

Lectures on quantum graphs, ideal, leaky, and generalized

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Course overview

The aim to review some recent results in the theory of quantum graphs, standard as well as non-standard

- *Lecture I*

Ideal graphs – their nontrivial aspect, or what is the meaning of the vertex coupling



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- *Lecture III*
Generalized graphs – or what happens if a quantum particle has to change its dimension



Quantum graphs

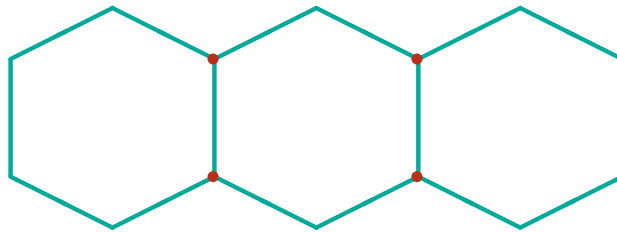
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Using “textbook” graphs such as



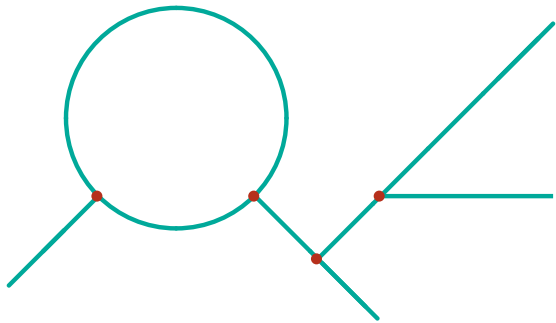
with “Kirchhoff” b.c. in combination with Pauli principle, they reproduced the actual spectra with a $\lesssim 10\%$ accuracy

A caveat: later naive generalizations were less successful

Ideal quantum graph concept

The beauty of theoretical physics resides in permanent oscillation between physical anchoring in reality and mathematical freedom of creating concepts

As a mathematically minded person you can imagine quantum particles confined to a graph of *arbitrary shape*



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

and, lo and behold, this turns out to be a *practically important* concept – after experimentalists learned in the last 15-20 years to fabricate tiny graph-like structure for which this is a good model



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- Moreover, from the stationary point of view a quantum graph is also equivalent to a *microwave network* built of optical cables – see [Hul et al.'04]
- In addition to graphs one can consider *generalized graphs* which consist of components of different dimensions, modelling things as different as combinations of nanotubes with fullerenes, scanning tunneling microscopy, etc. – we will do that in *Lecture III*



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- Graphs can support also *Dirac operators*, see e.g. [Bulla-Trenckler'90], although this remains so far a theoretical possibility only.

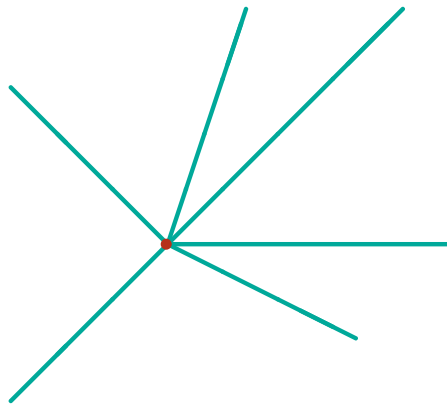


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- Graphs can support also *Dirac operators*, see e.g. [Bulla-Trenckler'90], although this remains so far a theoretical possibility only.
- The graph literature is extensive; let us refer just to a review [Kuchment'04] and other references in the recent topical issue of “*Waves in Random Media*”



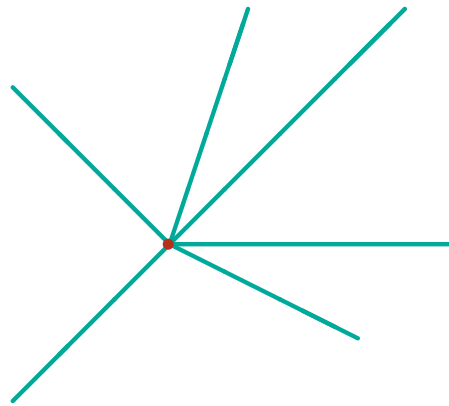
Wavefunction coupling at vertices



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 $\psi_j \mapsto -\psi_j''$



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

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

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

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



Unique boundary conditions

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

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

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One can derive them modifying the argument used in [Fülöp-Tsutsui'00] for generalized point interactions, $n = 2$. Self-adjointness requires vanishing of the boundary form,

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

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



Remarks

- The length parameter is not important because matrices corresponding to two different values are related by

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

The choice $\ell = 1$ just fixes the length scale



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- The unique b.c. help to simplify the analysis done in [\[Kostykin-Schrader'99\]](#), [\[Kuchment'04\]](#) and other previous work. It concerns, for instance, the null spaces of the matrices A, B
- or the *on-shell scattering matrix* for a star graph of n halflines with the considered coupling which equals

$$S_U(k) = \frac{(k - 1)I + (k + 1)U}{(k + 1)I + (k - 1)U}$$



Examples of vertex coupling

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

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

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

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

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



Further examples

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

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

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



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- 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.

$$(u - 1)(\psi_j(0) - \psi_k(0)) + i(u - 1)(\psi'_j(0) - \psi'_k(0)) = 0$$

$$(u - 1 + nv) \sum_{k=1}^n \psi_k(0) + i(u - 1 + nv) \sum_{k=1}^n \psi'_k(0) = 0$$



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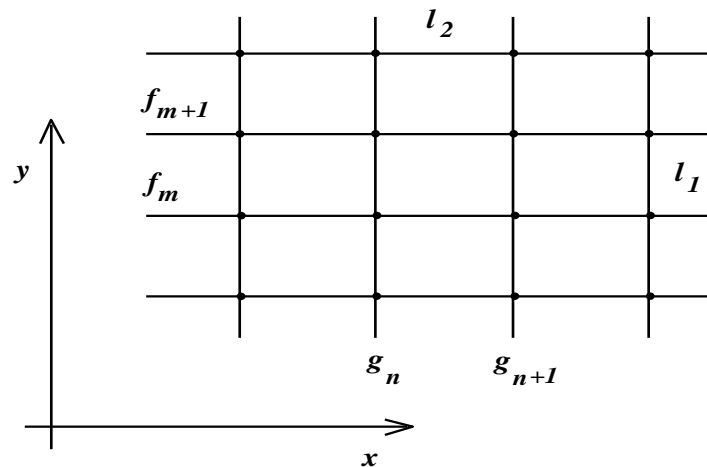
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- Recall also that in a rectangular lattice with δ coupling of nonzero α spectrum depends on *number theoretic properties* of model parameters [E.'95]



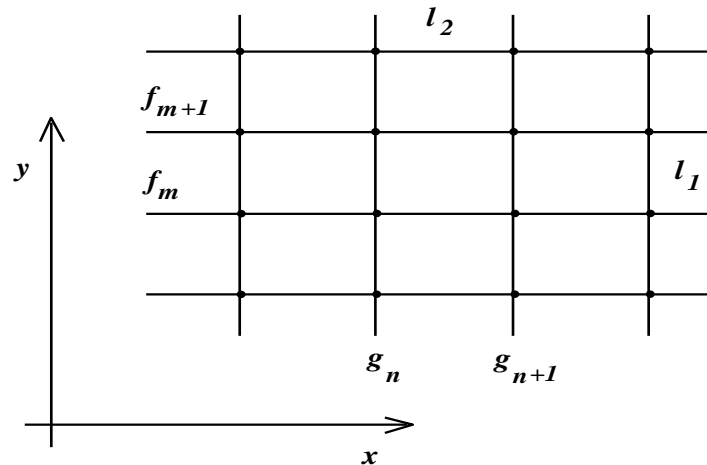
More on the lattice example

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



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Spectral condition for quasimomentum (θ_1, θ_2) reads

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



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 $\limsup_j a_j < \infty$
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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 $|\alpha|L > \frac{\pi^2}{\sqrt{5}}$



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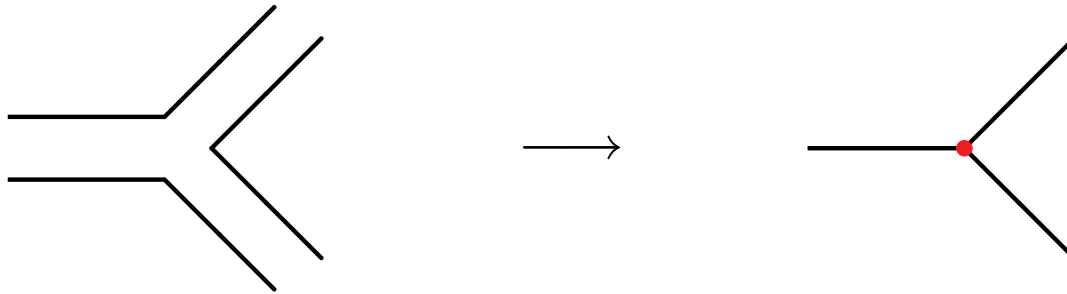
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This all illustrates why it is desirable to *understand vertex couplings*. This will be our main task in *Lecture I*



A head-on approach

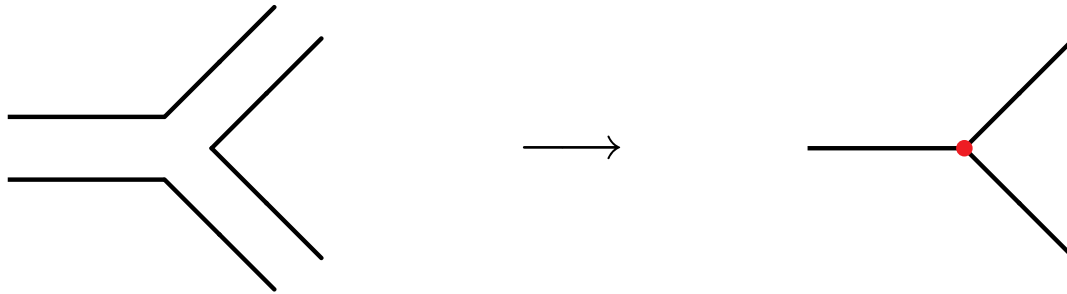
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Unfortunately, it is not so simple as it looks because

- after a long effort the *Neumann-like case* was solved [Kuchment-Zeng'01], [Rubinstein-Schatzmann'01], [Saito'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'06]?, but the full understanding has not yet been achieved here



Recall 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

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

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The form $u \mapsto \|u'\|_{M_0}^2 := \sum_{j \in J} \|u'\|_{I_j}^2$ 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 dX equal to $(\det g)^{1/2} dx$ in a fixed chart. For $u \in C_{\text{comp}}^\infty(X)$ we set

$$q_X(u) := \|du\|_X^2 = \int_X |du|^2 dX, \quad |du|^2 = \sum_{i,j} g^{ij} \partial_i u \partial_j \bar{u}$$

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

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



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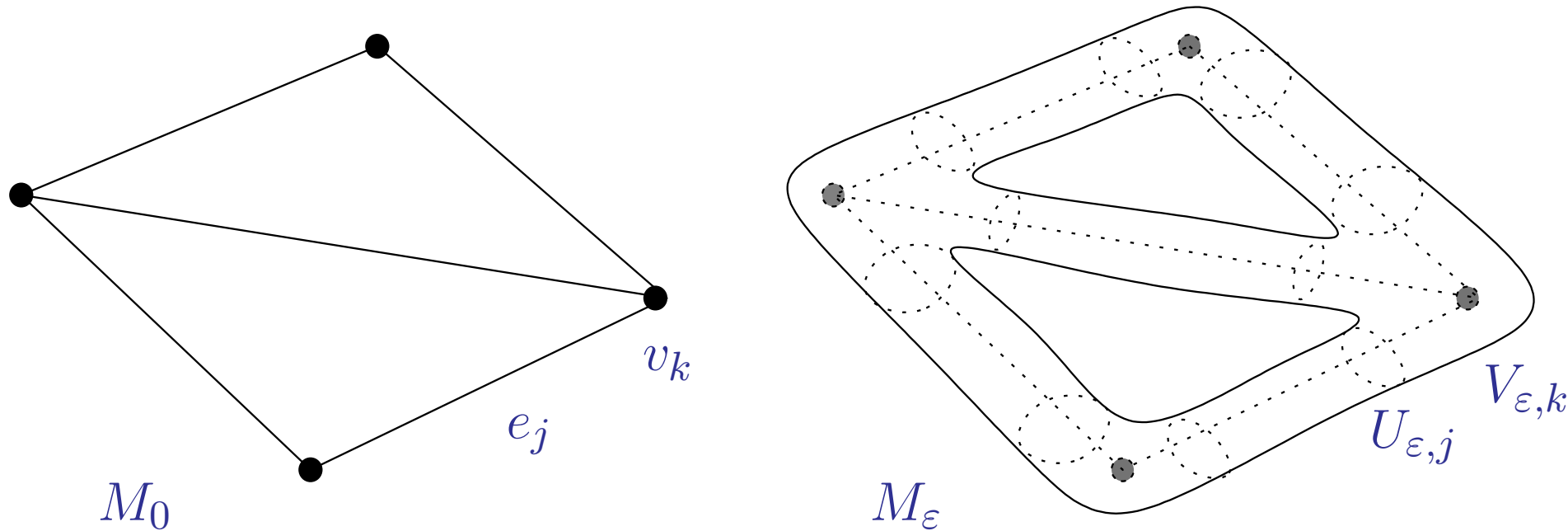
$$-\Delta_X u = -(\det g)^{-1/2} \sum_{i,j} \partial_i ((\det g)^{1/2} g^{ij} \partial_j u)$$

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



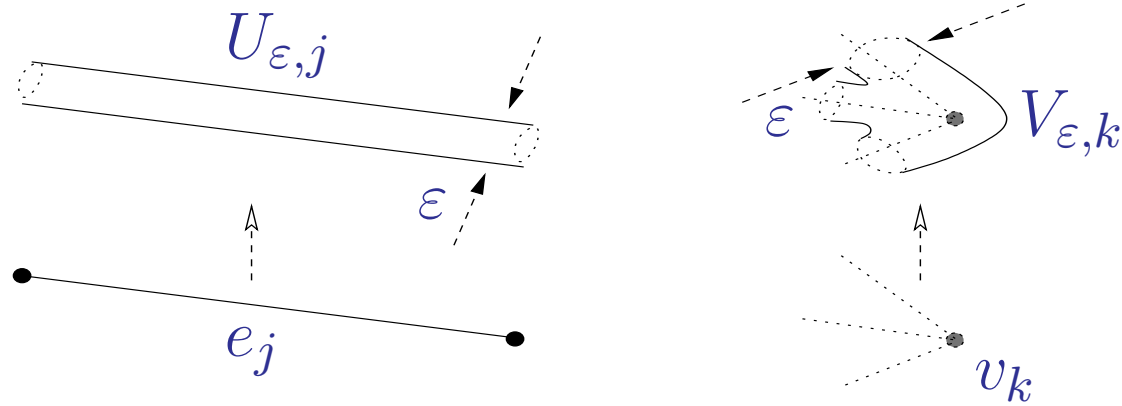
Fat graphs and sleeves: manifolds

We associate with the graph M_0 a family of manifolds M_ε

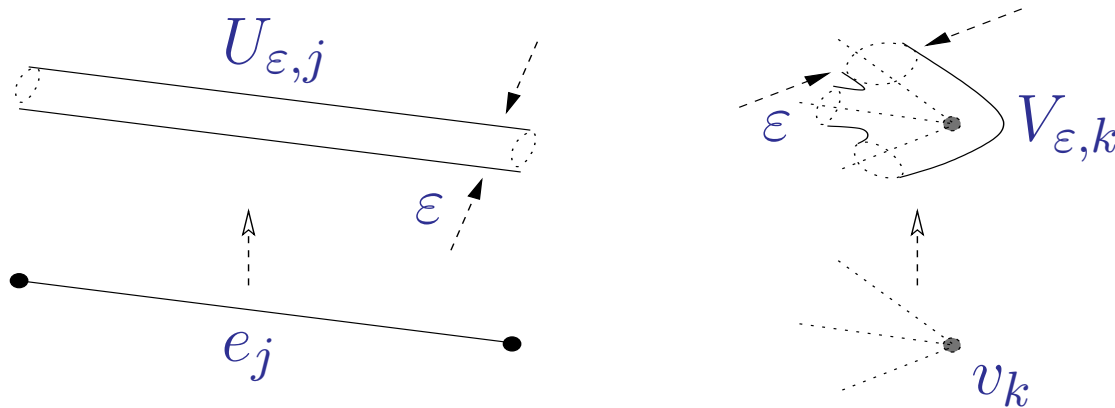


We suppose that M_ε is a union of compact edge and vertex components $U_{\varepsilon,j}$ and $V_{\varepsilon,k}$ such that their interiors are mutually disjoint for all possible $j \in J$ and $k \in K$

Manifold building blocks



Manifold building blocks



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

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

- for edge regions we assume that $U_{\epsilon,j}$ 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 $V_{\epsilon,k}$ is diffeomorphic to an ϵ -independent manifold V_k



Comparison of eigenvalues

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 $\|u\|_{Q,n}^2 := \|u\|^2 + \|Q^{n/2}u\|^2$.



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

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

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 $\delta_1, \delta_2 \rightarrow 0$, such that

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



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 $\text{vol } F = 1$. We define another metric \tilde{g}_ε on $U_{\varepsilon,j}$ by

$$\tilde{g}_\varepsilon := dx^2 + \varepsilon^2 h(y);$$

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}_ε) using product metric g_ε on the edges



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The sought result now looks as follows.

Theorem [E.-Post'05]: Under the stated assumptions
 $\lambda_k(M_\varepsilon) \rightarrow \lambda_k(M_0)$ as $\varepsilon \rightarrow 0$ (giving thus free b.c.!).



Sketch of the proof

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

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

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

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

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

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

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

$$N_j u(x) := \int_F u(x, \cdot) dF, \quad C_k u := \frac{1}{\text{vol } V_k} \int_{V_k} u dV_k$$

to build the comparison map by *interpolation*:

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

with a smooth ρ interpolating between zero and one



More general b.c.? Recall RS argument

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

$$\lambda \int_{V_\varepsilon} \phi \bar{u} \, dV_\varepsilon = \int_{V_\varepsilon} \langle d\phi, du \rangle \, dV_\varepsilon + \int_{\partial V_\varepsilon} \partial_n \phi \bar{u} \, d\partial V_\varepsilon$$

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



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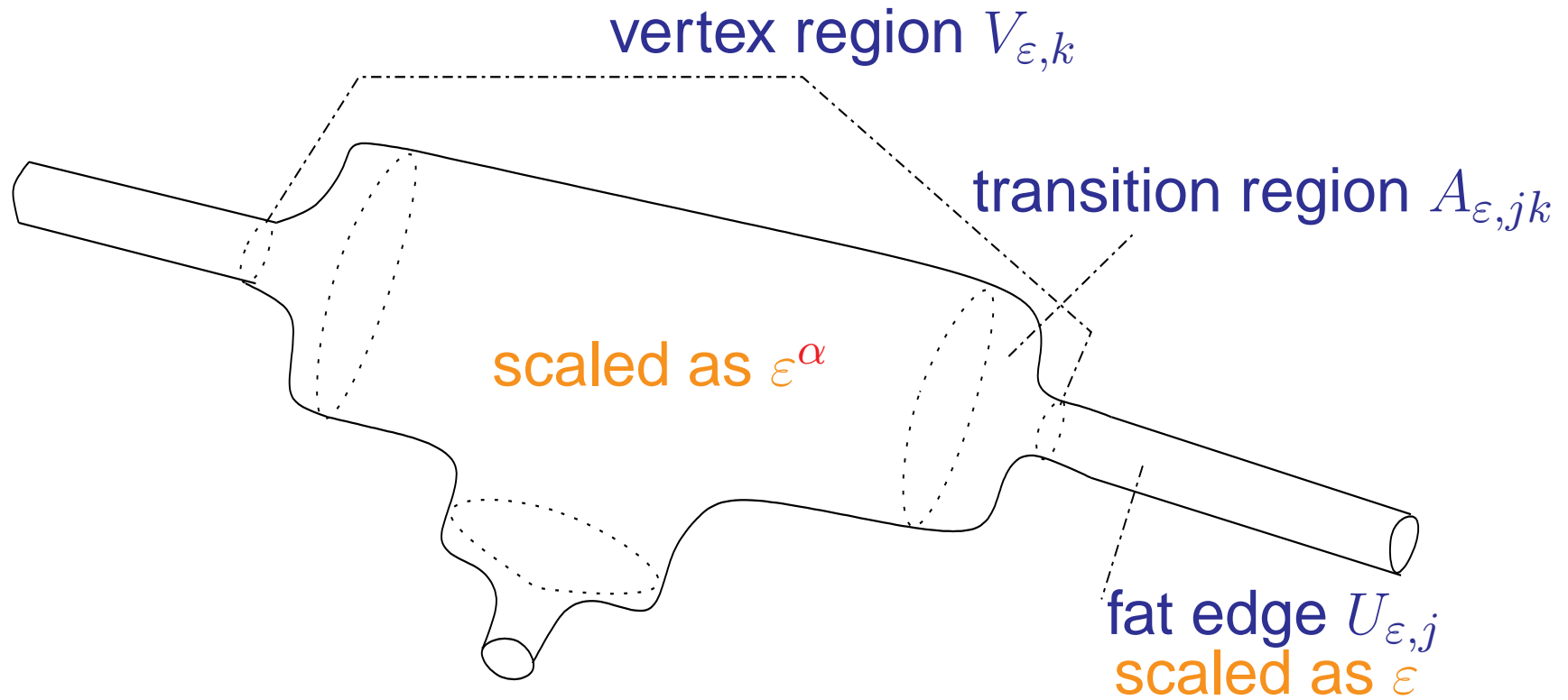
A way out could thus be to use *different* scaling rates of edges and vertices. Of a particular interest is the borderline case, $\text{vol}_d V_\varepsilon \approx \text{vol}_{d-1} \partial V_\varepsilon$, when the integral of $\langle d\phi, du \rangle$ is expected to be negligible and we hope to obtain

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



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

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

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

- 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 $q_0(u) := \sum_j \|u'_j\|_{I_j}^2$, 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 $(\text{vol}(V_k^-))^{1/2} u_j(v_k) = u_k$



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- 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*



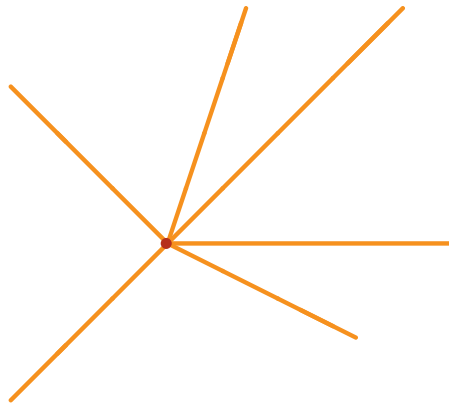
Potential approximation

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



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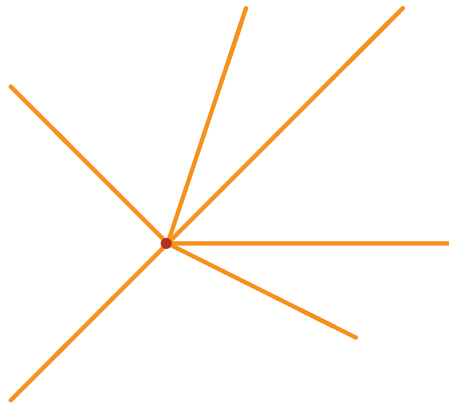
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We make the following assumptions:

- $V_j \in L^1_{\text{loc}}(\mathbb{R}_+)$, $j = 1, \dots, n$
- 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,

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

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

as $\varepsilon \rightarrow 0+$ in the norm resolvent sense, with the parameter

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



More singular couplings

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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*

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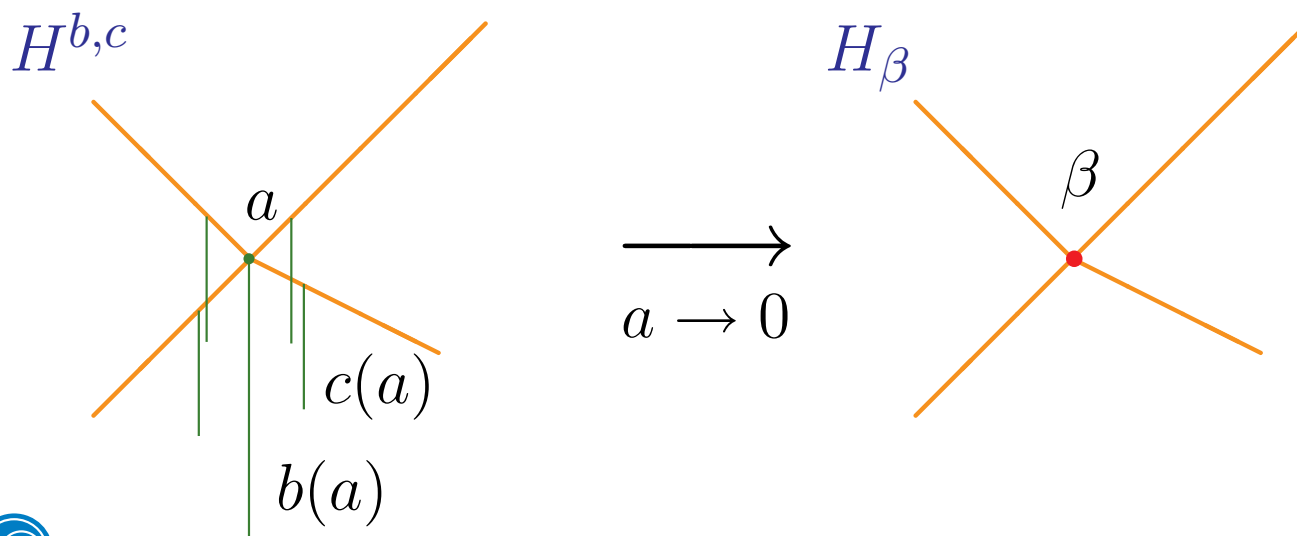
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This suggests the following scheme:



δ'_s approximation

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

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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

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



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- *Potential approximation to more singular coupling*: there are particular results showing the way, a deeper analysis needed



Some literature to Lecture I

- [CE04] T. Cheon, P.E.: An approximation to δ' couplings on graphs, *J. Phys. A: Math. Gen.* **A37** (2004), L329-335
- [E95] P.E.: Lattice Kronig–Penney models, *Phys. Rev. Lett.* **75** (1995), 3503-3506
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- [EHŠ06] P.E., P. Hejčík, P. Šeba: Approximations by graphs and emergence of global structures, *Rep. Math. Phys.* **57** (2006), 445-455
- [ENZ01] P.E., H. Neidhardt, V.A. Zagrebnov: Potential approximations to δ' : an inverse Klauder phenomenon with norm-resolvent convergence, *CMP* **224** (2001), 593-612
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- [ET06] P.E., O. Turek: Approximations of permutation-symmetric vertex couplings in quantum graphs, *Proceedings Snowbird 2005*, to appear; math-ph/0508046, and in preparation

and references therein, see also <http://www.ujf.cas.cz/~exner>



Lecture II

Leaky graphs – what they are, and their spectral and resonance properties



Lecture overview

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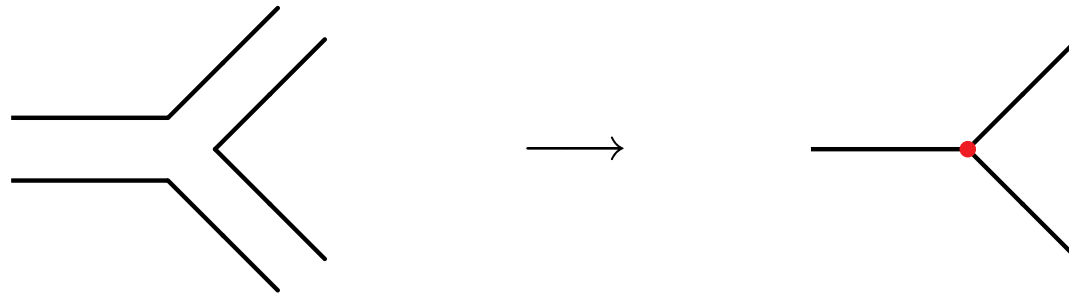
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- *How to find spectrum numerically*: an approximation by point interaction Hamiltonians
- *A solvable resonance model*: interaction supported by a line and a family of points – a caricature but solvable



Drawbacks of ideal graphs

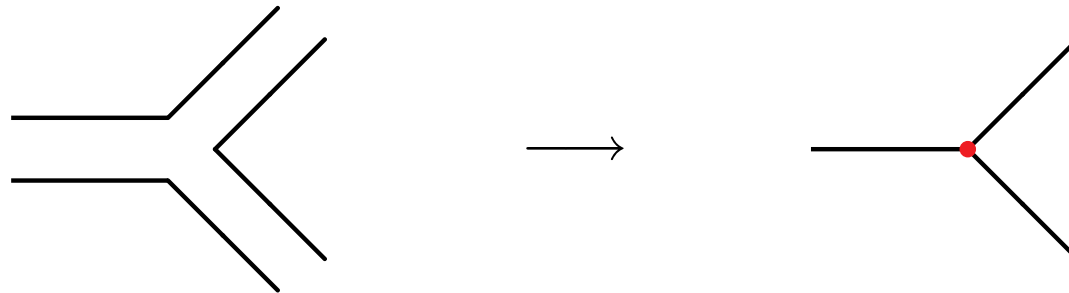
- Presence of *ad hoc parameters* in the b.c. describing branchings. A natural remedy: fit these using an approximation procedure, e.g.



As we have seen in *Lecture 1* it is possible but not quite easy and a lot of work remains to be done

Drawbacks of ideal graphs

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As we have seen in *Lecture 1* 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

We consider “*leaky*” graphs 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.



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

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

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 $W_{\text{loc}}^{2,1}(\mathbb{R}^2 \setminus \Gamma)$, which are continuous and exhibit a normal-derivative jump,

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



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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 $\text{codim } \Gamma$ does not exceed three



Geometrically induced spectrum

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



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- $|\Gamma(s) - \Gamma(s')| \geq c|s - s'|$ 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

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

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

- *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, 2001]: Under these assumptions, $\sigma_{\text{ess}}(H_{\alpha,\Gamma}) = [-\frac{1}{4}\alpha^2, \infty)$ and $H_{\alpha,\Gamma}$ has *at least one eigenvalue* below the threshold $-\frac{1}{4}\alpha^2$



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- The same for *curves in \mathbb{R}^3* , under stronger regularity, with $-\frac{1}{4}\alpha^2$ 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 $H_{\alpha,\tilde{\Gamma}} \leq H_{\alpha,\Gamma}$. If the essential spectrum threshold is the same for both graphs and Γ fits the above assumptions, we have $\sigma_{\text{disc}}(H_{\alpha,\Gamma}) \neq \emptyset$ 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 $\mathcal{R}_{\alpha,\Gamma}^\kappa$ on $L^2(\mathbb{R})$ with the kernel

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

has an eigenvalue equal to one



Sketch of the proof

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

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The curvature-induced perturbation is *sign-definite*: we have $(\mathcal{R}_{\alpha,\Gamma}^{\kappa} - \mathcal{R}_{\alpha,\Gamma_0}^{\kappa})(s, s') \geq 0$, 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 $\sup \sigma(\mathcal{R}_{\alpha,\Gamma}^{\kappa}) > \frac{\alpha}{2\kappa}$



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



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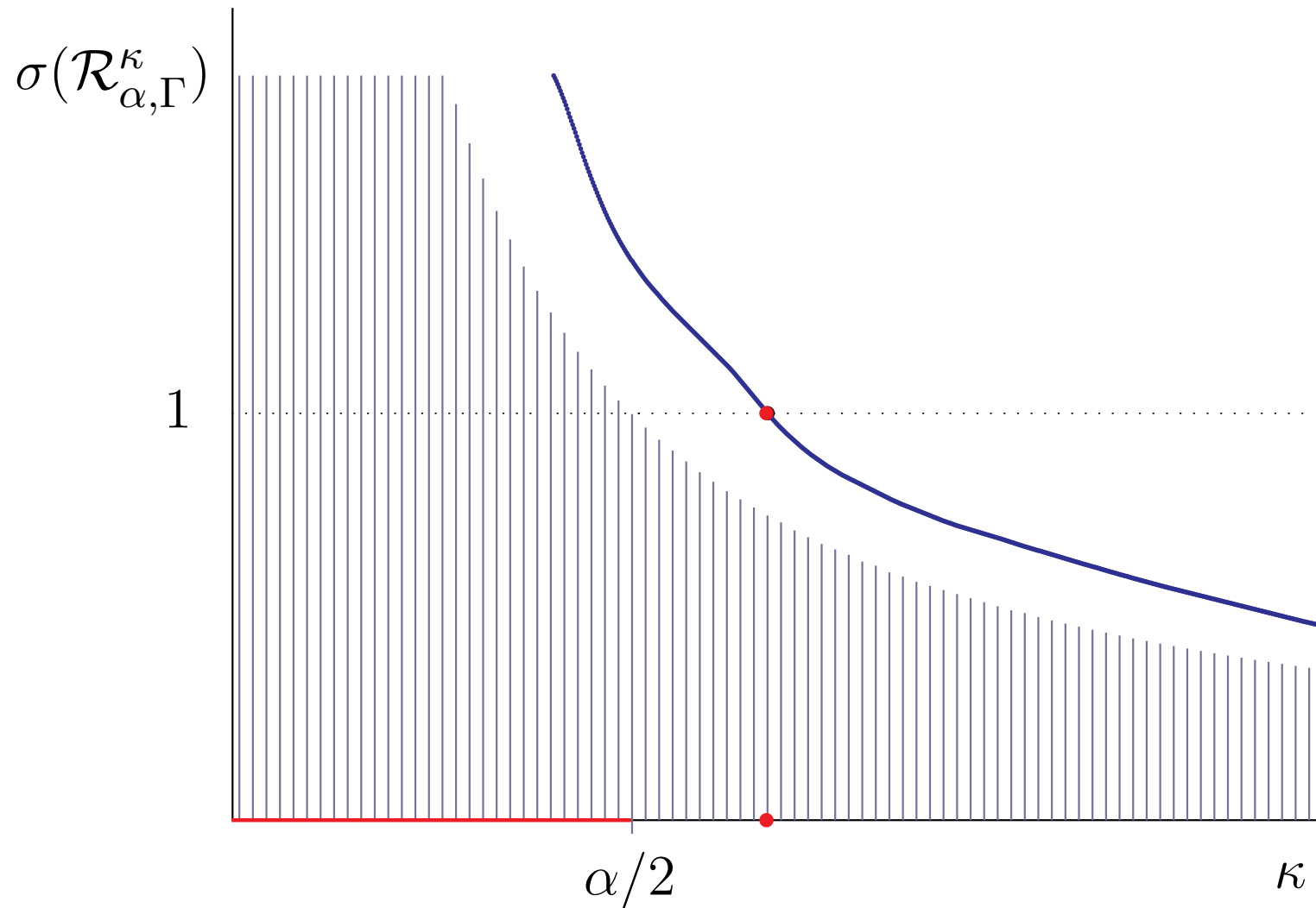
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To conclude we employ continuity and $\lim_{\kappa \rightarrow \infty} \|\mathcal{R}_{\alpha, \Gamma}^{\kappa}\| = 0$.

The argument can be pictorially expressed as follows:



Pictorial sketch of the proof



More geometrically induced properties

(b) *Perturbation theory for punctured manifolds:*

let $\Gamma : \mathbb{R} \rightarrow \mathbb{R}^2$ be as above, C^2 -smooth, and let Γ_ε differ by ε -long hiatus around a fixed point $x_0 \in \Gamma$. Let φ_j be the ef of $H_{\alpha,\Gamma}$ corresponding to a simple ev $\lambda_j \equiv \lambda_j(0)$ of $H_{\alpha,\Gamma}$.

Theorem [E.-Yoshitomi, 2003]: The j -th ev of $H_{\alpha,\Gamma_\varepsilon}$ is

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Remarks: Similarly one can express perturbed *degenerate* ev's. Analogous results hold for ev's for punctured compact, $(d-1)$ -dimensional, $C^{1+[d/2]}$ -smooth manifolds in \mathbb{R}^d .

Formally a small hole acts as *repulsive δ interaction* with coupling α times $(d-1)$ -Lebesgue measure of the hole



Strongly attractive curves

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

Theorem [E.-Yoshitomi, 2001]: The j -th ev of $H_{\alpha,\Gamma}$ is

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Strongly attractive curves

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

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



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



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- 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 $-\Delta_{LB} + K - M^2$, where K, M , respectively, are the corresponding Gauss and mean curvatures



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- *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

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2D point interactions

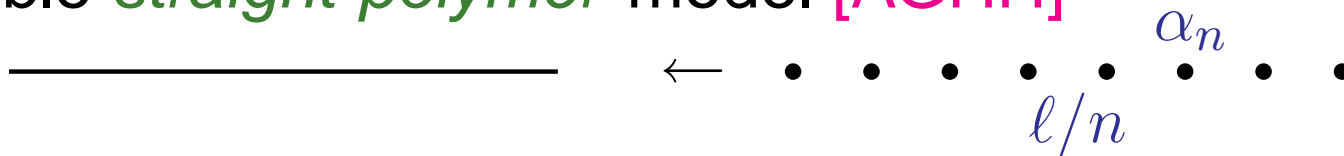
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For our purpose, the coupling should depend on the set Y approximating Γ . To see how compare a line Γ with the solvable *straight-polymer* model [AGHH]



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 $|Y_n| := \#Y_n$.

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Theorem [E.-Němcová, 2003]: Let a family $\{Y_n\}$ of finite sets $Y_n \subset \Gamma \subset \mathbb{R}^2$ be such that

$$\frac{1}{|Y_n|} \sum_{y \in Y_n} f(y) \rightarrow \int_{\Gamma} f \, dm$$

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



Comments on the approximation

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- *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's constant*.



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

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



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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 $n \rightarrow \infty$ \square



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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



An interlude: scattering on leaky graphs

Let Γ be a graph with *semi-infinite “leads”*, e.g. an infinite asymptotically straight curve. What we know about scattering in such systems? **Not much.**

- *First question:* What is the “free” operator? $-\Delta$ is not a good candidate, rather $H_{\alpha, \Gamma}$ for a straight line Γ . Recall that we are particularly interested in energy interval $(-\frac{1}{4}\alpha^2, 0)$, i.e. 1D transport of states laterally bound to Γ



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- On the other hand, in general, the **global geometry** of Γ is expected to determine the S-matrix



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:



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- *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



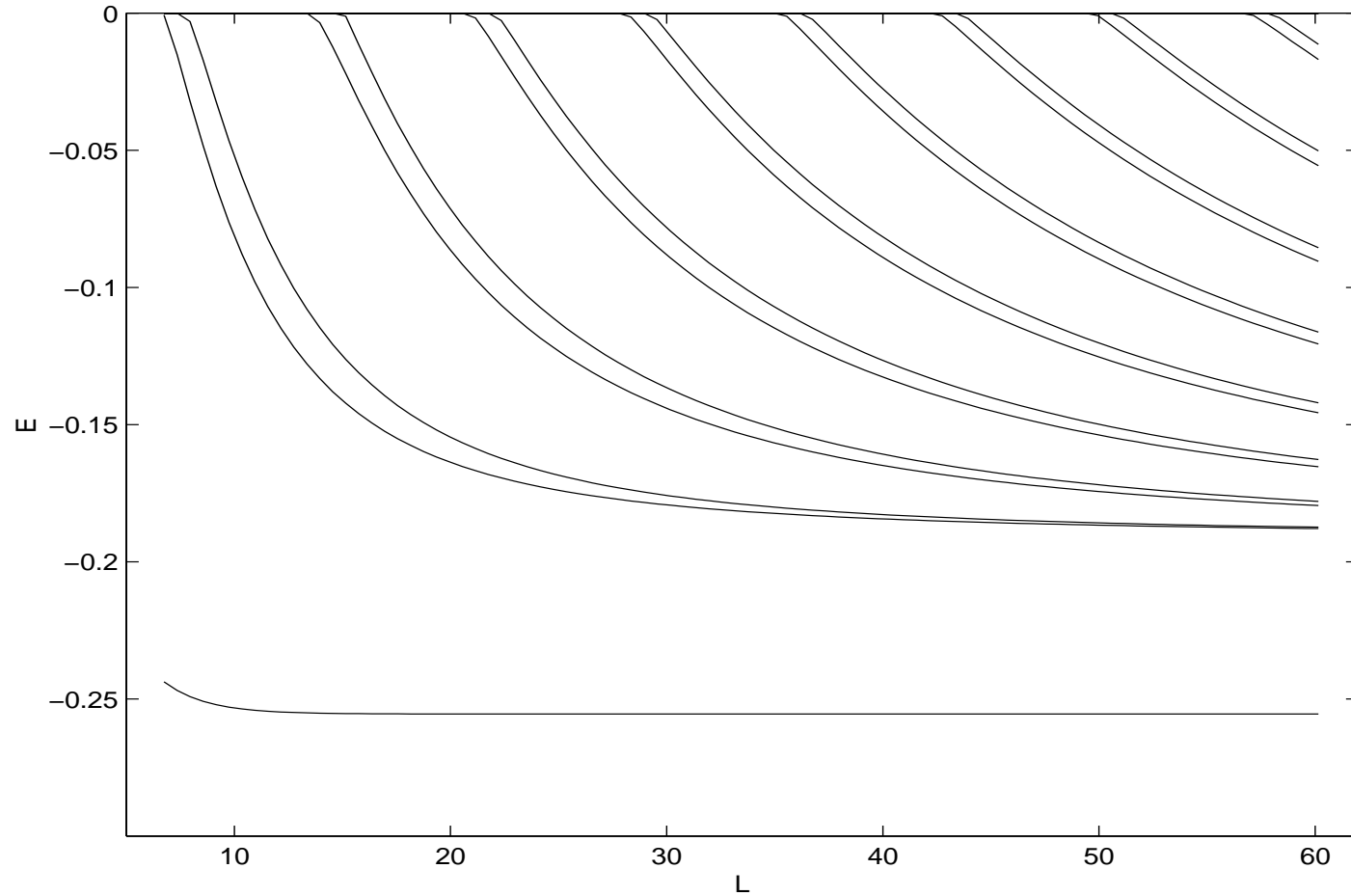
Broken line


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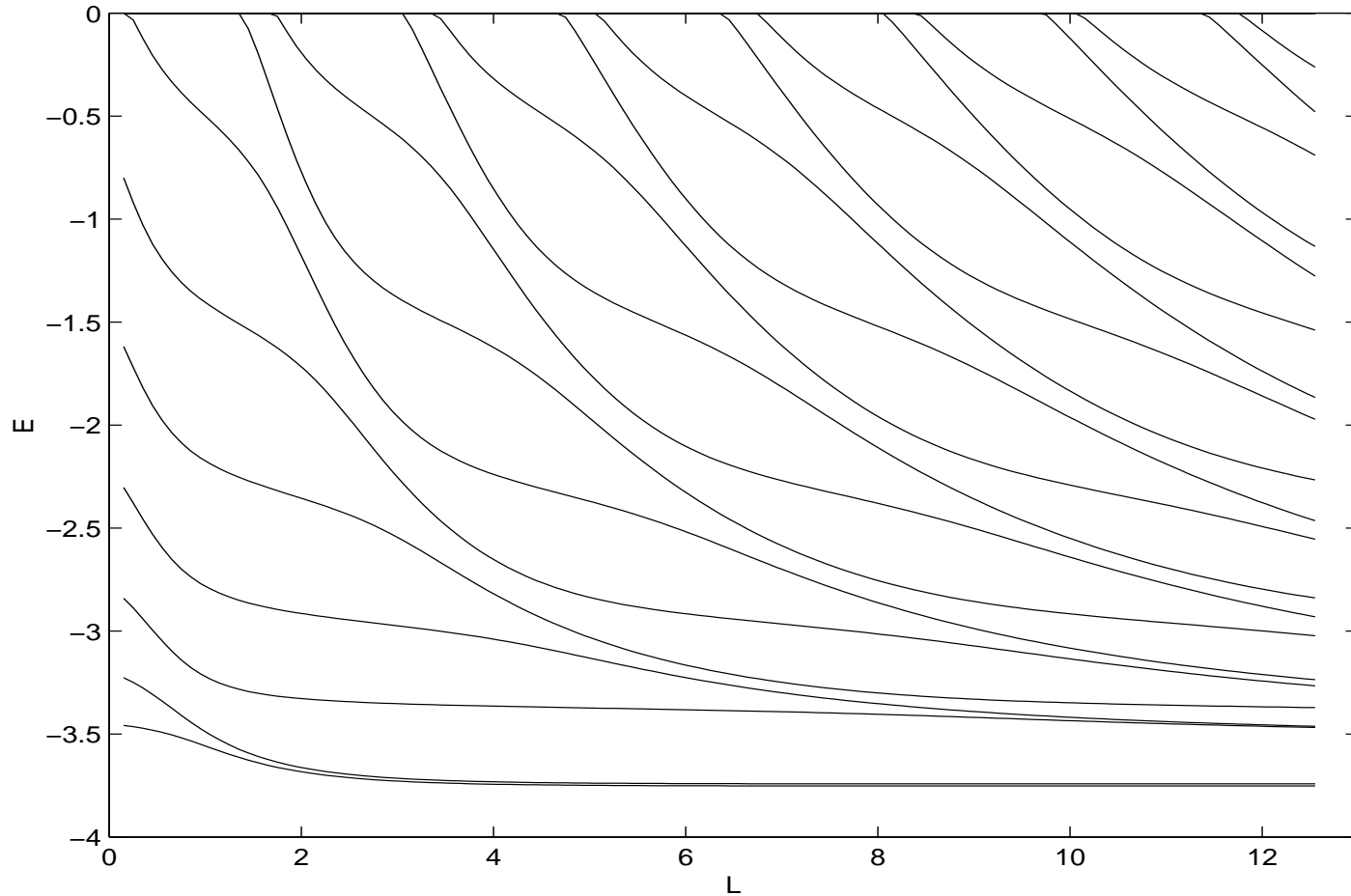


Z shape with $\theta = \frac{\pi}{2}$

$$\left. \begin{array}{l} L_c = 10 \\ \alpha = 5 \end{array} \right\}$$

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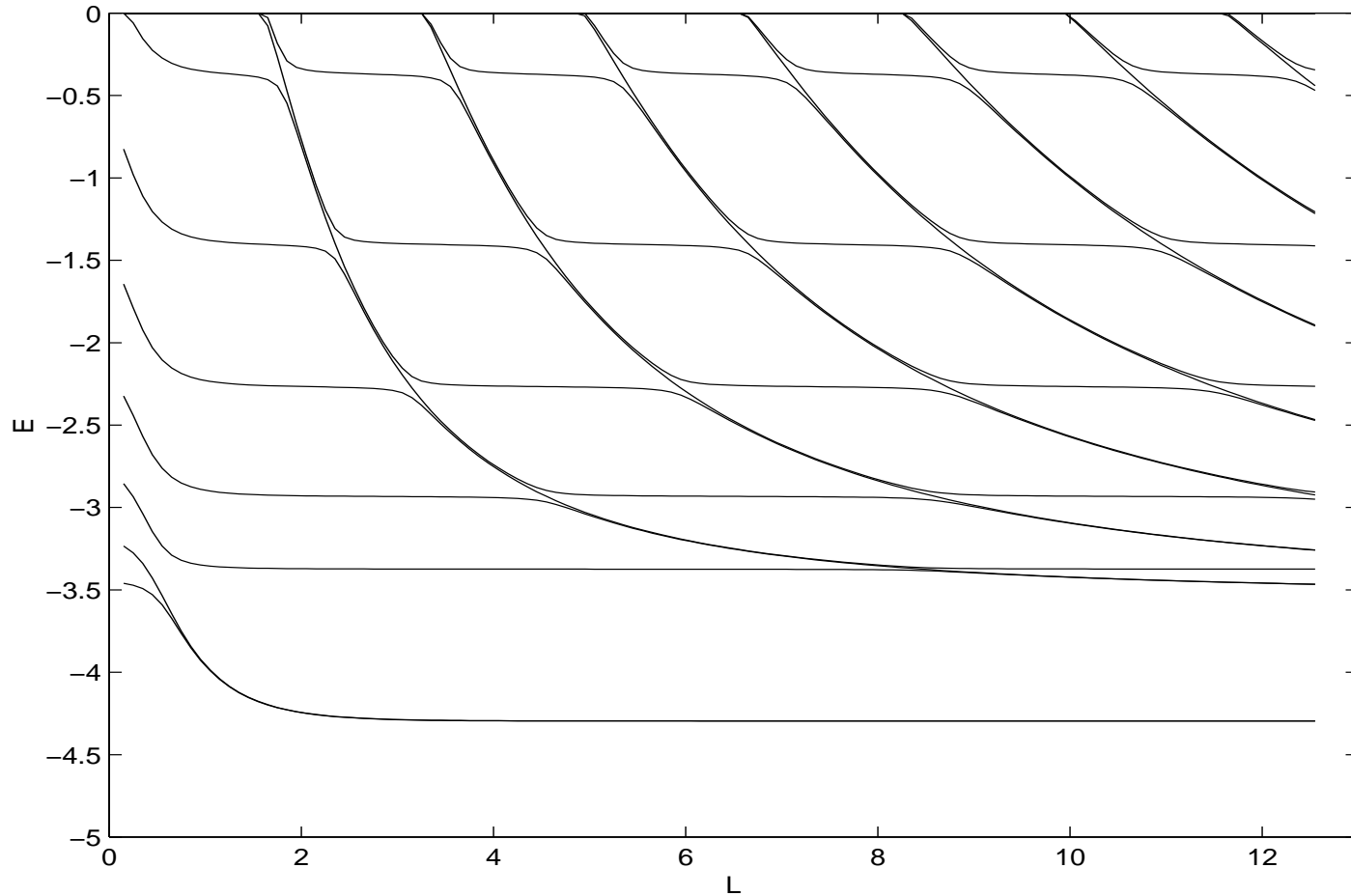
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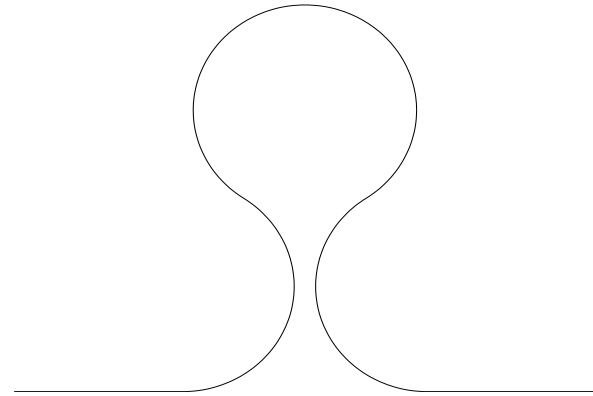
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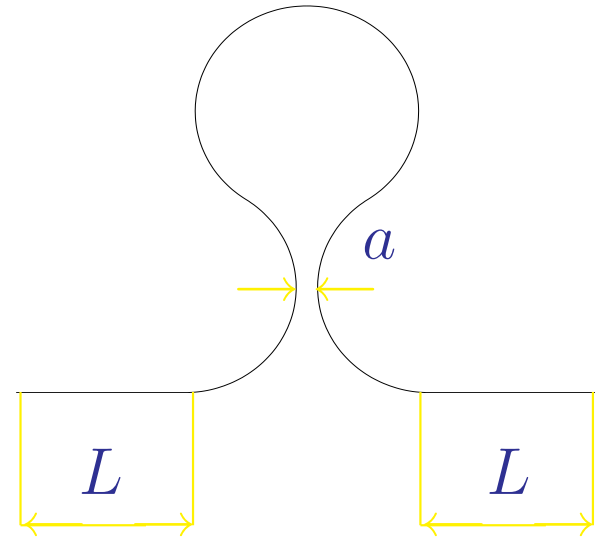
A bottleneck curve

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



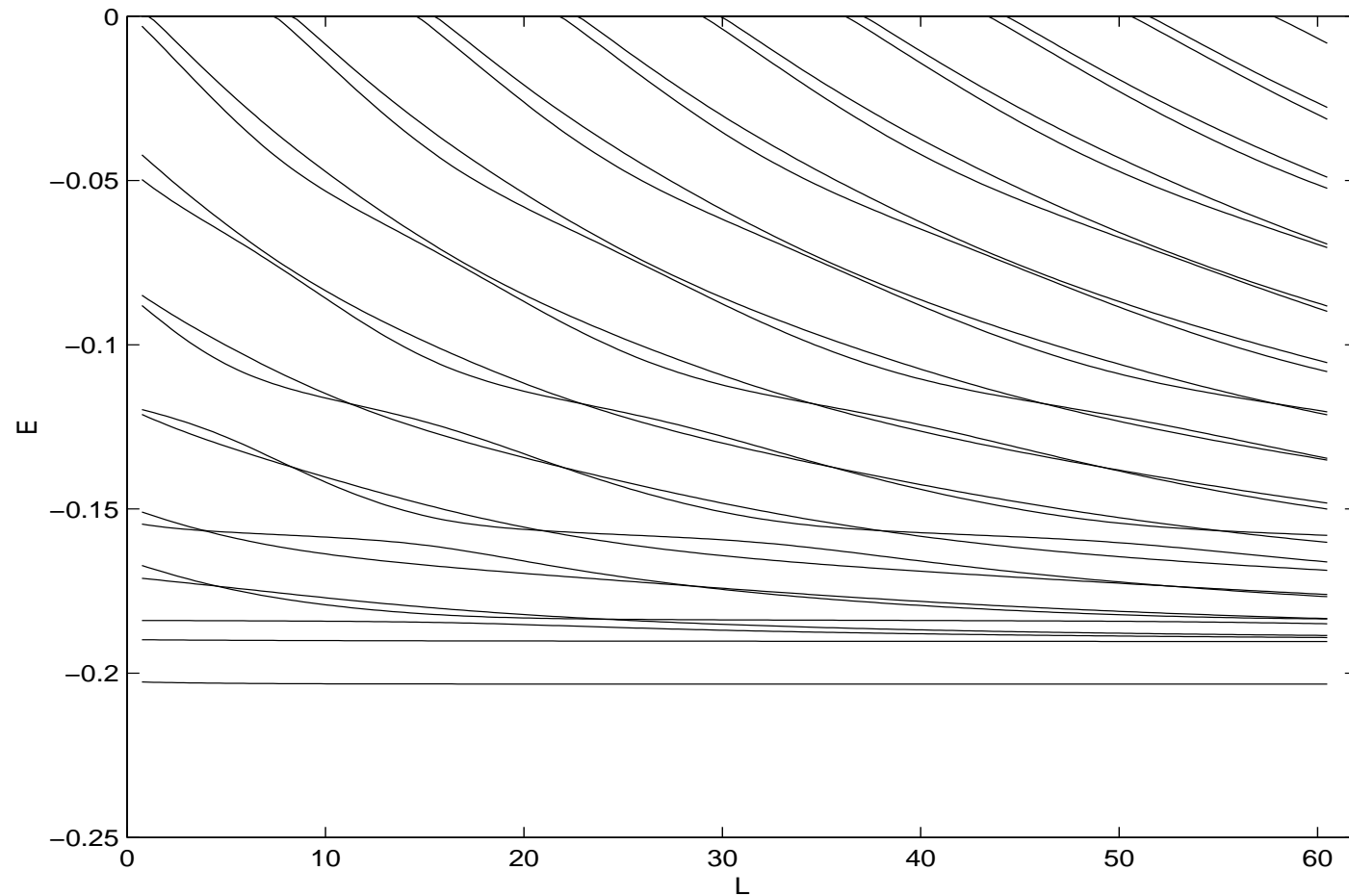
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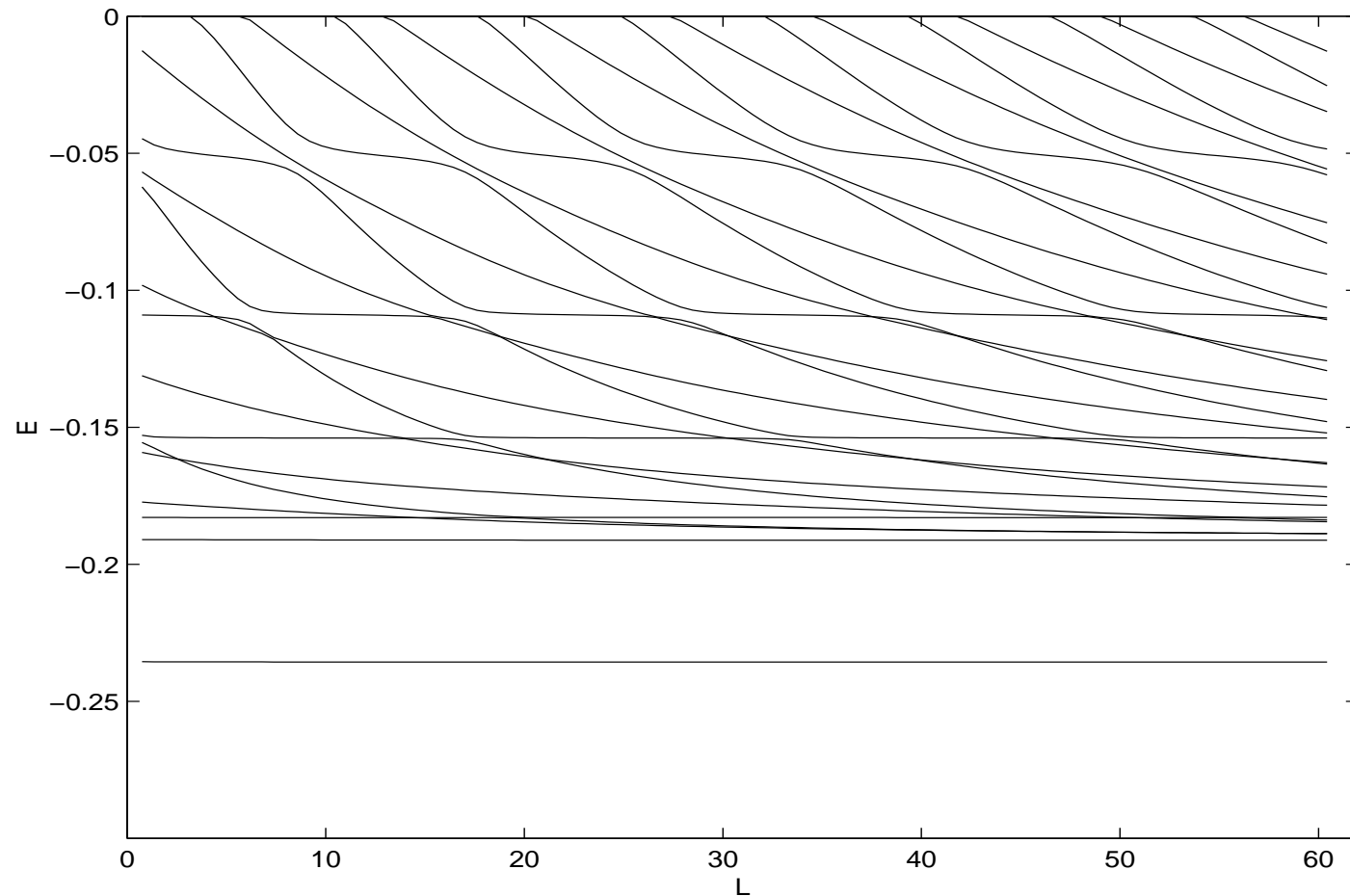


If Γ is a straight line, the transverse eigenfunction is $e^{-\alpha|y|/2}$, hence the distance at which tunneling becomes significant is $\approx 4\alpha^{-1}$. In the example, we choose $\alpha = 1$

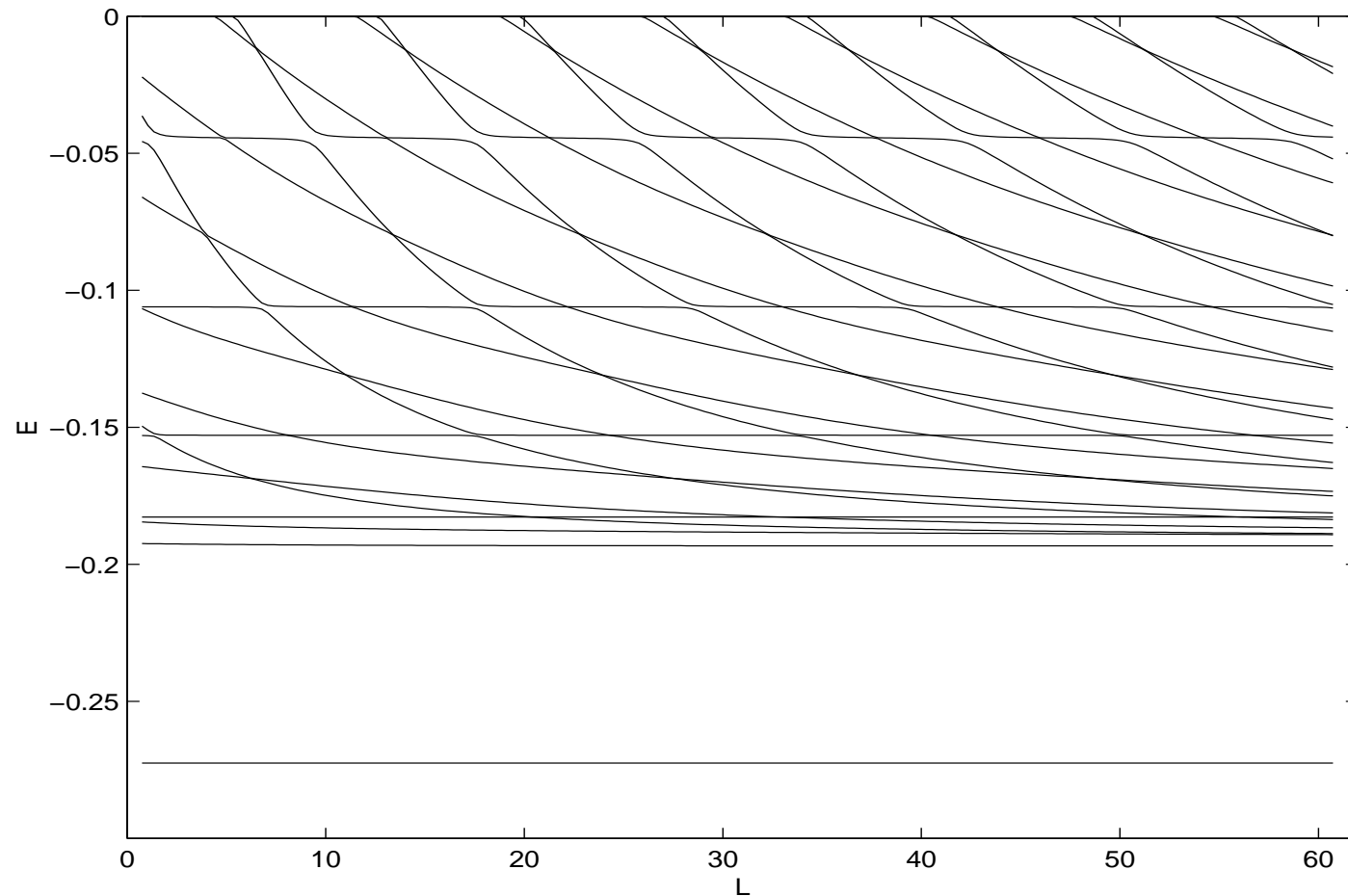
Bottleneck with $a = 5.2$



Bottleneck with $a = 2.9$



Bottleneck with $a = 1.9$



A caricature but solvable model

Let us pass to a simple model in which existence of resonances can be proved: a straight *leaky wire* and a family of *leaky dots*.



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$$-\Delta - \alpha\delta(x - \Sigma) + \sum_{i=1}^n \tilde{\beta}_i \delta(x - y^{(i)})$$

in $L^2(\mathbb{R}^2)$ with $\alpha > 0$. The 2D point interactions at $\Pi = \{y^{(i)}\}$ with couplings $\beta = \{\beta_1, \dots, \beta_n\}$ are properly introduced through b.c. mentioned above, giving Hamiltonian $H_{\alpha, \beta}$



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Resolvent by Krein-type formula: given $z \in \mathbb{C} \setminus [0, \infty)$ we start from the free resolvent $R(z) := (-\Delta - z)^{-1}$, also interpreted as unitary $\mathbf{R}(z)$ acting from L^2 to $W^{2,2}$. Then



Resolvent by Krein-type formula

- we introduce auxiliary Hilbert spaces, $\mathcal{H}_0 := L^2(\mathbb{R})$ and $\mathcal{H}_1 := \mathbb{C}^n$, and trace maps $\tau_j : W^{2,2}(\mathbb{R}^2) \rightarrow \mathcal{H}_j$ defined by $\tau_0 f := f \upharpoonright_{\Sigma}$ and $\tau_1 f := f \upharpoonright_{\Pi}$,

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- then we define canonical embeddings of $\mathbf{R}(z)$ to \mathcal{H}_i by $\mathbf{R}_{i,L}(z) := \tau_i R(z) : L^2 \rightarrow \mathcal{H}_i$, $\mathbf{R}_{L,i}(z) := [\mathbf{R}_{i,L}(z)]^*$, and $\mathbf{R}_{j,i}(z) := \tau_j \mathbf{R}_{L,i}(z) : \mathcal{H}_i \rightarrow \mathcal{H}_j$, and



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- operator-valued matrix $\Gamma(z) : \mathcal{H}_0 \oplus \mathcal{H}_1 \rightarrow \mathcal{H}_0 \oplus \mathcal{H}_1$ by

$$\Gamma_{ij}(z)g := -\mathbf{R}_{i,j}(z)g \quad \text{for } i \neq j \quad \text{and } g \in \mathcal{H}_j,$$

$$\Gamma_{00}(z)f := [\alpha^{-1} - \mathbf{R}_{0,0}(z)]f \quad \text{if } f \in \mathcal{H}_0,$$

$$\Gamma_{11}(z)\varphi := \left(s_{\beta}(z)\delta_{kl} - G_z(y^{(k)}, y^{(l)})(1 - \delta_{kl}) \right) \varphi,$$

with $s_{\beta}(z) := \beta + s(z) := \beta + \frac{1}{2\pi} (\ln \frac{\sqrt{z}}{2i} - \psi(1))$



Resolvent by Krein-type formula

To invert it we define the “reduced determinant”

$$D(z) := \Gamma_{11}(z) - \Gamma_{10}(z)\Gamma_{00}(z)^{-1}\Gamma_{01}(z) : \mathcal{H}_1 \rightarrow \mathcal{H}_1,$$



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then an easy algebra yields expressions for “blocks” of $[\Gamma(z)]^{-1}$ in the form

$$[\Gamma(z)]_{11}^{-1} = D(z)^{-1},$$

$$[\Gamma(z)]_{00}^{-1} = \Gamma_{00}(z)^{-1} + \Gamma_{00}(z)^{-1}\Gamma_{01}(z)D(z)^{-1}\Gamma_{10}(z)\Gamma_{00}(z)^{-1},$$

$$[\Gamma(z)]_{01}^{-1} = -\Gamma_{00}(z)^{-1}\Gamma_{01}(z)D(z)^{-1},$$

$$[\Gamma(z)]_{10}^{-1} = -D(z)^{-1}\Gamma_{10}(z)\Gamma_{00}(z)^{-1};$$

thus to determine singularities of $[\Gamma(z)]^{-1}$ one has to find the null space of $D(z)$



Resolvent by Krein-type formula

With this notation we can state the sought formula:

Theorem [E.-Kondej, 2004]: For $z \in \rho(H_{\alpha,\beta})$ with $\text{Im } z > 0$ the resolvent $R_{\alpha,\beta}(z) := (H_{\alpha,\beta} - z)^{-1}$ equals

$$R_{\alpha,\beta}(z) = R(z) + \sum_{i,j=0}^1 \mathbf{R}_{L,i}(z) [\Gamma(z)]_{ij}^{-1} \mathbf{R}_{j,L}(z)$$



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Remark: One can also compare resolvent of $H_{\alpha,\beta}$ to that of $H_{\alpha} \equiv H_{\alpha,\Sigma}$ using trace maps of the latter,

$$R_{\alpha,\beta}(z) = R_{\alpha}(z) + \mathbf{R}_{\alpha;L1}(z) D(z)^{-1} \mathbf{R}_{\alpha;1L}(z)$$



Spectral properties of $H_{\alpha,\beta}$

It is easy to check that

$$\sigma_{\text{ess}}(H_{\alpha,\beta}) = \sigma_{\text{ac}}(H_{\alpha,\beta}) = \left[-\frac{1}{4}\alpha^2, \infty\right)$$

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σ_{disc} given by *generalized Birman-Schwinger principle*:

$$\dim \ker \Gamma(z) = \dim \ker R_{\alpha,\beta}(z),$$

$$H_{\alpha,\beta}\phi_z = z\phi_z \Leftrightarrow \phi_z = \sum_{i=0}^1 \mathbf{R}_{L,i}(z)\eta_{i,z},$$

where $(\eta_{0,z}, \eta_{1,z}) \in \ker \Gamma(z)$. Moreover, it is clear that $0 \in \sigma_{\text{disc}}(\Gamma(z)) \Leftrightarrow 0 \in \sigma_{\text{disc}}(D(z))$; this reduces the task of finding the spectrum to an algebraic problem



Spectral properties of $H_{\alpha,\beta}$

Theorem [E.-Kondej, 2004]: (a) Let $n = 1$ and denote $\text{dist}(\sigma, \Pi) =: a$, then $H_{\alpha,\beta}$ has one isolated eigenvalue $-\kappa_a^2$. The function $a \mapsto -\kappa_a^2$ is increasing in $(0, \infty)$,

$$\lim_{a \rightarrow \infty} (-\kappa_a^2) = \min \left\{ \epsilon_\beta, -\frac{1}{4}\alpha^2 \right\},$$

where $\epsilon_\beta := -4e^{2(-2\pi\beta + \psi(1))}$, while $\lim_{a \rightarrow 0} (-\kappa_a^2)$ is finite.



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(b) For any $\alpha > 0$, $\beta \in \mathbb{R}^n$, and $n \in \mathbb{N}_+$ the operator $H_{\alpha,\beta}$ has N isolated eigenvalues, $1 \leq N \leq n$. If all the point interactions are strong enough, we have $N = n$



Spectral properties of $H_{\alpha,\beta}$

Theorem [E.-Kondej, 2004]: (a) Let $n = 1$ and denote $\text{dist}(\sigma, \Pi) =: a$, then $H_{\alpha,\beta}$ has one isolated eigenvalue $-\kappa_a^2$. The function $a \mapsto -\kappa_a^2$ is increasing in $(0, \infty)$,

$$\lim_{a \rightarrow \infty} (-\kappa_a^2) = \min \left\{ \epsilon_\beta, -\frac{1}{4}\alpha^2 \right\},$$

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Remark: Embedded eigenvalues due to mirror symmetry w.r.t. Σ possible if $n \geq 2$



Resonance for $n = 1$

Assume the point interaction eigenvalue *becomes embedded* as $a \rightarrow \infty$, i.e. that $\epsilon_\beta > -\frac{1}{4}\alpha^2$



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Observation: Birman-Schwinger works in the complex domain too; it is enough to look for analytical continuation of $D(\cdot)$, which acts for $z \in \mathbb{C} \setminus [-\frac{1}{4}\alpha^2, \infty)$ as a multiplication by

$$d_a(z) := s_\beta(z) - \phi_a(z) = s_\beta(z) - \int_0^\infty \frac{\mu(z, t)}{t - z - \frac{1}{4}\alpha^2} dt ,$$

$$\mu(z, t) := \frac{i\alpha}{16\pi} \frac{(\alpha - 2i(z-t)^{1/2}) e^{2ia(z-t)^{1/2}}}{t^{1/2}(z-t)^{1/2}}$$

Thus we have a situation reminiscent of **Friedrichs model**, just the functions involved are more complicated



Analytic continuation

Take a region Ω_- of the other sheet with $(-\frac{1}{4}\alpha^2, 0)$ as a part of its boundary. Put $\mu^0(\lambda, t) := \lim_{\varepsilon \rightarrow 0} \mu(\lambda + i\varepsilon, t)$, define

$$I(\lambda) := \mathcal{P} \int_0^\infty \frac{\mu^0(\lambda, t)}{t - \lambda - \frac{1}{4}\alpha^2} dt,$$

and furthermore, $g_{\alpha, a}(z) := \frac{i\alpha}{4} \frac{e^{-\alpha a}}{(z + \frac{1}{4}\alpha^2)^{1/2}}$.



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Lemma: $z \mapsto \phi_a(z)$ is continued analytically to Ω_- as

$$\phi_a^0(\lambda) = I(\lambda) + g_{\alpha,a}(\lambda) \quad \text{for } \lambda \in \left(-\frac{1}{4}\alpha^2, 0\right),$$

$$\phi_a^-(z) = - \int_0^\infty \frac{\mu(z, t)}{t - z - \frac{1}{4}\alpha^2} dt - 2g_{\alpha,a}(z), \quad z \in \Omega_-$$



Analytic continuation

Proof: By a direct computation one checks

$$\lim_{\varepsilon \rightarrow 0^+} \phi_a^\pm(\lambda \pm i\varepsilon) = \phi_a^0(\lambda), \quad -\frac{1}{4}\alpha^2 < \lambda < 0,$$

so the claim follows from edge-of-the-wedge theorem. \square



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The continuation of d_a is thus the function $\eta_a : M \mapsto \mathbb{C}$, where $M = \{z : \text{Im } z > 0\} \cup (-\frac{1}{4}\alpha^2, 0) \cup \Omega_-$, acting as

$$\eta_a(z) = s_\beta(z) - \phi_a^{l(z)}(z),$$

and our problem reduces to solution of the implicit function problem $\eta_a(z) = 0$.



Resonance for $n = 1$

Theorem [E.-Kondej, 2004]: Assume $\epsilon_\beta > -\frac{1}{4}\alpha^2$. For any a large enough the equation $\eta_a(z) = 0$ has a unique solution $z(a) = \mu(a) + i\nu(a) \in \Omega_-$, i.e. $\nu(a) < 0$, with the following asymptotic behaviour as $a \rightarrow \infty$,

$$\mu(a) = \epsilon_\beta + \mathcal{O}(e^{-a\sqrt{-\epsilon_\beta}}), \quad \nu(a) = \mathcal{O}(e^{-a\sqrt{-\epsilon_\beta}})$$

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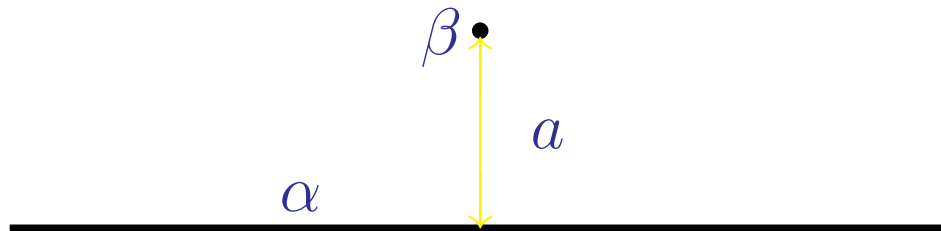
$$\mu(a) = \epsilon_\beta + \mathcal{O}(e^{-a\sqrt{-\epsilon_\beta}}), \quad \nu(a) = \mathcal{O}(e^{-a\sqrt{-\epsilon_\beta}})$$

Remark: We have $|\phi_a^-(z)| \rightarrow 0$ uniformly in a and $|s_\beta(z)| \rightarrow \infty$ as $\text{Im } z \rightarrow -\infty$. Hence the imaginary part $z(a)$ is bounded as a function of a , in particular, *the resonance pole survives* as $a \rightarrow 0$.



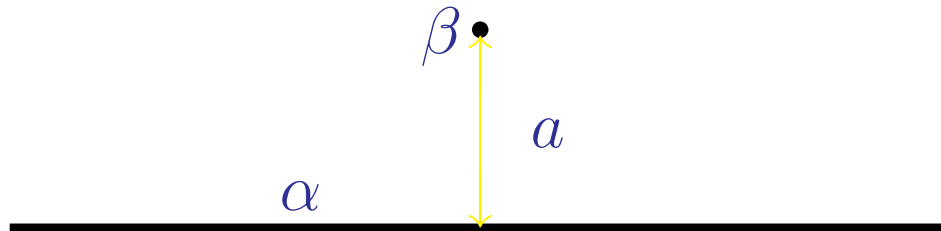
Scattering for $n = 1$

The same as scattering problem for $(H_{\alpha,\beta}, H_\alpha)$



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The same as scattering problem for $(H_{\alpha,\beta}, H_\alpha)$



Existence and completeness by Birman-Kuroda theorem; we seek on-shell S-matrix in $(-\frac{1}{4}\alpha^2, 0)$. By Krein formula, resolvent for $\text{Im } z > 0$ expresses as

$$R_{\alpha,\beta}(z) = R_\alpha(z) + \eta_a(z)^{-1}(\cdot, v_z)v_z,$$

where $v_z := R_{\alpha;L,1}(z)$



Scattering for $n = 1$

Apply this operator to vector

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

and take limit $\varepsilon \rightarrow 0+$ in the sense of distributions; then a straightforward calculation give generalized eigenfunction of $H_{\alpha,\beta}$. In particular, we have



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Proposition: For any $\lambda \in (-\frac{1}{4}\alpha^2, 0)$ the reflection and transmission amplitudes are

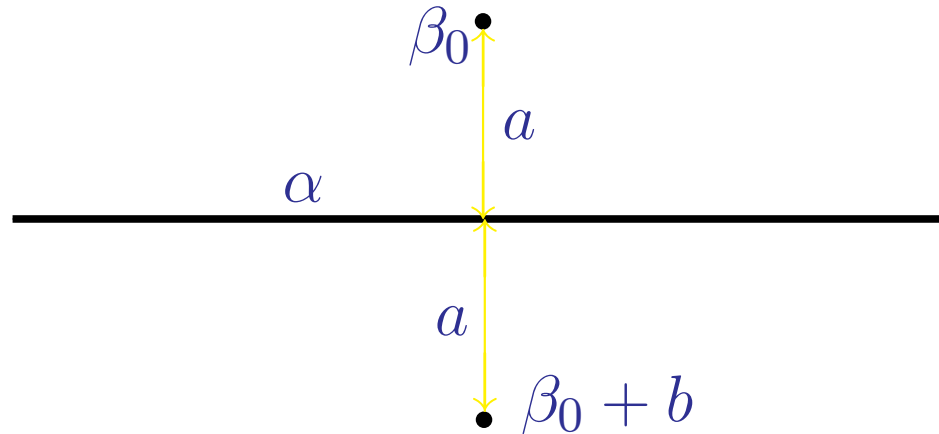
$$\mathcal{R}(\lambda) = \mathcal{T}(\lambda) - 1 = \frac{i}{4} \alpha \eta_a(\lambda)^{-1} \frac{e^{-\alpha a}}{(\lambda + \frac{1}{4}\alpha^2)^{1/2}} ;$$

they have the same pole in the analytical continuation to Ω_- as the continued resolvent



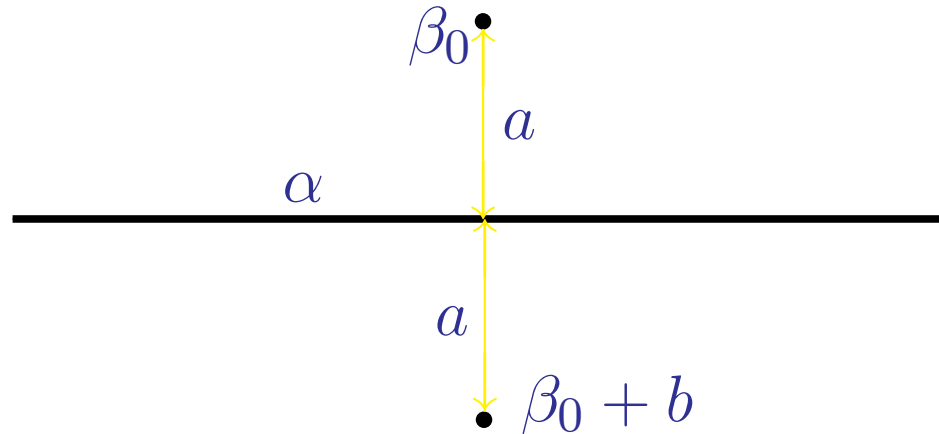
Resonances from perturbed symmetry

Take the simplest situation, $n = 2$



Resonances from perturbed symmetry

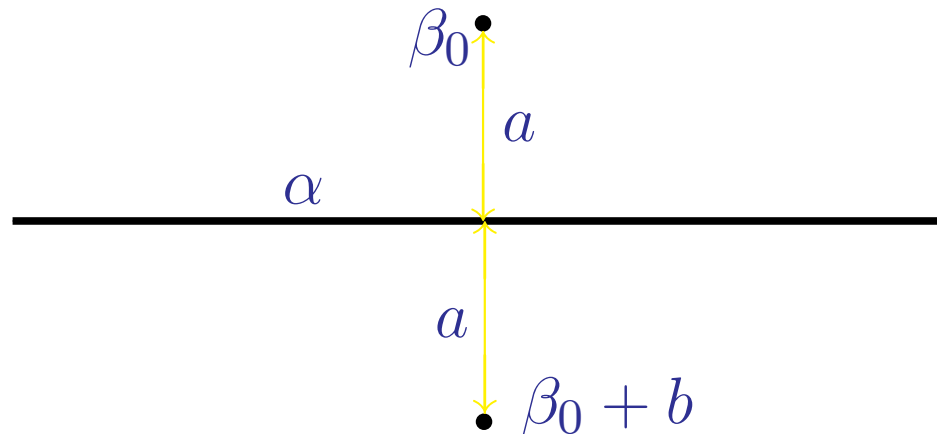
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Let $\sigma_{\text{disc}}(H_{0,\beta_0}) \cap (-\frac{1}{4}\alpha^2, 0) \neq \emptyset$, so that Hamiltonian H_{0,β_0} has two eigenvalues, the larger of which, ϵ_2 , exceeds $-\frac{1}{4}\alpha^2$. Then H_{α,β_0} has the same eigenvalue ϵ_2 embedded in the negative part of continuous spectrum

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One has now to continue analytically the 2×2 matrix function $D(\cdot)$. Put $\kappa_2 := \sqrt{-\epsilon_2}$ and $\check{s}_\beta(\kappa) := s_\beta(-\kappa^2)$



Resonances from perturbed symmetry

Proposition: Assume $\epsilon_2 \in (-\frac{1}{4}\alpha^2, 0)$ and denote $\tilde{g}(\lambda) := -ig_{\alpha,a}(\lambda)$. Then for all b small enough the continued function has a unique zero $z_2(b) = \mu_2(b) + i\nu_2(b) \in \Omega_-$ with the asymptotic expansion

$$\mu_2(b) = \epsilon_2 + \frac{\kappa_2 b}{\check{s}'_{\beta}(\kappa_2) + K'_0(2a\kappa_2)} + \mathcal{O}(b^2),$$

$$\nu_2(b) = -\frac{\kappa_2 \tilde{g}(\epsilon_2) b^2}{2(\check{s}'_{\beta}(\kappa_2) + K'_0(2a\kappa_2)) |\check{s}'_{\beta}(\kappa_2) - \phi_a^0(\epsilon_2)|} + \mathcal{O}(b^3)$$



Unstable state decay, $n = 1$

Complementary point of view: investigate decay of unstable state associated with the resonance; assume again $n = 1$. We found that if the “unperturbed” ev ϵ_β of H_β is embedded in $(-\frac{1}{4}\alpha^2, 0)$ and a is large, the corresponding resonance has a long half-life. In analogy with *Friedrichs model* [Demuth, 1976] one conjectures that in weak coupling case, the resonance state would be similar up to normalization to the eigenvector $\xi_0 := K_0(\sqrt{-\epsilon_\beta} \cdot)$ of H_β , with the *decay law being dominated by the exponential term*



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At the same time, $H_{\alpha,\beta}$ has always an isolated ev with ef which is *not* orthogonal to ξ_0 for any a (recall that both functions are positive). Consequently, the decay law $|(\xi_0, U(t)\xi_0)|^2 \|\xi_0\|^{-2}$ *has always a nonzero limit as $t \rightarrow \infty$*



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Summarizing Lecture II

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- *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



Some literature to Lecture II

- [EI01] P.E., T. Ichinose: Geometrically induced spectrum in curved leaky wires, *J. Phys.* **A34** (2001), 1439-1450.
- [EK02] 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.
- [EK03] P.E., S. Kondej: Bound states due to a strong δ interaction supported by a curved surface, *J. Phys.* **A36** (2003), 443-457.
- [EK04] P.E., S. Kondej: Schrödinger operators with singular interactions: a model of tunneling resonances, *J. Phys.* **A37** (2004), 8255-8277.
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- [EN03] P.E., K. Němcová: Leaky quantum graphs: approximations by point interaction Hamiltonians, *J. Phys.* **A36** (2003), 10173-10193.
- [EY01] 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.
- [EY02a] 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.
- [EY02b] P.E., K. Yoshitomi: Persistent currents for 2D Schrödinger operator with a strong δ -interaction on a loop, *J. Phys.* **A35** (2002), 3479-3487.
- [EY03] 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 references therein, see also <http://www.ujf.cas.cz/~exner>



Lecture III

Generalized graphs – or what happens if a quantum particle has to change its dimension



Lecture overview

- Motivation – a nontrivial configuration space



Lecture overview

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- Coupling by means of s-a extensions

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- A model: point-contact spectroscopy
- A model: single-mode geometric scatterers
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- An illustration on microwave experiments



Lecture overview

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- Coupling by means of s-a extensions
- A model: point-contact spectroscopy
- A model: single-mode geometric scatterers
- Large gaps in periodic systems
- A heuristic way to choose the coupling
- An illustration on microwave experiments
- And something else: spin conductance oscillations



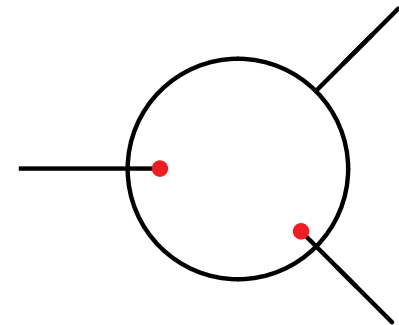
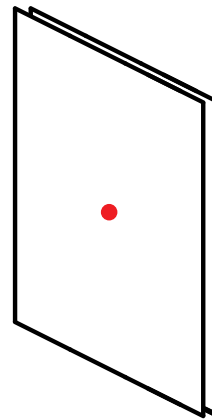
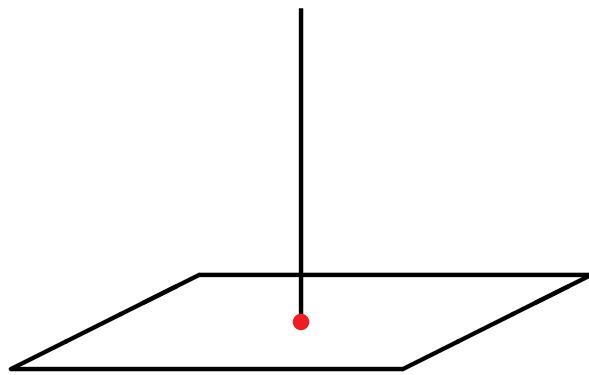
A nontrivial configuration space

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In contrast, QM offers interesting examples, e.g.

- *point-contact* spectroscopy,
- *STEM-type devices*,
- compositions of *nanotubes* with *fulleren* molecules,

etc. Similarly one can consider some *electromagnetic systems* such as flat microwave resonators with attached antennas; we will comment on that later in the lecture



Coupling by means of s-a extensions

Among other things we owe to J. von Neumann the theory of self-adjoint extensions of symmetric operators is not the least. Let us apply it to our problem.



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The idea: Quantum dynamics on $M_1 \cup M_2$ coupled by a point contact $x_0 \in M_1 \cap M_2$. Take Hamiltonians H_j on the *isolated* manifold M_j and restrict them to functions vanishing in the vicinity of x_0



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The operator $H_0 := H_{1,0} \oplus H_{2,0}$ is symmetric, in general not s-a. We seek admissible Hamiltonians of the coupled system among *its self-adjoint extensions*



Coupling by means of s-a extensions

Limitations: In nonrelativistic QM considered here, where H_j is a *second-order operator* the method works for $\dim M_j \leq 3$ (more generally, codimension of the contact should not exceed *three*), since otherwise the restriction is *e.s.a.* [similarly for Dirac operators we require the codimension to be at most *one*]



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Non-uniqueness: Apart of the trivial case, there are many s-a extensions. A junction where n configuration-space components meet contributes typically by n to deficiency indices of H_0 , and thus adds n^2 parameters to the resulting Hamiltonian class; recall a similar situation in *Lecture 1*



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Physical meaning: The construction guarantees that the *probability current is conserved* at the junction



Different dimensions

In distinction to quantum graphs “1 + 1” situation, we will be mostly concerned with cases “2+1” and “2+2”, i.e. manifolds of these dimensions coupled through *point contacts*. Other combinations are similar

We use “rational” units, in particular, the Hamiltonian acts at each configuration component as $-\Delta$ (or Laplace-Beltrami operator if M_j has a nontrivial metric)

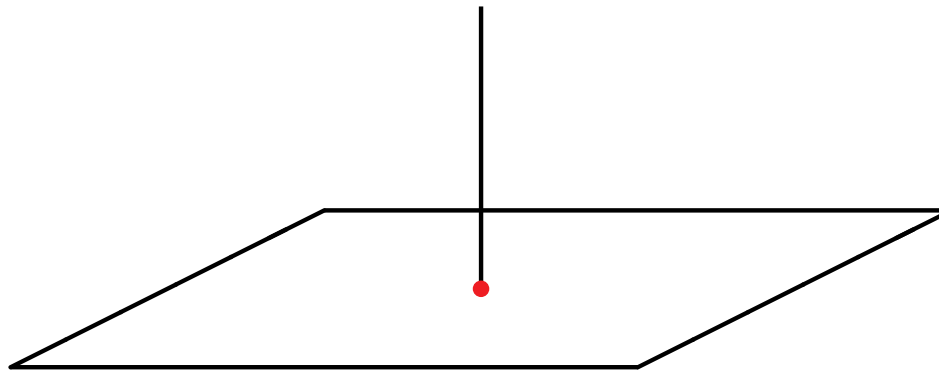


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An archetypal example, $\mathcal{H} = L^2(\mathbb{R}_-) \oplus L^2(\mathbb{R}^2)$, so the wavefunctions are pairs $\phi := \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$ of square integrable functions



A model: *point-contact spectroscopy*

Restricting $\left(-\frac{d^2}{dx^2}\right)_D \oplus -\Delta$ to functions vanishing in the vicinity of the junction gives symmetric operator with deficiency indices $(2, 2)$.



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von Neumann theory gives a general prescription to construct the s-a extensions, however, it is practical to characterize the by means of *boundary conditions*. We need *generalized boundary values*

$$L_0(\Phi) := \lim_{r \rightarrow 0} \frac{\Phi(\vec{x})}{\ln r}, \quad L_1(\Phi) := \lim_{r \rightarrow 0} [\Phi(\vec{x}) - L_0(\Phi) \ln r]$$

(in view of the 2D character, in three dimensions L_0 would be the coefficient at the pole singularity)



2 + 1 point-contact coupling

Typical b.c. determining a s-a extension

$$\begin{aligned}\phi_1'(0-) &= A\phi_1(0-) + BL_0(\Phi_2), \\ L_1(\Phi_2) &= C\phi_1(0-) + DL_0(\Phi_2),\end{aligned}$$



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The easiest way to see that is to compute the boundary form to H_0^* , recall that the latter is given by the same differential expression.

Notice that *only the s-wave part* of Φ in the plane, $\Phi_2(r, \varphi) = (2\pi)^{-1/2}\phi_2(r)$ can be coupled nontrivially to the halfline



2 + 1 point-contact coupling

An integration by parts gives

$$\begin{aligned}(\phi, H_0^* \psi) - (H_0^* \phi, \psi) &= \bar{\phi}'_1(0) \psi_1(0) - \bar{\phi}_1(0) \psi'_1(0) \\ &+ \lim_{\varepsilon \rightarrow 0^+} \varepsilon (\bar{\phi}_2(\varepsilon) \psi'_1(\varepsilon) - \bar{\phi}'_2(\varepsilon) \psi_2(\varepsilon)) ,\end{aligned}$$



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and using the asymptotic behaviour

$$\phi_2(\varepsilon) = \sqrt{2\pi} [L_0(\Phi_2) \ln \varepsilon + L_1(\Phi_2) + \mathcal{O}(\varepsilon)] ,$$



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and using the asymptotic behaviour

$$\phi_2(\varepsilon) = \sqrt{2\pi} [L_0(\Phi_2) \ln \varepsilon + L_1(\Phi_2) + \mathcal{O}(\varepsilon)] ,$$

we can express the above limit term as

$$2\pi [L_1(\Phi_2) L_0(\Psi_2) - L_0(\Phi_2) L_1(\Psi_2)] ,$$

so the form vanishes under the stated boundary conditions



Transport through point contact

Using the b.c. we match plane wave solution $e^{ikx} + r(k)e^{-ikx}$ on the halfline with $t(k)(\pi kr/2)^{1/2}H_0^{(1)}(kr)$ in the plane obtaining

$$r(k) = -\frac{\mathcal{D}_-}{\mathcal{D}_+}, \quad t(k) = \frac{2iCk}{\mathcal{D}_+}$$

Transport through point contact

Using the b.c. we match plane wave solution $e^{ikx} + r(k)e^{-ikx}$ on the halfline with $t(k)(\pi kr/2)^{1/2} H_0^{(1)}(kr)$ in the plane obtaining

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Remark: More general coupling, $\mathcal{A}(\frac{\phi_1}{L_0}) + \mathcal{B}(\frac{\phi_1'}{L_1}) = 0$, gives rise to similar formulae (an invertible \mathcal{B} can be put to one)



Transport through point contact

Let us finish discussion of this “*point contact spectroscopy*” model by a few remarks:

- Scattering is *nontrivial* if $\mathcal{A} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ is not diagonal. For any choice of s-a extension, the on-shell S-matrix is *unitary*, in particular, we have $|r(k)|^2 + |t(k)|^2 = 1$



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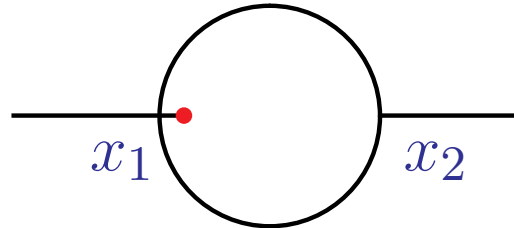
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- Notice that *reflection dominates at high energies*, since $|t(k)|^2 = \mathcal{O}((\ln k)^{-2})$ holds as $k \rightarrow \infty$
- For some \mathcal{A} there are also *bound states* decaying exponentially away of the junction, at most two



Single-mode geometric scatterers

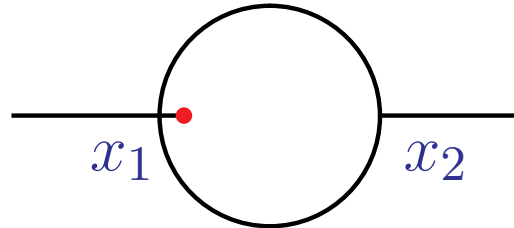
Consider a sphere with two leads attached



with the coupling at both vertices given by the same \mathcal{A}

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Three one-parameter families of \mathcal{A} were investigated [Kiselev, 1997; E.-Tater-Vaněk, 2001; Brüning-Geyler-Margulis-Pyataev, 2002]; it appears that scattering properties *en gross* are not very sensitive to the coupling:

- there numerous resonances
- in the background reflection dominates as $k \rightarrow \infty$



Geometric scatterer transport

Let us describe the argument in more details: construction of generalized eigenfunctions means to couple plane-wave solution at leads with

$$u(x) = a_1 G(x, x_1; k) + a_2 G(x, x_2; k),$$

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where $G(\cdot, \cdot; k)$ is Green's function of Δ_{LB} on the sphere
The latter has a logarithmic singularity so $L_j(u)$ express in terms of $g := G(x_1, x_2; k)$ and

$$\xi_j \equiv \xi(x_j; k) := \lim_{x \rightarrow x_j} \left[G(x, x_j; k) + \frac{\ln |x - x_j|}{2\pi} \right]$$



Geometric scatterer transport

Introduce $Z_j := \frac{D_j}{2\pi} + \xi_j$ and $\Delta := g^2 - Z_1 Z_2$, and consider, e.g., $\mathcal{A}_j = \begin{pmatrix} (2a)^{-1} & (2\pi/a)^{1/2} \\ (2\pi a)^{-1/2} & -\ln a \end{pmatrix}$ with $a > 0$. Then the solution of the matching condition is given by



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$$r(k) = - \frac{\pi\Delta + Z_1 + Z_2 - \pi^{-1} + 2ika(Z_2 - Z_1) + 4\pi k^2 a^2 \Delta}{\pi\Delta + Z_1 + Z_2 - \pi^{-1} + 2ika(Z_1 + Z_2 + 2\pi\Delta) - 4\pi k^2 a^2 \Delta},$$

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Geometric scatterers: needed quantities

So far formulae are valid for any compact manifold G . To make use of them we need to know g, Z_1, Z_2, Δ . The spectrum $\{\lambda_n\}_{n=1}^{\infty}$ of Δ_{LB} on G is purely discrete with eigenfunctions $\{\phi(x)_n\}_{n=1}^{\infty}$. Then we find easily

$$g(k) = \sum_{n=1}^{\infty} \frac{\phi_n(x_1) \overline{\phi_n(x_2)}}{\lambda_n - k^2}$$



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and

$$\xi(x_j, k) = \sum_{n=1}^{\infty} \left(\frac{|\phi_n(x_j)|^2}{\lambda_n - k^2} - \frac{1}{4\pi n} \right) + c(G),$$

where $c(G)$ depends of the manifold only (changing it is equivalent to a coupling constant renormalization)



A symmetric spherical scatterer

Theorem [Kiselev, 1997, E.-Tater-Vaněk, 2001]: For any l large enough the interval $(l(l-1), l(l+1))$ contains a point μ_l such that $\Delta(\sqrt{\mu_l}) = 0$. Let $\varepsilon(\cdot)$ be a positive, strictly increasing function which tends to ∞ and obeys the inequality $|\varepsilon(x)| \leq x \ln x$ for $x > 1$. Furthermore, denote $K_\varepsilon := \mathbb{R} \setminus \bigcup_{l=2}^{\infty} (\mu_l - \varepsilon(l)(\ln l)^{-2}, \mu_l + \varepsilon(l)(\ln l)^{-2})$.



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$$|t(k)|^2 \leq c\varepsilon(l)^{-2}$$

in the *background*, i.e. for $k^2 \in K_\varepsilon \cap (l(l-1), l(l+1))$ and any l large enough. On the other hand, there are *resonance peaks* localized outside K_ε with the property

$$|t(\sqrt{\mu_l})|^2 = 1 + \mathcal{O}((\ln l)^{-1}) \quad \text{as } l \rightarrow \infty$$



A *symmetric* spherical scatterer

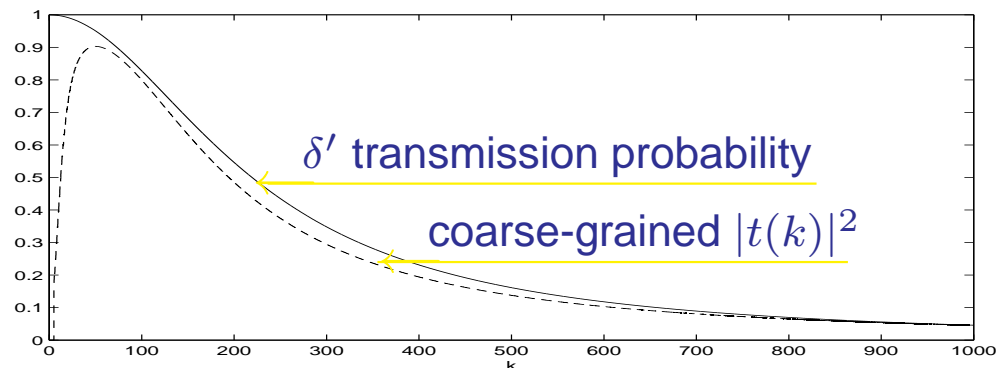
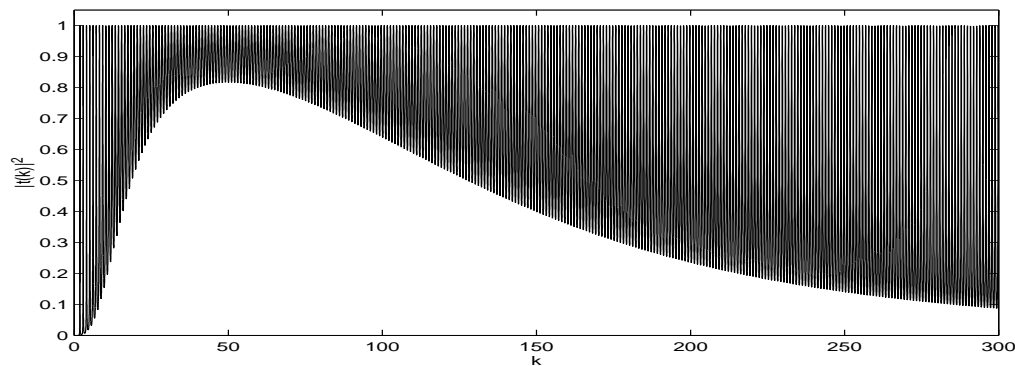
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Figure 7



An *asymmetric* spherical scatterer

While the above general features are expected to be the same if the angular distance of junctions is less than π , the detailed transmission plot changes [Brüning et al., 2002]:



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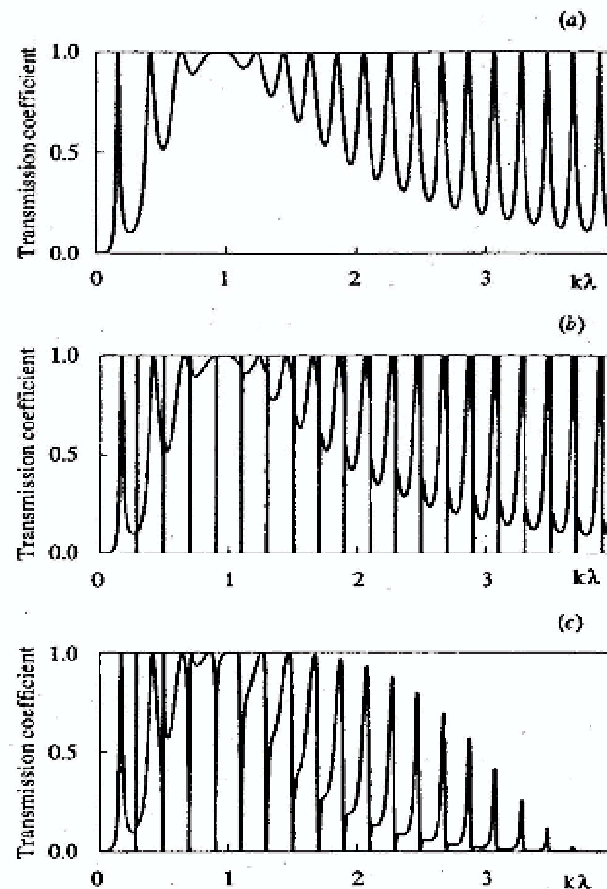


Figure 2. The transmission coefficient as a function of $k\lambda$ at $\alpha = 10\lambda$: (a) $r = \pi\alpha$; (b) $r = 0.98\pi\alpha$; (c) $r = 0.96\pi\alpha$.



Arrays of geometric scatterers

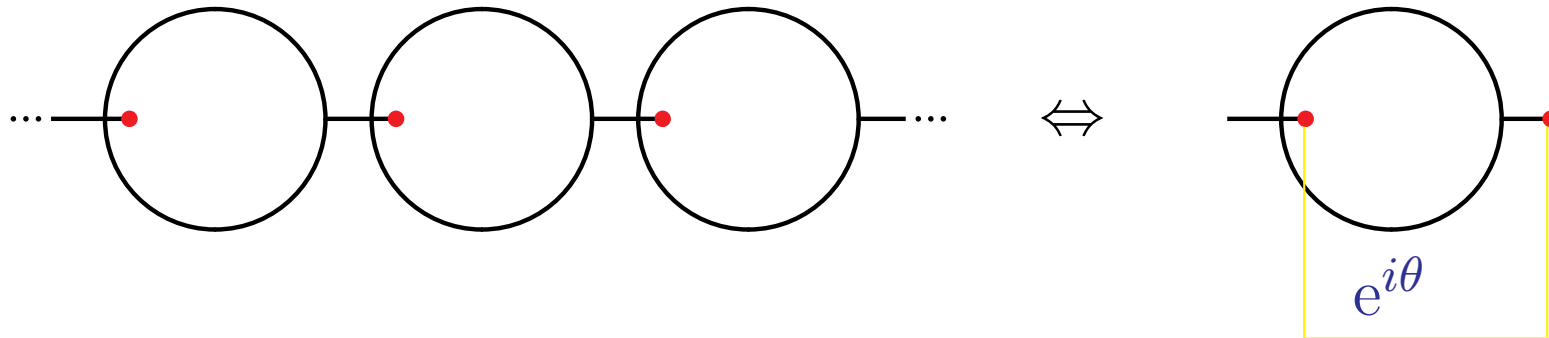
In a similar way one can construct *general scattering theory* on such “hedgehog” manifolds composed of compact scatterers, connecting edges and external leads
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Furthermore, infinite periodic systems can be treated by Floquet-Bloch decomposition



Sphere array spectrum

A band spectrum example from [E.-Tater-Vaněk, 2001]:
radius $R = 1$, segment length $\ell = 1, 0.01$ and coupling ρ



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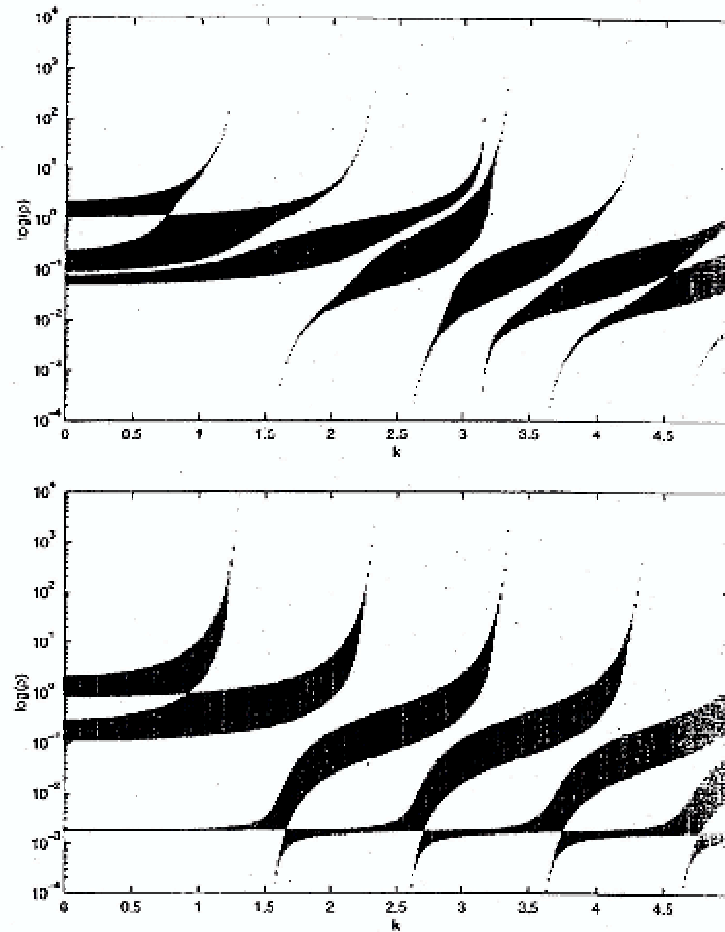


FIG. 8. Band spectrum of an infinite "bubble" array. The spheres are of unit radius, the spacing is $1=1$ (upper figure) and $1=0.01$ (lower figure), ρ is the contact radius.



How do gaps behave as $k \rightarrow \infty$?

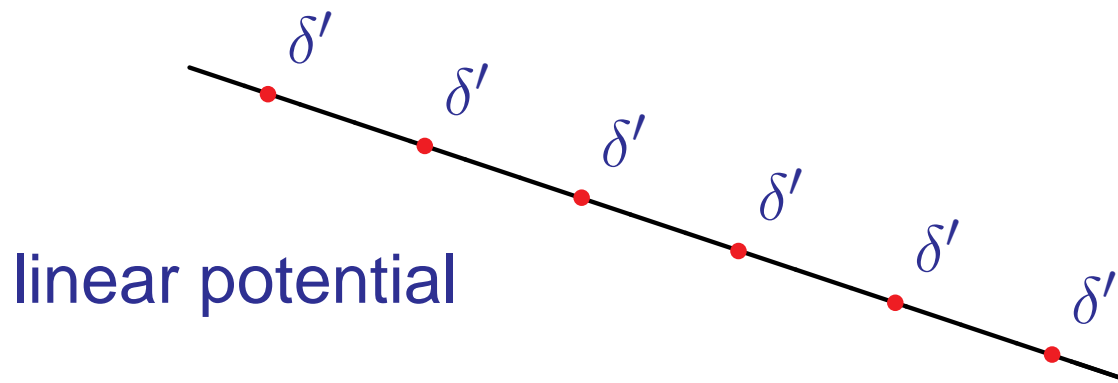
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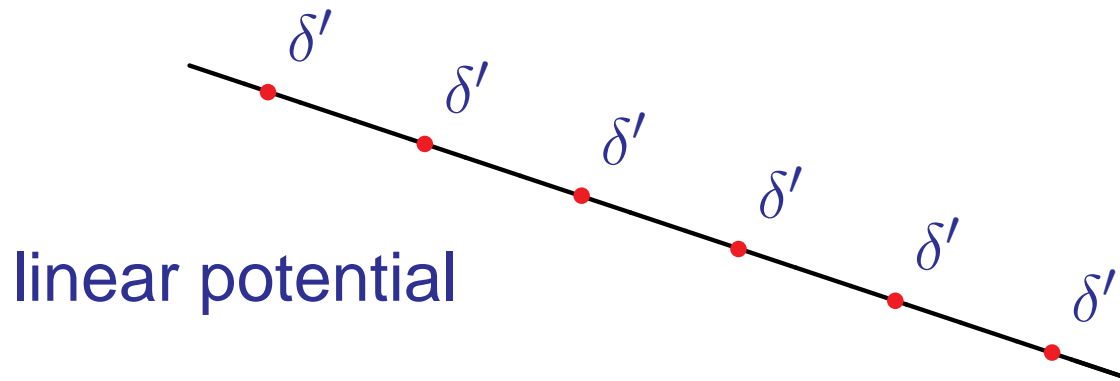
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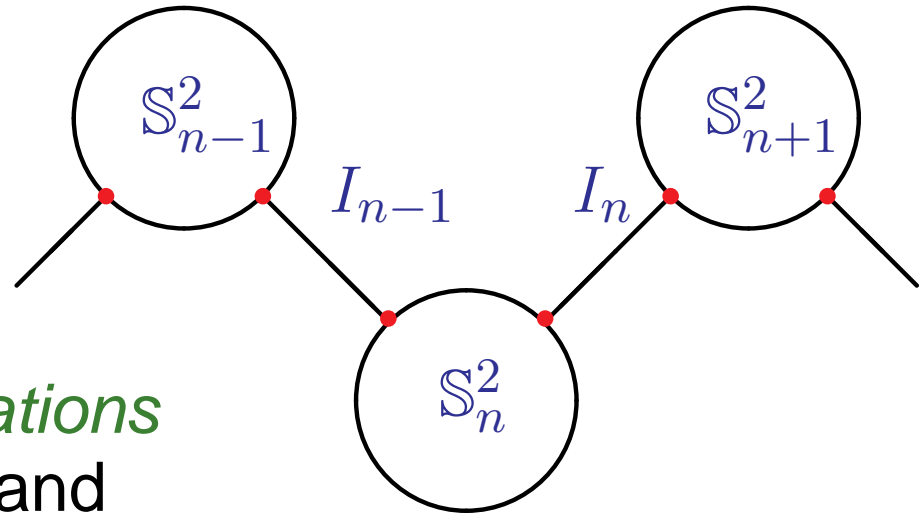
Recall properties of *singular Wannier-Stark* systems:



Spectrum of such systems is *purely discrete* which is proved for “most” values of the parameters [Asch-Duclos-E., 1998] and conjectured for *all* values. The reason behind are *large gaps* of δ' Kronig-Penney systems



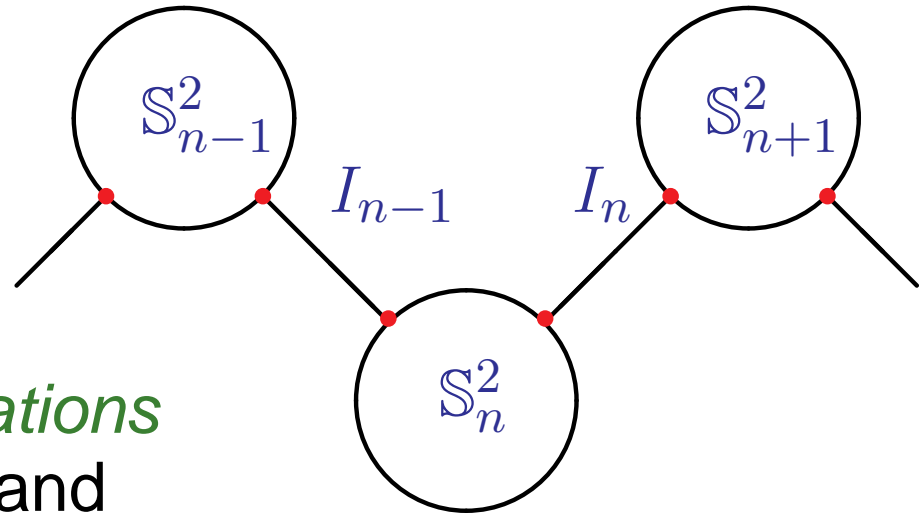
Periodic systems – assumptions



Consider *periodic combinations of spheres and segments* and adopt the following assumptions:

- periodicity in one or two directions (one can speak about “bead arrays” and “bead carpets”)

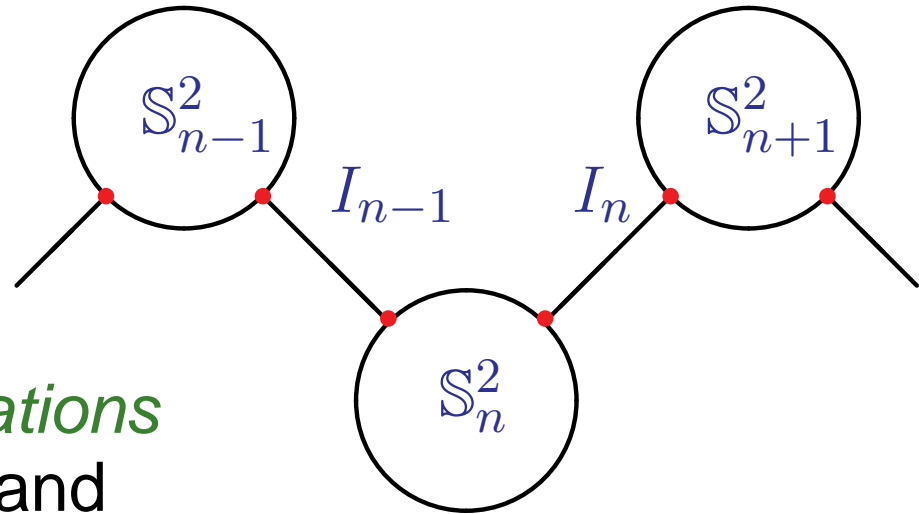
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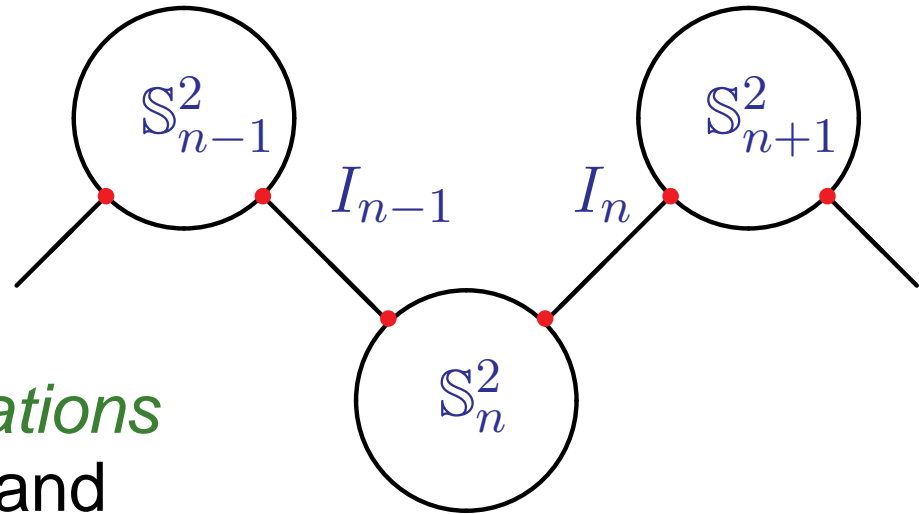
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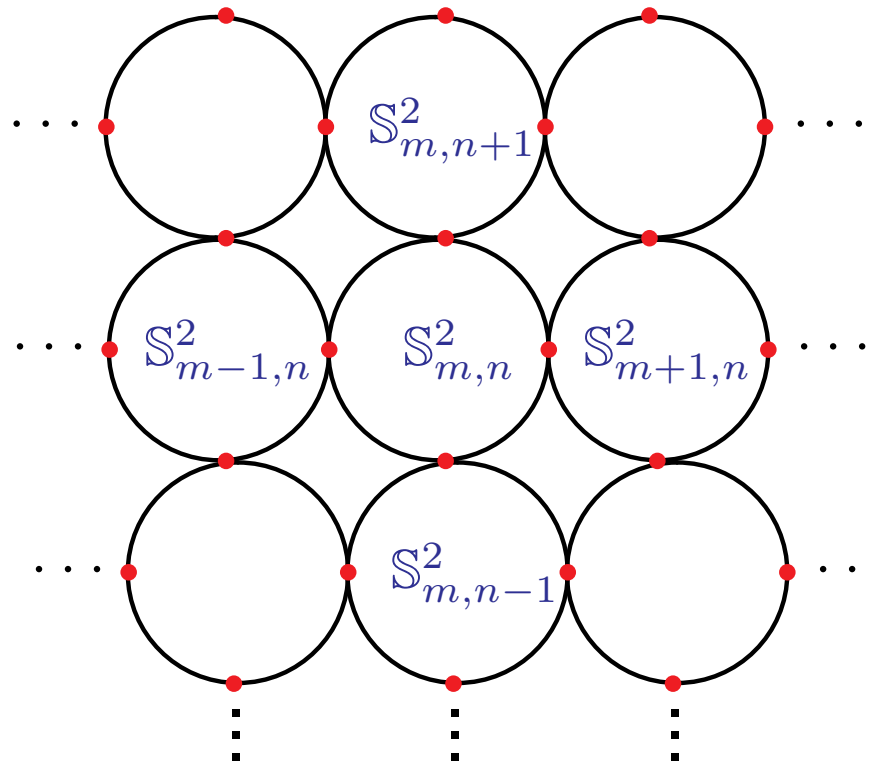


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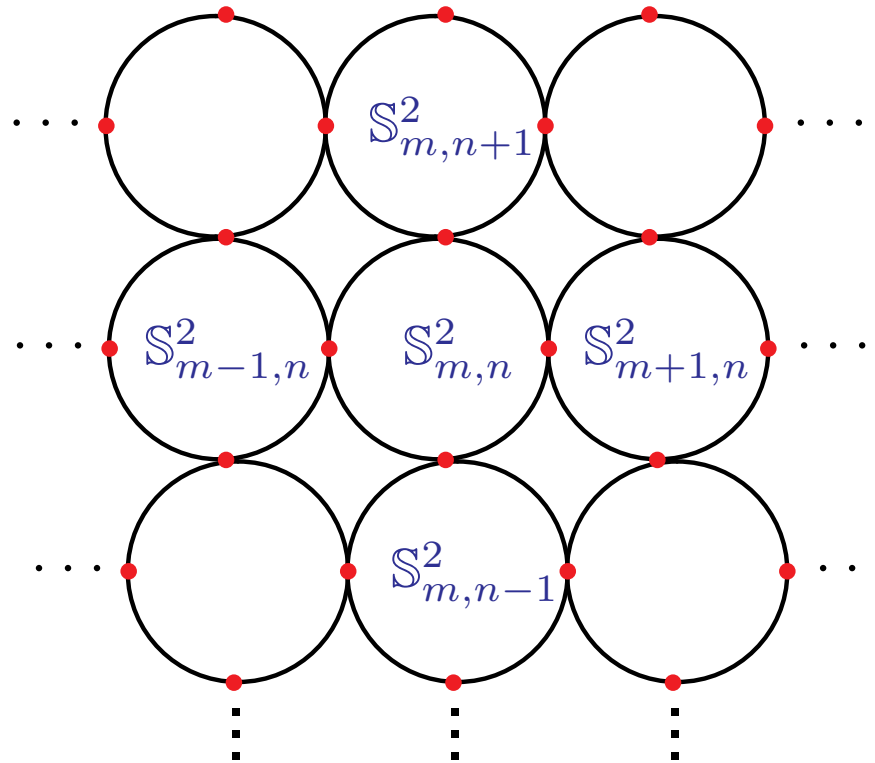
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- we allow also *tight coupling* when the spheres touch



Tightly coupled spheres



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The tight-coupling boundary conditions will be

$$L_1(\Phi_1) = AL_0(\Phi_1) + CL_0(\Phi_2),$$

$$L_1(\Phi_2) = \bar{C}L_0(\Phi_1) + DL_0(\Phi_2)$$

with $A, D \in \mathbb{R}$, $C \in \mathbb{C}$. For simplicity we put $A = D = 0$



Large gaps in periodic manifolds

We analyze how spectra of the fibre operators depend on quasimomentum θ . Denote by B_n, G_n the widths of the n th band and gap, respectively; then we have



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holds as $n \rightarrow \infty$ for *loosely connected* systems, where $\epsilon = \frac{1}{2}$ for arrays and $\epsilon = \frac{1}{4}$ for carpets. For *tightly coupled* systems to any $\epsilon \in (0, 1)$ there is a $\tilde{c} > 0$ such that the inequality $B_n/G_n \leq \tilde{c} (\ln n)^{-\epsilon}$ holds as $n \rightarrow \infty$



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Conjecture: Similar results hold for other couplings and angular distances of the junctions. The problem is just technical; the dispersion curves are less regular in general



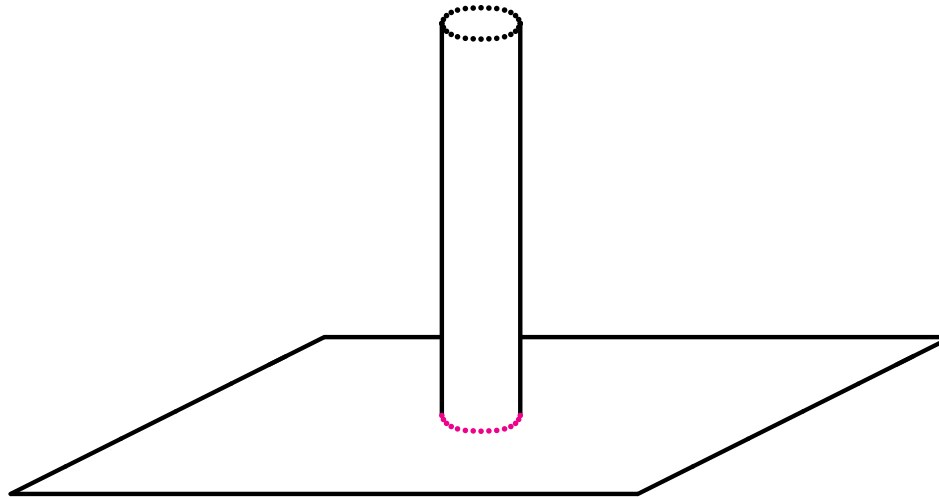
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Plane plus tube scattering

Rotational symmetry allows us again to treat each partial wave separately. Given orbital quantum number ℓ one has to match smoothly the corresponding solutions

$$\psi(x) := \begin{cases} e^{ikx} + r_a^{(\ell)}(k) e^{-ikx} & \dots & x \leq 0 \\ \sqrt{\frac{\pi kr}{2}} t_a^{(\ell)}(k) H_\ell^{(1)}(kr) & \dots & r \geq a \end{cases}$$



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This yields

$$r_a^{(\ell)}(k) = -\frac{\mathcal{D}_-^a}{\mathcal{D}_+^a}, \quad t_a^{(\ell)}(k) = 4i \sqrt{\frac{2ka}{\pi}} (\mathcal{D}_+^a)^{-1}$$

with

$$\mathcal{D}_\pm^a := (1 \pm 2ika) H_\ell^{(1)}(ka) + 2ka \left(H_\ell^{(1)} \right)'(ka)$$



Plane plus point: low energy behavior

Wronskian relation $W(J_\nu(z), Y_\nu(z)) = 2/\pi z$ implies scattering unitarity, in particular, it shows that

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Using asymptotic properties of Bessel functions with for small values of the argument we get

$$|t_a^{(\ell)}(k)|^2 \approx \frac{4\pi}{((\ell - 1)!)^2} \left(\frac{ka}{2}\right)^{2\ell-1}$$

for $\ell \neq 0$, so the *transmission probability vanishes fast* as $k \rightarrow 0$ for higher partial waves



Heuristic choice of coupling parameters

The situation is different for $\ell = 0$ where

$$H_0^{(1)}(z) = 1 + \frac{2i}{\pi} \left(\gamma + \ln \frac{ka}{2} \right) + \mathcal{O}(z^2 \ln z)$$



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Notice that the “right” s-a extensions depend on a *single parameter*, namely radius of the “thin” component



Illustration on *microwave experiments*

Our models do not apply to QM only. Consider an *electromagnetic resonator*. If it is *very flat*, Maxwell equations simplify: TE modes effectively decouple from TM ones and one can describe them by Helmholtz equation



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The reflection amplitude for a compact manifold with one lead attached at x_0 is found as above: we have

$$r(k) = - \frac{\pi Z(k)(1 - 2ika) - 1}{\pi Z(k)(1 + 2ika) - 1},$$

where $Z(k) := \xi(\vec{x}_0; k) - \frac{\ln a}{2\pi}$



Finding the resonances

To evaluate regularized Green's function we use ev's and ef's of Dirichlet Laplacian in $M = [0, c_1] \times [0, c_2]$, namely

$$\phi_{nm}(x, y) = \frac{2}{\sqrt{c_1 c_2}} \sin\left(n \frac{\pi}{c_1} x\right) \sin\left(m \frac{\pi}{c_2} y\right),$$

$$\lambda_{nm} = \frac{n^2 \pi^2}{c_1^2} + \frac{m^2 \pi^2}{c_2^2}$$



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Resonances are given by complex zeros of the denominator of $r(k)$, i.e. by solutions of the algebraic equation

$$\xi(\vec{x}_0, k) = \frac{\ln(a)}{2\pi} + \frac{1}{\pi(1 + ika)}$$



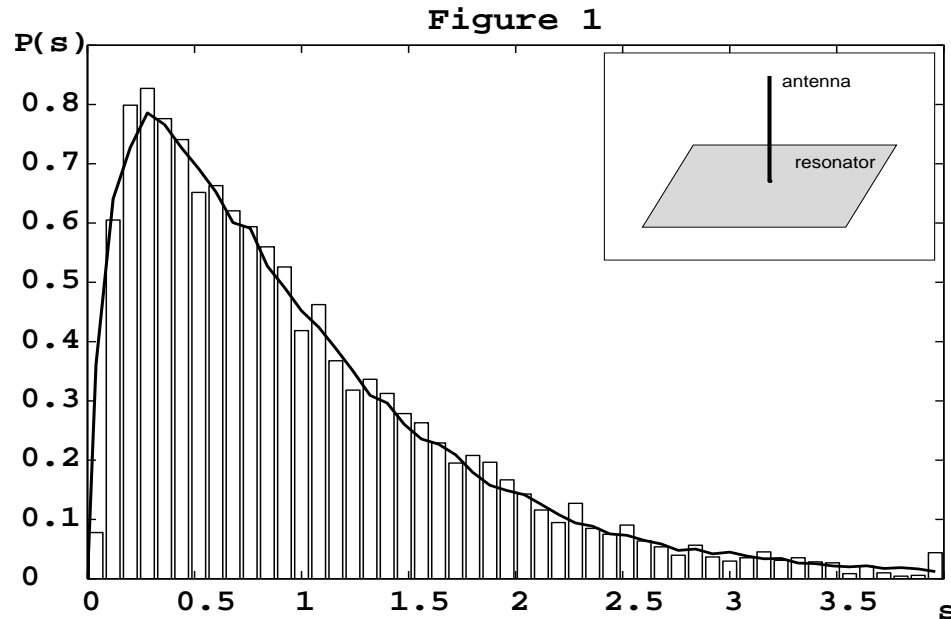
Comparison with experiment

Compare now *experimental results* obtained at University of Marburg with the model for $a = 1$ mm, averaging over x_0 and $c_1, c_2 = 20 \sim 50$ cm



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Important: An agreement is achieved with the *lower third* of measured frequencies – confirming thus validity of our approximation, since shorter wavelengths are comparable with the antenna radius a and $ka \ll 1$ is no longer valid



Spin conductance oscillations

Finally, manifolds we consider need not be separate spatial entities. Illustration: a spin conductance problem:

[Hu et al., 2001] measured conductance of polarized electrons through an InAs sample; the results *depended on length L* of the semiconductor “bar”, in particular, that for some L *spin-flip processes dominated*



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Physical mechanism of the spin flip is the *spin-orbit interaction with impurity atoms*. It is complicated and no realistic transport theory of that type was constructed



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Finally, manifolds we consider need not be separate spatial entities. Illustration: a spin conductance problem:

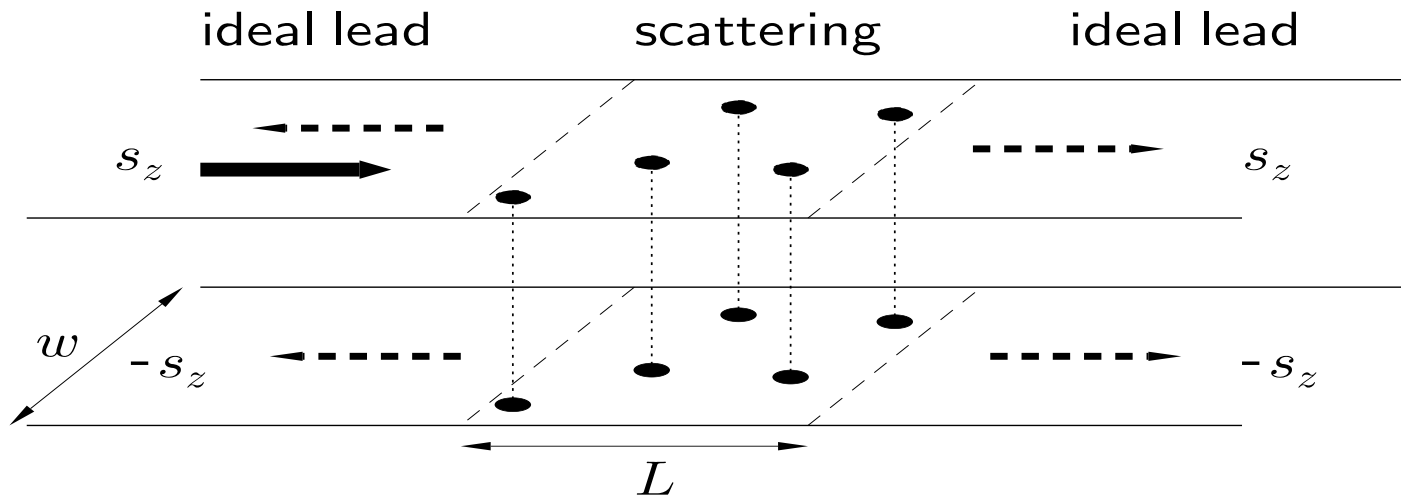
[Hu et al., 2001] measured conductance of polarized electrons through an InAs sample; the results *depended on length L* of the semiconductor “bar”, in particular, that for some L *spin-flip processes dominated*

Physical mechanism of the spin flip is the *spin-orbit interaction with impurity atoms*. It is complicated and no realistic transport theory of that type was constructed

We construct a *model* in which spin-flipping interaction has a *point character*. Semiconductor bar is described as *two strips coupled at the impurity sites* by the boundary condition described above



Spin-orbit coupled strips



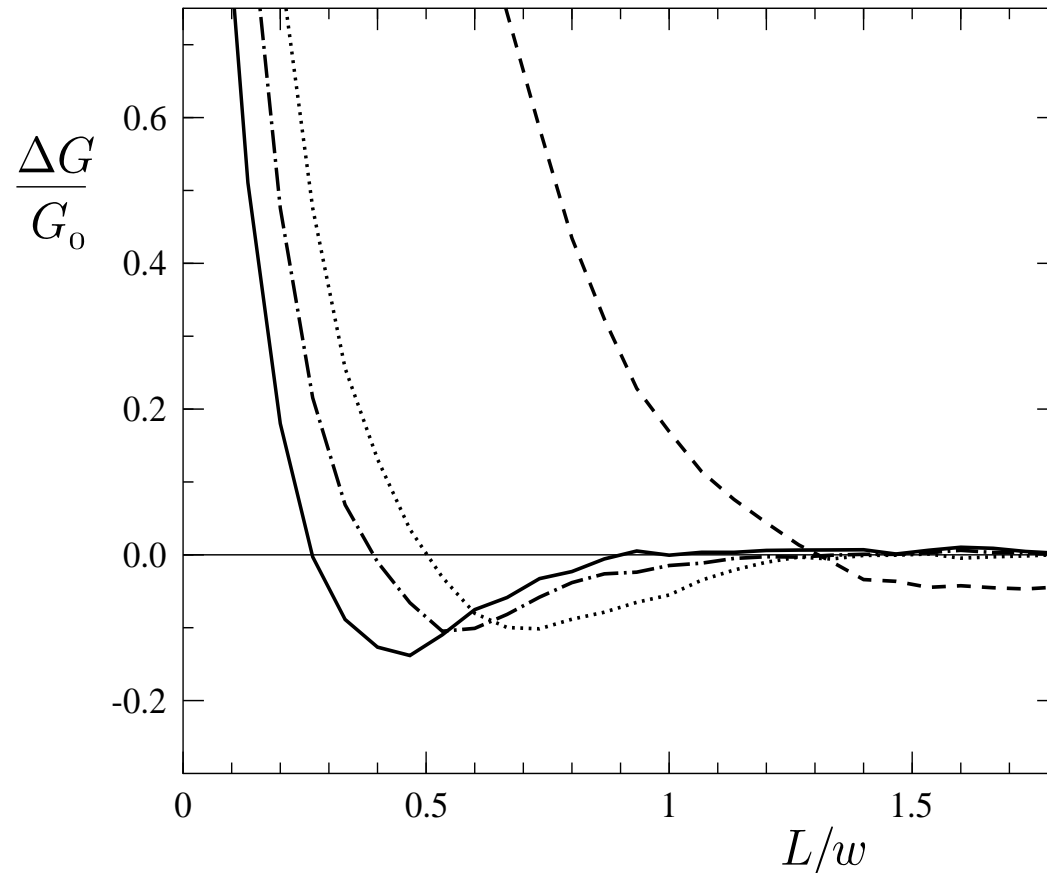
We assume that impurities are randomly distributed with the same coupling, $A = D$ and $C \in \mathbb{R}$. Then we can instead study a pair of decoupled strips,

$$L_1(\Phi_1 \pm \Phi_2) = (A \pm C)L_0(\Phi_1 \pm \Phi_2),$$

which have naturally different localization lengths

Compare with measured conductance

Returning to original functions Φ_j , *spin conductance oscillations* are expected. This is indeed what we see if the parameters assume realistic values:



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- In QM there is an *efficient technique to model them* generalizing ideal quantum graphs of *Lecture I*
- A typical feature of such systems is a *suppression of transport at high energies*
- This has consequences for spectral properties of *periodic and WS-type systems*
- Finally, concerning the *justification of coupling choice* a lot of work remains to be done; the situation is less understood than for quantum graphs of *Lecture I*



Some literature to Lecture III

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- [ETV01] P.E., M. Tater, D. Vaněk: A single-mode quantum transport in serial-structure geometric scatterers, *J. Math. Phys.* **42** (2001), 4050-4078
- [EŠ86] P.E., P. Šeba: Quantum motion on two planes connected at one point, *Lett. Math. Phys.* **12** (1986), 193-198
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- [EŠ97] P.E., P. Šeba: Resonance statistics in a microwave cavity with a thin antenna, *Phys. Lett.* **A228** (1997), 146-150
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and references therein, see also <http://www.ujf.cas.cz/~exner>



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- 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

