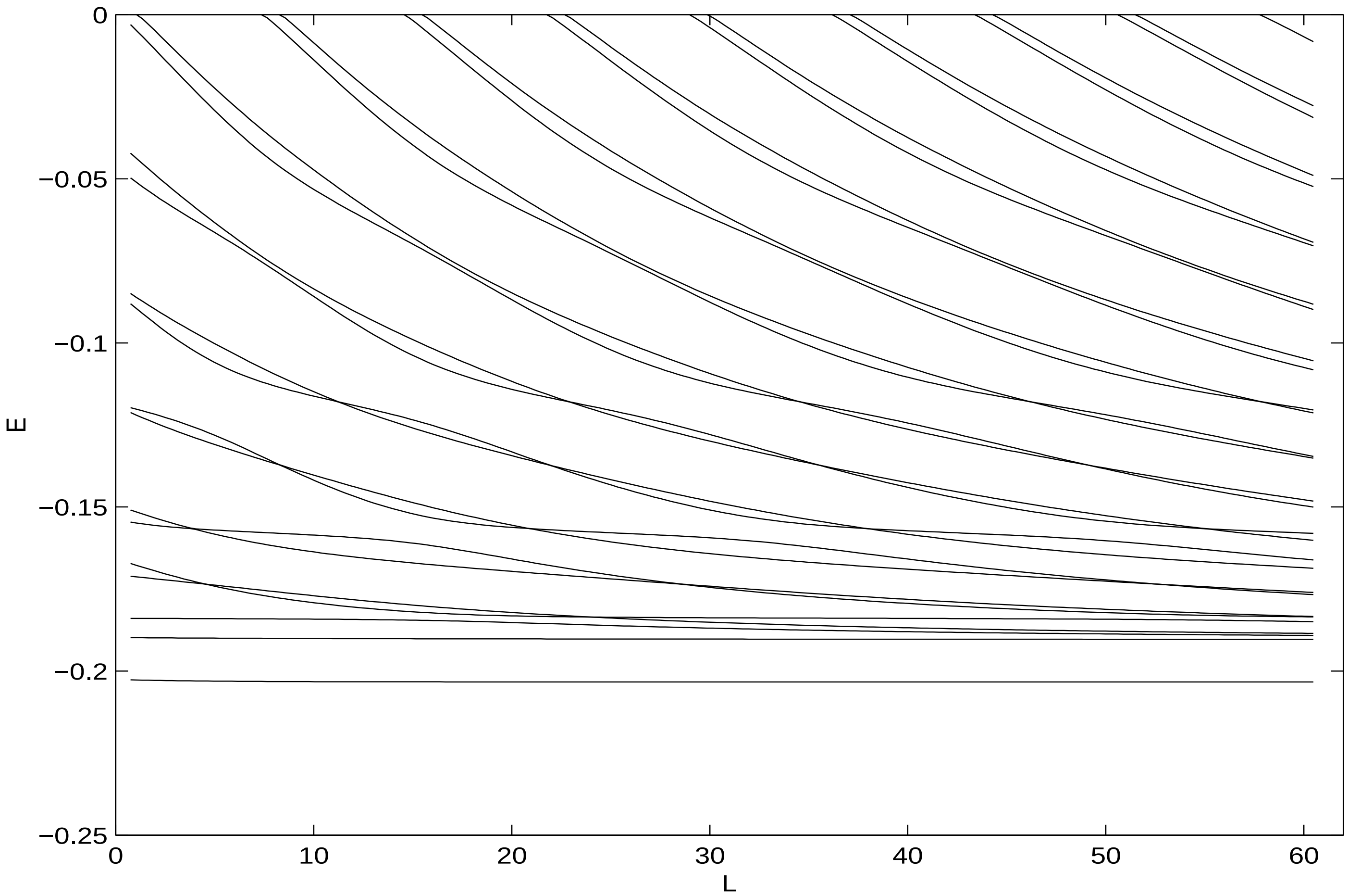
A bottleneck curve

Consider a straight line deformation which shaped as an open loop with a bottleneck the width a of which we will vary

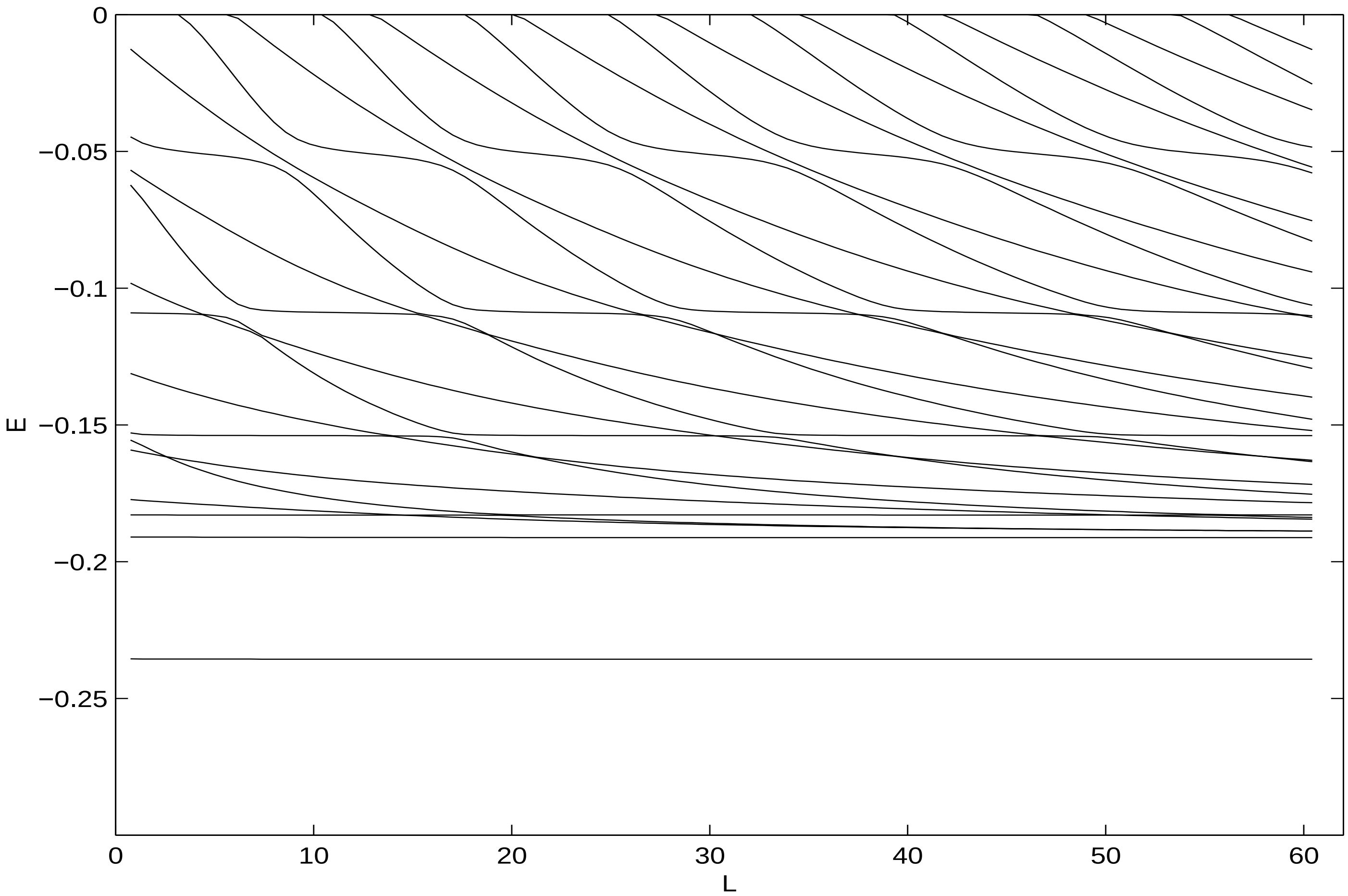


If Γ is a straight line, the transverse eigenfunction is $\mathrm{e}^{-\alpha|y|/2}$, hence the distance at which tunneling becomes significant is $\approx 4\alpha^{-1}$. In the example, we choose $\alpha = 1$

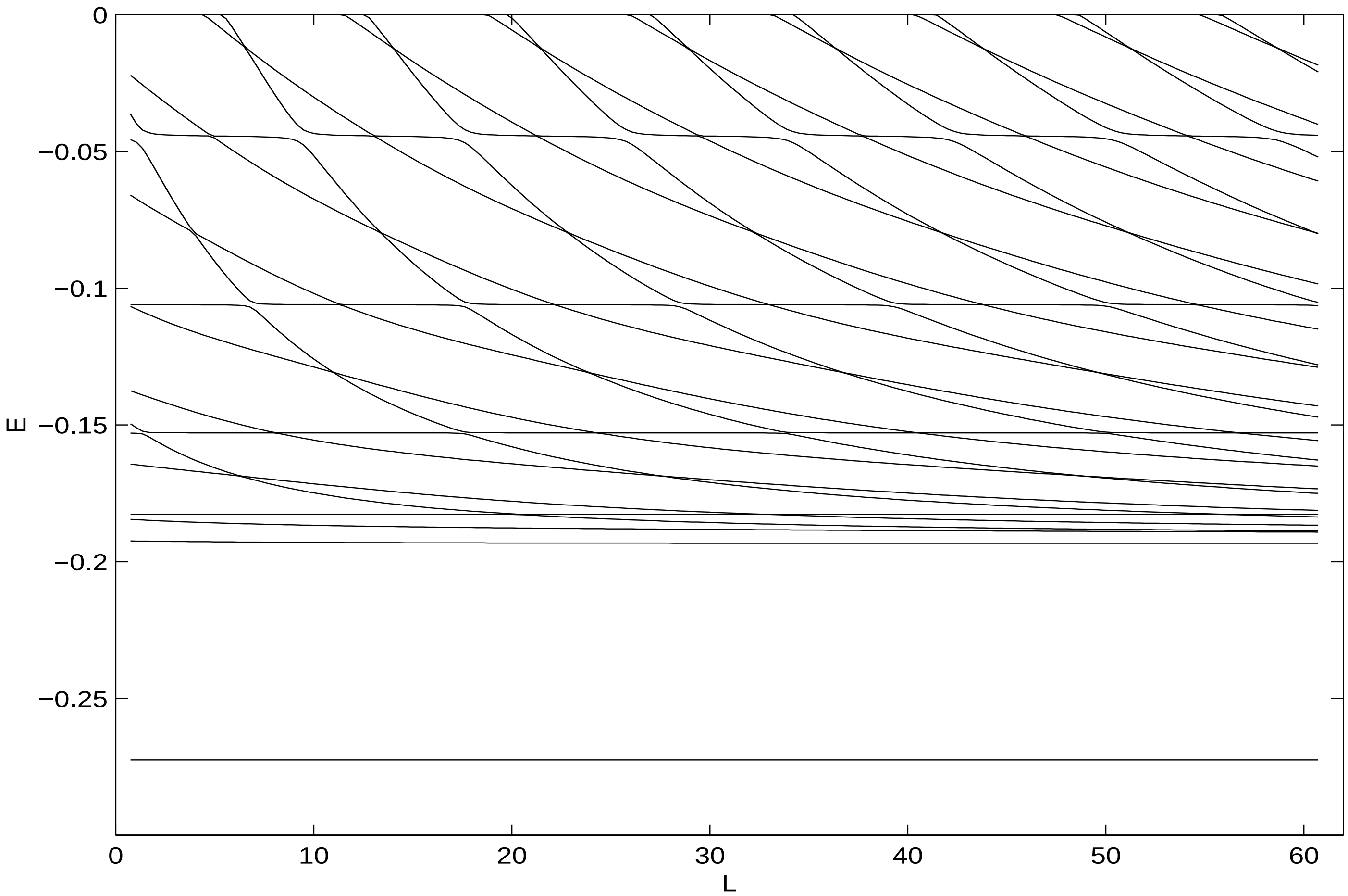
Bottleneck with $a = 5.2$



Bottleneck with $a = 2.9$



Bottleneck with $a = 1.9$



Some references

[AGHH'05] S. Albeverio, F. Gesztesy, R. Høegh-Krohn, H. Holden, *Solvable Models in Quantum Mechanics*, 2nd edition, AMS Chelsea, Providence, RI, 2005

[BFT'98] J.F. Brasche, R. Figari, A. Teta: Singular Schrödinger operators as limits of point interaction Hamiltonians, *Potential Anal.* **8** (1998), 163-178

[BO'06] J.F. Brasche, K. Ožanová: Convergence of Schrödinger operators, `math-ph/0511029`

[BT'92] J.F. Brasche, A. Teta: Spectral analysis and scattering theory for Schrödinger operators with an interaction supported by a regular curve, in *Ideas and Methods in Quantum and Statistical Physics*, ed. S. Albeverio, et al., CUP 1992, pp. 197-211

[EK'05] P.E., S. Kondej: Scattering by local deformations of a straight leaky wire, *J. Phys.* **A38** (2005), 4865-4874

[EN'03] P.E., K. Němcová: Leaky quantum graphs: approximations by point interaction Hamiltonians, *J. Phys.* **A36** (2003), 10173-10193

[HM'00] G.A. Hagedorn, B. Meller: Resonances in a box, *J. Math. Phys.* **41** (2000), 103-117

[Ož'06] K. Ožanová: Approximation by point potentials in a magnetic field , *J. Phys.* **A39** (2006), 3071-3083

Summarizing Lecture V

- *"Leaky" graphs* are a more realistic model of graph-like nanostructures because they take quantum tunneling into account

Summarizing Lecture V

- *"Leaky" graphs* are a more realistic model of graph-like nanostructures because they take quantum tunneling into account
- *Geometry plays essential role* in determining spectral and scattering properties of such systems

Summarizing Lecture V

- *"Leaky" graphs* are a more realistic model of graph-like nanostructures because they take quantum tunneling into account
- *Geometry plays essential role* in determining spectral and scattering properties of such systems
- There are *efficient numerical methods* to determine spectra of leaky graphs

Summarizing Lecture V

- *"Leaky" graphs* are a more realistic model of graph-like nanostructures because they take quantum tunneling into account
- *Geometry plays essential role* in determining spectral and scattering properties of such systems
- There are *efficient numerical methods* to determine spectra of leaky graphs
- *Rigorous results* on spectra and scattering are available so far in simple situations only

Summarizing Lecture V

- *"Leaky" graphs* are a more realistic model of graph-like nanostructures because they take quantum tunneling into account
- *Geometry plays essential role* in determining spectral and scattering properties of such systems
- There are *efficient numerical methods* to determine spectra of leaky graphs
- *Rigorous results* on spectra and scattering are available so far in simple situations only
- The theory described in the lecture is far from complete, various *open questions* persist

Summarizing the course

- Quantum graphs and various generalizations of them offer a *wide variety of solvable models*

Summarizing the course

- Quantum graphs and various generalizations of them offer a *wide variety of solvable models*
- They describe numerous systems *of physical importance*, both of quantum and classical nature

Summarizing the course

- Quantum graphs and various generalizations of them offer a *wide variety of solvable models*
- They describe numerous systems *of physical importance*, both of quantum and classical nature
- The field offers many *open questions*, some of them difficult, presenting thus a challenge for ambitious young people