Quantum networks modelled by graphs

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Talk overview

- Quantum graphs: a short review

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- Vertex coupling parametrization, examples

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- Summary and outlook

Quantum graph concept

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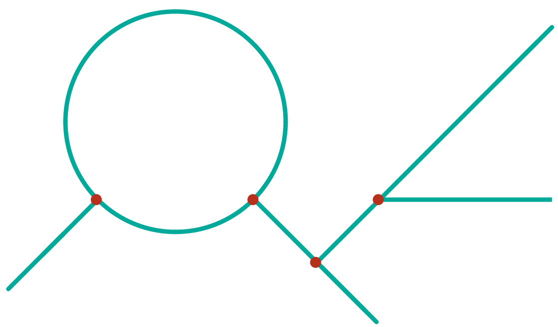
The concept extends, however, to graphs of *arbitrary shape*



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

and what is important, it became *practically important* after experimentalists learned in the last two decades 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 one can consider *generalized graphs* which consist of components of different dimensions
- Now when the microstructures reach *molecular size* quantum graphs "return" in a sense to their origin!

More remarks

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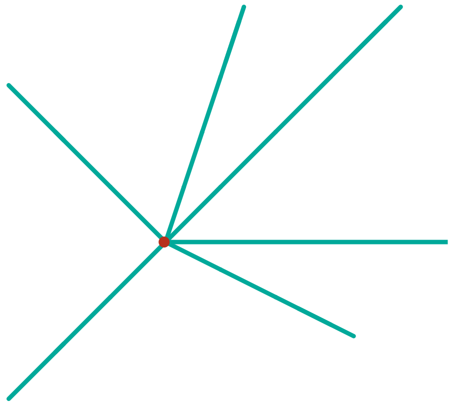
- Graphs can support also *Dirac operators*, see [Bulla-Trenckler'90], [Bolte-Harrison'03], although this remains so far a theoretical possibility only.
- The graph literature is extensive; recall just a review [Kuchment'04], proceedings of Snowbird'05 conference, and present AGA Programme at INI Cambridge

Vertex coupling



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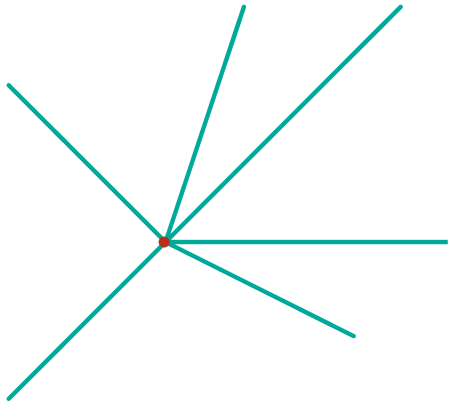

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Since it is second-order, the boundary condition involve $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$ being of the form

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

by [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

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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

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

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- 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*,

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

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

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

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

Further examples

- Another generalization of 1D δ' is the δ' *coupling*:
$$\sum_{j=1}^{n} \psi_j'(0) = 0\,, \quad \psi_j(0) - \psi_k(0) = \frac{\beta}{n}(\psi_j'(0) - \psi_k'(0))\,, \; 1 \le j,k \le n$$
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

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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.

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

Why are vertices interesting?

Apart of a general mathematical interest, there are specific reasons related to various use of such models, e.g.

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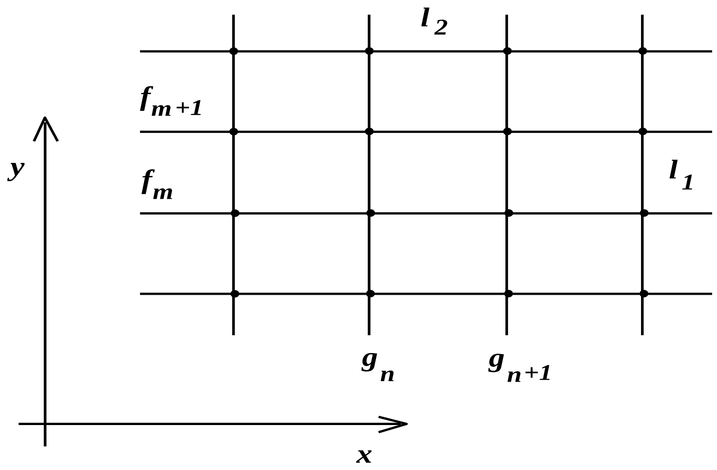
- A nontrivial vertex coupling can lead to *number theoretic properties* of graph spectrum; I will show a simple example below
- On more practical side, the conductivity of graph nanostructures is controlled typically by external fields, vertex coupling can serve the same purpose
- In particular, the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



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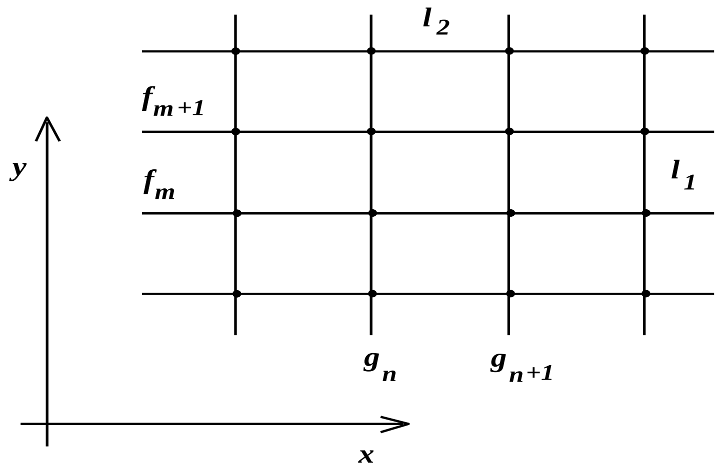

Spectral condition for quasimomentum (θ_1, θ_2) reads

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

Lattice band spectrum

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

- *"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)

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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 $|\alpha| < \alpha_0$

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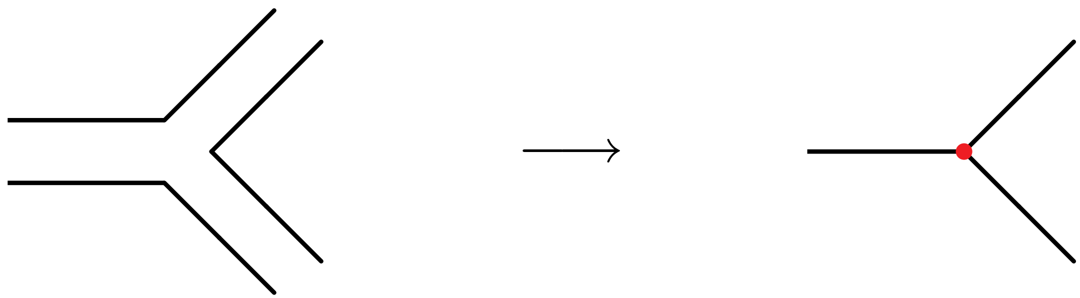
Clearly, *understanding of vertex couplings* is needed when one wants to model real physical systems by such graphs

A head-on approach

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



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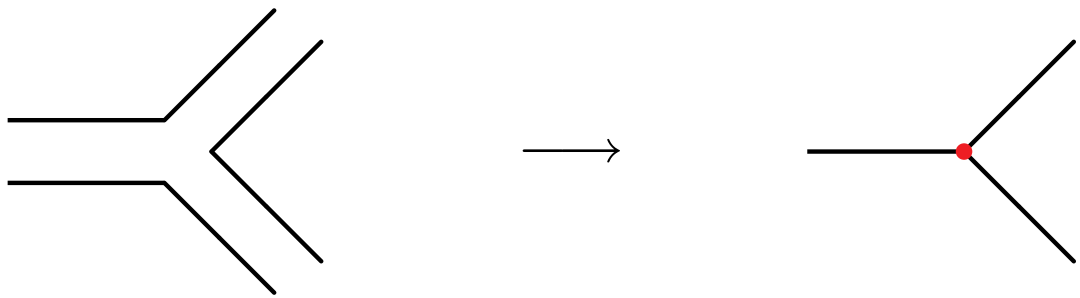

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- after a long effort the *Neumann-like case* was solved [Freidlin-Wentzell'93], [Freidlin'96], [Saito'01], [Kuchment-Zeng'01], [Rubinstein-Schatzmann'01], [E.-Post'05], [Post'06] giving free b.c. only
- there is a recent progress in *Dirichlet case*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

More on the Dirichlet case

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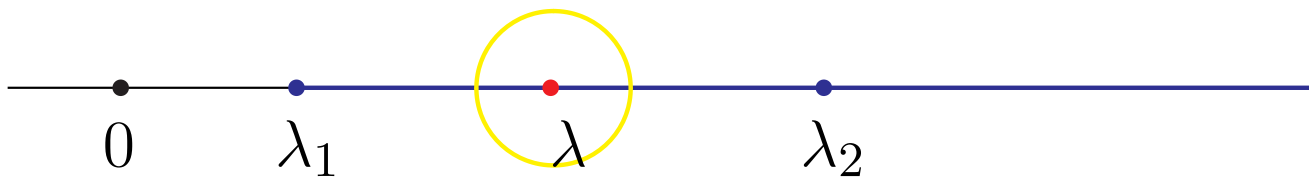
More on the Dirichlet case

- *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]

Back to the Neumann case: first, the graph

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 $u \mapsto \|u'\|^2_{M_0} := \sum_{j \in J} \|u'\|^2_{I_j}$ 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 Δ_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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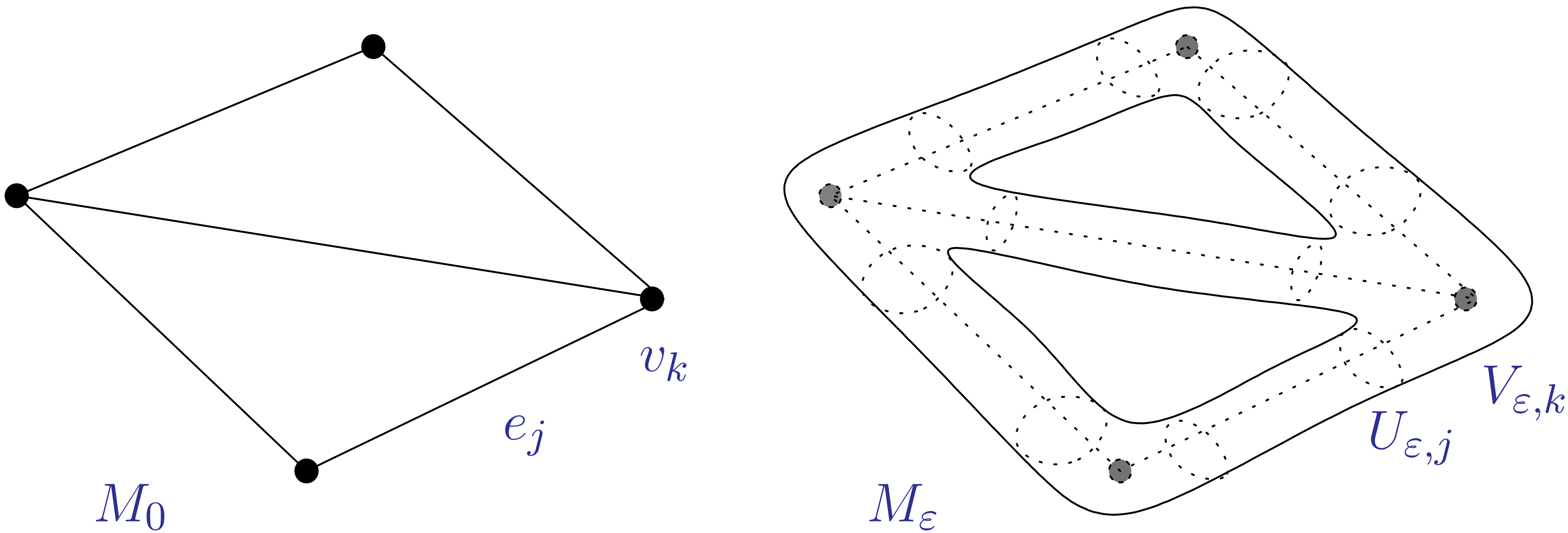
If X is compact with piecewise smooth boundary, one starts from the form defined on $C^\infty(X)$. This yields Δ_X as the *Neumann* Laplacian on X and allows us to treat “fat graphs” and “sleeves” on the same footing

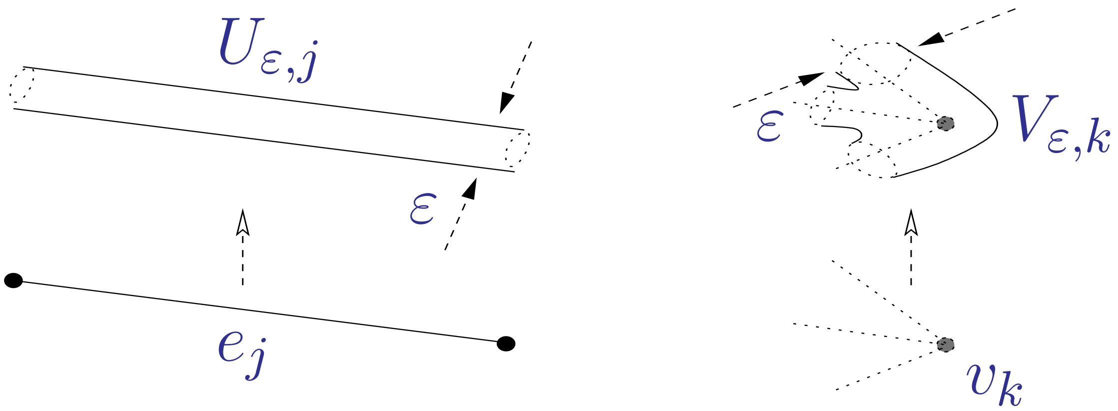
Fat graphs and sleeves: manifolds

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



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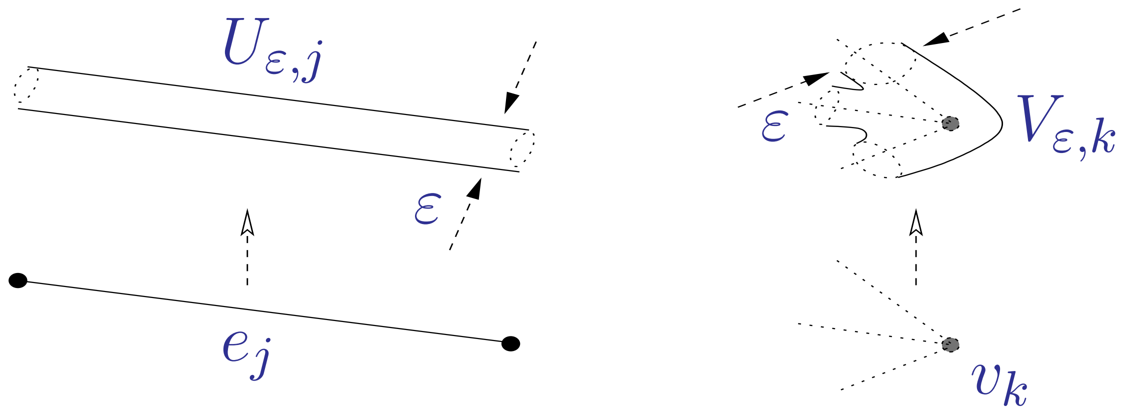

However, M_ε *need not be embedded* in some $\mathbb{R}^d$.

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 $\mathrm{vol}\, F = 1$. 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

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

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

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

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

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

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

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:

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

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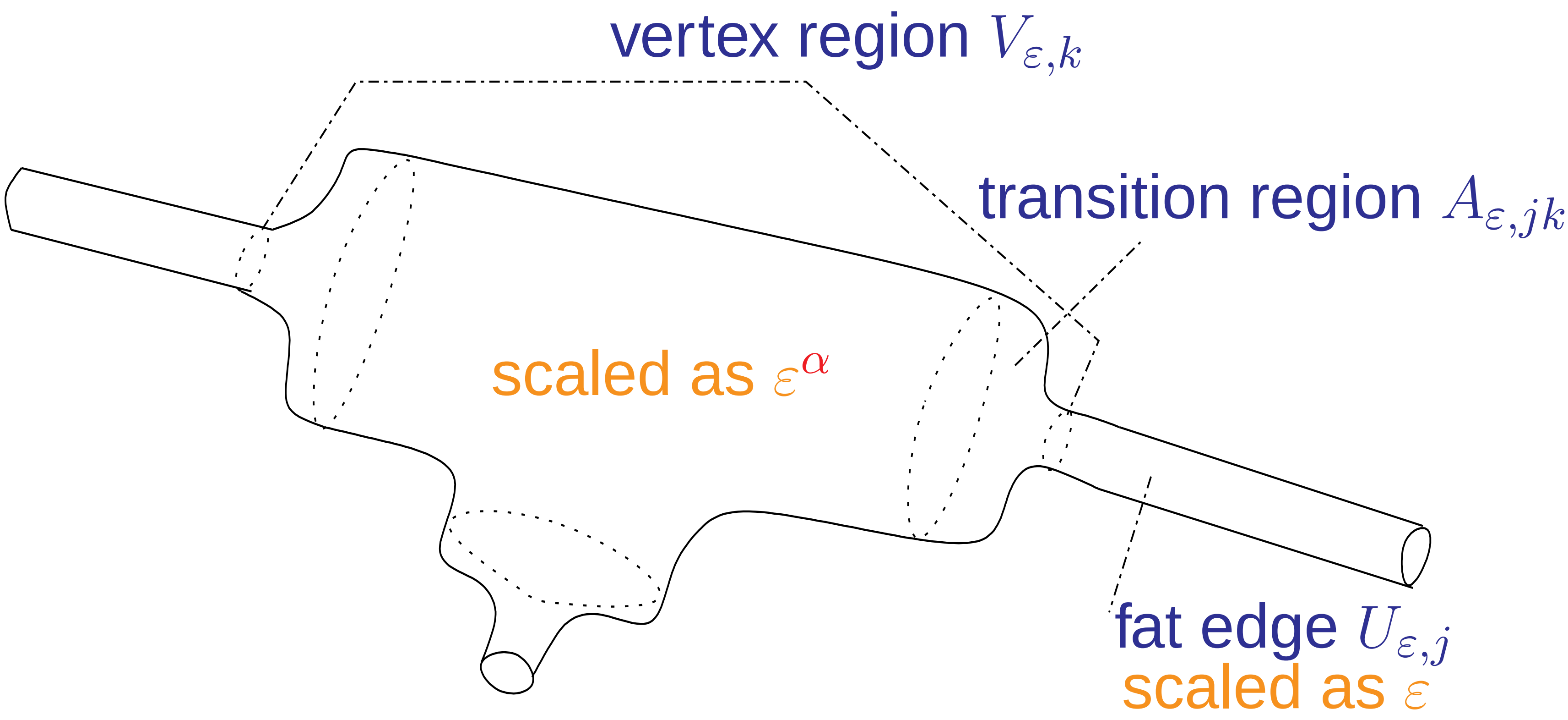
A way out could thus be to use *different* scaling rates of edges and vertices. Of a particular interest is the borderline case, $\mathrm{vol}_d V_\varepsilon \approx \mathrm{vol}_{d-1} \partial V_\varepsilon$, when the integral of $\langle \mathrm{d}\phi, \mathrm{d}u \rangle$ is expected to be negligible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

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- 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 $(\mathrm{vol}\,(V_k^-)^{1/2} u_j(v_k) = u_k$

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- finally, if vertex regions do not scale at all, $\alpha = 0$, the manifold components decouple in the limit again,

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

Thus scaling trick gives just free b.c.: to get more either *manifold geometry* or *external potentials* must be added

A stronger convergence

The b.c. are not the only problem. The ev convergence for finite graphs is rather weak. Fortunately, one can do better.

Theorem [Post'06]: Let M_ε be graphlike manifolds associated with a metric graph M_0, *not necessarily finite*. Under some natural uniformity conditions, $\Delta_{M_\varepsilon} \to \Delta_{M_0}$ as $\varepsilon \to 0+$ in the *norm-resolvent sense* (with suitable identification), in particular, the σ_{disc} and σ_{ess} converge uniformly in an bounded interval, and ef's converge as well.

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The *natural uniformity conditions* mean (i) existence of nontrivial bounds on vertex degrees and volumes, edge lengths, and the second Neumann eigenvalues at vertices, (ii) appropriate scaling (analogous to the described above) of the metrics at the edges and vertices.

Proof is based on an abstract convergence result.

Convergence of resonances

In a similar way we can treat convergence of resonances. As a motivating example one can think of a *“fat lasso”* graph, with the ε-squeezing setting the same as before:

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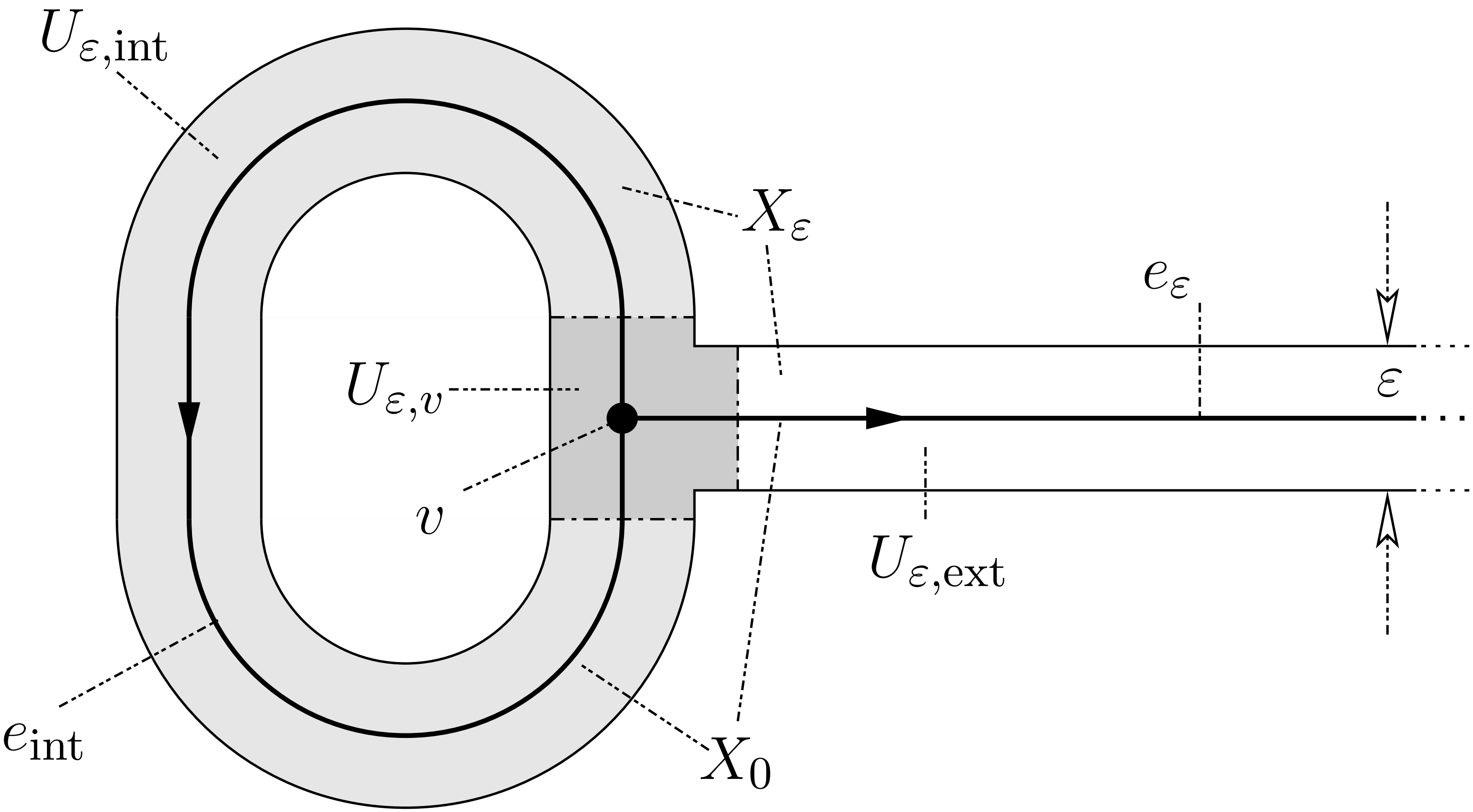

Convergence of resonances, continued

Let H_0, with free b.c., and H_ε will be as above. We use an *exterior complex scaling* extending to complex θ the map

$$U^\theta f := (\det D\Phi^\theta)^{1/2}(f \circ \Phi^\theta)$$

where $\Phi_e^\theta(x) := \mathrm{e}^\theta x$ on external edges, and $(\det D\Phi^\theta)^{1/2}$ equals one and $\mathrm{e}^{\theta/2}$, respectively, on $X_{0,\mathrm{int}}$ and $X_{0,\mathrm{ext}}$.

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Theorem [E.-Post'07]: Let $\lambda(0)$ be a resonance of H_0 of multiplicity $m > 0$, then for small enough $\varepsilon > 0$ there is m resonances $\lambda_1(\varepsilon), \dots, \lambda_m(\varepsilon)$ of H_ε, not necessarily distinct, which all converge to $\lambda(0)$ as $\varepsilon \to 0$. The same is true for embedded ev's of H_0, when $\mathrm{Im}\,\lambda_j(\varepsilon) \le 0$ holds in general.

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Remarks: (i) The above Φ^θ can have a shifted discontinuity, or be replaced by a smooth flow, with the same result
(ii) The result persists if a magnetic field is added

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

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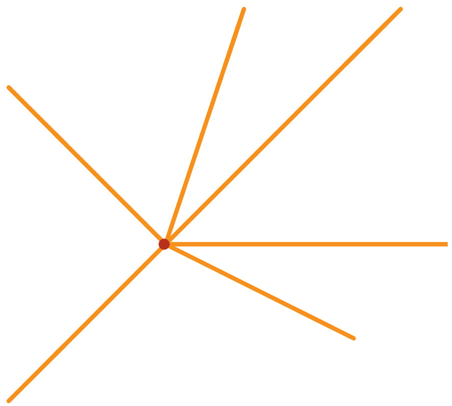

Consider once more *star graph* with $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and Schrödinger operator acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j'' + V_j\psi_j$

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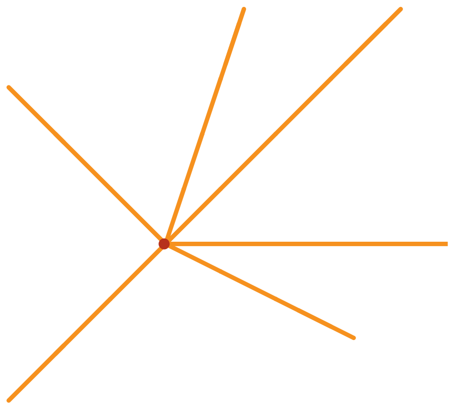

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We make the following assumptions:

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

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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*

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  In that case, its asymptotic behavior is given by

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

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

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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* [Albeverio-Nizhnik'00], [E.-Neidhardt-Zagrebnov'01]

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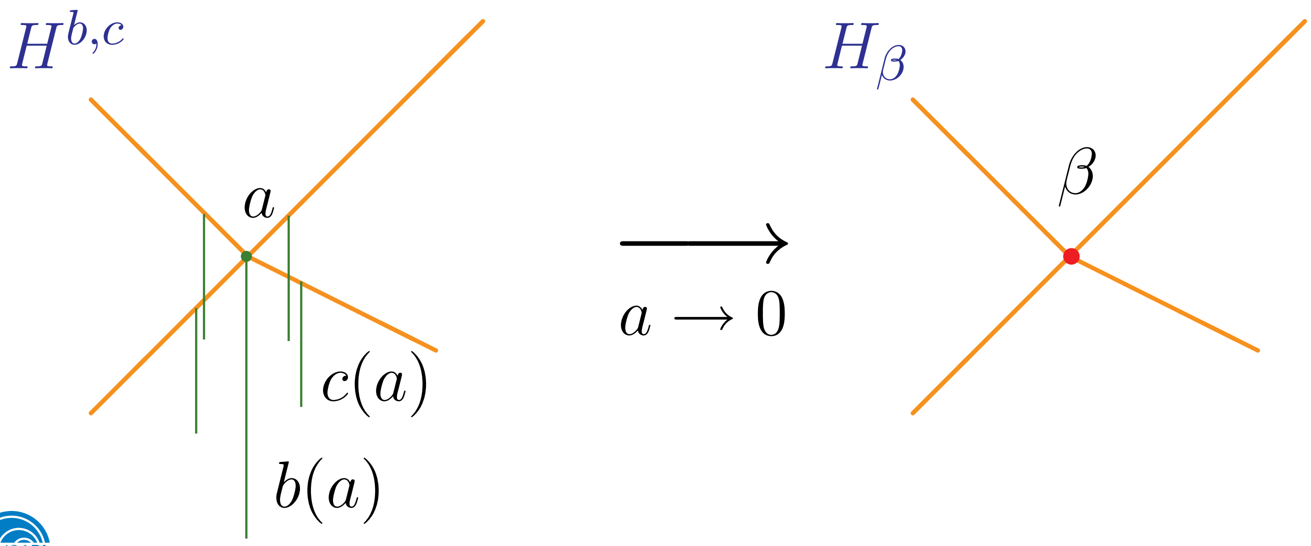
This suggests the following scheme:



A heuristic argument

In the symmetric sector, $\psi_j = \psi_k$, we can drop the indices. The boundary values at $x = 0$ and $x = a$ are related by

$$\psi(a) = \psi(0) + a\psi'(0) + \mathcal{O}(a^2)\,, \quad \psi'(a-) = \psi'(0+) + \mathcal{O}(a)\,,$$
$$\psi'(a+) = \psi'(a-) + c\psi(a)\,, \quad n\psi'(0+) = b\psi(0)$$

Eliminating $\psi(0)$ and $\psi'(0+)$ from here, we get in the leading order the relation $B(a)\psi(a) = \psi'(a+)$, where

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Hence $\beta\psi'(0+) = n\psi(0)$, is achieved as $a \to 0+$ if we choose

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

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In the orthogonal complement we again drop the index, because the operators act in the same way on all the linear combinations of $\sum_{j=1}^{n} d_j \psi_j(x)$ with $\sum_{j=1}^{n} d_j = 0$. The b.c. at origin is now replaced by $\psi(0) = 0$

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Eliminating then the boundary values at $x = 0$ we get in the leading order the relation $\psi'(a+) = (c + a^{-1})\psi(a) + \mathcal{O}(a)$. The right-hand side vanishes if we choose again

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giving Neumann condition, $\psi'(0+) = 0$, in the limit

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

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Proof: By symmetry the task is reduces to a pair of halfline problems. Consider first the one with Dirichlet condition at the origin, so the free Green's function at energy k^2 is $G_k(x,y) = \frac{\sin kx_<}{k}\,\mathrm{e}^{ikx_>}$ for $x, y \geq 0$

The Green's function of the operator with the δ interaction at $x = a$ is obtained easily by Krein's formula

$$G_k^c(x,y) = G_k(x,y) + \frac{G_k(x,a)G_k(a,y)}{-c^{-1} - G_k(a,a)}$$

Proof

The Neumann Green's function is $G_k^N(x,y) = \frac{\cos kx_<}{k}\, \mathrm{e}^{ikx_>}$; the two have to converge to each other for some $k^2 \in \mathbb{C}$.

Choose $k = i\kappa$ with $\kappa > 0$, then the denominator is nonzero for a small enough. It is sufficient to compute the difference in the case when neither of the arguments is smaller than a; for definiteness suppose that $a \le x \le y$; then

$$G_{i\kappa}^c(x,y) - G_{i\kappa}^N(x,y) = \frac{\mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y}}{\kappa} \left[-1 + \frac{\sinh^2 \kappa a}{-\kappa c^{-1} - \mathrm{e}^{-\kappa x} \sinh^2 \kappa a} \right]$$

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If $c = -a^{-1}$ the last term is $1 + \mathcal{O}(a)$ for $a \to 0+$, so

$$\lim_{a\to 0+} G_{i\kappa}^c(x,y) = G_{i\kappa}^N(x,y)$$

holds for all $x, y > 0$

Proof, continued

Consider next δ coupling at the origin using the same values of parameters, $k = i\kappa$ and $a \le x \le y$. We need the following two Green's functions,

$$G^b_{i\kappa}(x,y) = \frac{\mathrm{e}^{-\kappa y}}{\kappa(b+\kappa)}\left(b \sinh \kappa x + \kappa \cosh \kappa x\right),$$

$$G^\beta_{i\kappa}(x,y) = \frac{\mathrm{e}^{-\kappa y}}{\kappa(n+\beta\kappa)}\left(n \sinh \kappa x + \beta\kappa \cosh \kappa x\right)$$

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The first of them determines the full approximating Green's function by Krein's formula,

$$G^{b,c}_k(x,y) = G^b_k(x,y) + \frac{G^b_k(x,a)G^b_k(a,y)}{-c^{-1} - G^b_k(a,a)}$$

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$$\left. + \frac{\frac{\mathrm{e}^{-\kappa x}}{(b+\kappa)^2}(b\sinh\kappa x + \kappa\cosh\kappa x)^2}{\kappa a - \frac{\mathrm{e}^{-\kappa a}}{b+\kappa}(b\sinh\kappa x + \kappa\cosh\kappa x)} - \frac{n\sinh\kappa x + \beta\kappa\cosh\kappa x}{n+\beta\kappa} \right]$$

Proof, continued

$$G^{b,c}_{i\kappa}(x,y) - G^{\beta}_{i\kappa}(x,y) = \frac{\mathrm{e}^{-\kappa y}}{\kappa}\left[\frac{b\sinh\kappa x + \kappa\cosh\kappa x}{b+\kappa}\right.$$

$$\left. + \frac{\frac{\mathrm{e}^{-\kappa x}}{(b+\kappa)^2}(b\sinh\kappa x + \kappa\cosh\kappa x)^2}{\kappa a - \frac{\mathrm{e}^{-\kappa a}}{b+\kappa}(b\sinh\kappa x + \kappa\cosh\kappa x)} - \frac{n\sinh\kappa x + \beta\kappa\cosh\kappa x}{n+\beta\kappa}\right]$$

The first term tends to $\sinh\kappa x$ as $a \to 0+$, while the third one is independent of a, so their sum in the limit gives $-\frac{\beta\kappa\,\mathrm{e}^{-\kappa x}}{n+\beta\kappa}$. Next we take the middle term without the factor $\mathrm{e}^{-\kappa x}$ and expand the numerator and denominator to the second power in a; this together gives

$$\lim_{a\to 0+} G^{b,c}_{i\kappa}(x,y) = G^{\beta}_{i\kappa}(x,y)\,, \qquad x,y>0$$

Finally, the pointwise convergence implies convergence of the resolvents in the HS-norm $\square$

Permutation symmetry

We have employed the fact that each of the Hamiltonians H_β and $H^{b,c}(a)$ decomposes into a nontrivial part which acts on the *one-dimensional subspace* of $\mathcal{H} = \bigoplus_{j=1}^n L^2(\mathbb{R}_+)$ of functions symmetric w.r.t. permutations, $\psi_j(x) = \psi_k(x)$ for all j, k, and the $(n-1)$-dimensional part corresponding to *Dirichlet* and *Neumann condition* at the central vertex for the δ and δ'_s coupling, respectively

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A similar reduction to a halfline problem can be used also for all permutation-symmetric couplings – cf. [E.-Turek'06]. In the generic case the scheme works with

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

other appropriate choices of $b(a),\, c(a)$ cover the exceptions

Nonsymmetric singular couplings

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Proposition [E.-Turek'07]: Let Γ be an n-edged star graph and $\Gamma(d)$ obtained by adding a finite number of δ's at each edge, uniformly in d, at the distances $\mathcal{O}(d)$ as $d \to 0_+$. Suppose that the approximations gives KS conditions with some $A,\, B$ as $d \to 0$. The family which can be obtained in this way *depends on $2n$ parameters* if $n > 2$, and on three parameters for $n = 2$.

Number of CS parameters

Let us *sketch the proof:* as before we can use Taylor expansion to express boundary values of a δ through those of the neighbouring one. Using it recursively, we write $\psi(0),\, \Psi'(0+)$ through $\psi_j(d_j),\, \psi_j'(d_{j+})$ where d_j means distance of the last δ on j-th halfline

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Using the δ coupling in the centre of Γ we get

$$\begin{aligned} c_j\psi_j(0) - c_k\psi_k(0) + t_j\psi_j'(0_+) - t_k\psi_k'(0_+) &= 0\,, \quad 1 \le j, h \le n\,, \\ \sum_{j=1}^n \gamma_j\psi_j(0) + \sum_{j=1}^n \tau_j\psi_j'(0_+) &= 0\,, \end{aligned}$$

which be written as $A\Psi(0) + B\Psi'(0) = 0$ with coefficients dependent on $2n$ parameters.

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In the particular case $n = 2$ the number of independent parameters is three, see also [Shigehara et al.'99]

A concrete approximation

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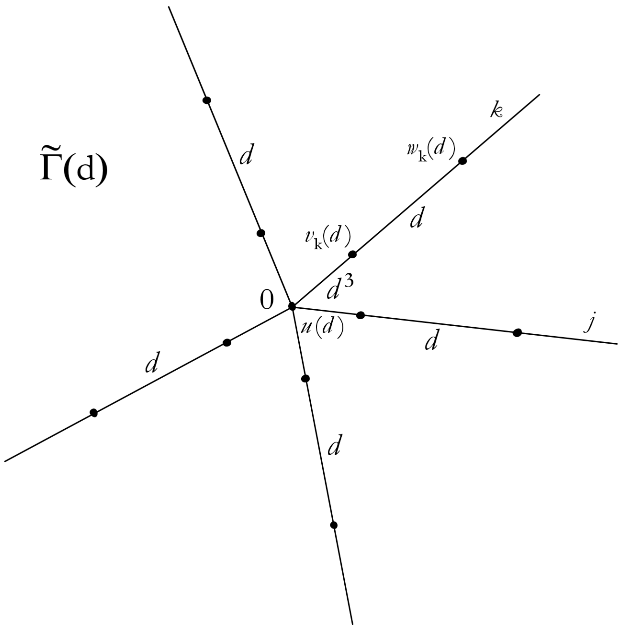

CS-type approximation of star graphs

Theorem [E.-Turek'07]: Choose the above quantities as

$$u(d) = \frac{\omega}{d^4}\,, \quad v_j(d) = -\frac{1}{d^3} + \frac{\alpha_j}{d^2}\,, \quad w_j(d) = -\frac{1}{d} + \beta_j\,.$$

Then the corresponding $H^{u,\vec{v},\vec{w}}(d)$ converges as $d \to 0_+$ in the norm-resolvent sense to some $H^{\omega,\vec{\alpha},\vec{\beta}}$ depending explicitly on $2n$ parameters (notice that, say, α_1 and β_1 cannot be chosen independently here)

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Proof is rather tedious but straightforward; one has to construct both resolvents and compare them. $\square$

It is clear that to get a wider class of couplings one must employ other objects as approximants

More general approximations

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Proposition [E.-Turek'07]: Consider graphs $\tilde\Gamma(d)$ obtained from Γ by adding edges connection pairwise the halflines, a finite of them independent of d. Suppose that $\tilde\Gamma(d)$ supports only δ couplings and δ interactions, their number again independent of d, and that the distances between all their sites are $\mathcal{O}(d)$ as $d \to 0_+$. The family of conditions $A\Psi(0) + B\Psi'(0) = 0$ which can be obtained in this way has *real-valued coefficients*, $A, B \in \mathbb{R}^{n,n}$, depending thus on at most $\binom{n+1}{2}$ parameters.

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Remark: The requirement $A, B \in \mathbb{R}^{n,n}$ means that the corresponding coupling is *time-reversal invariant*

An approximation arrangement

For simplicity, consider the generic case with B regular, so that $\Psi'(0) = -B^{-1}A\Psi(0)$, where $-B^{-1}A$ is symmetric. We divide into *diagonal* and *off-diagonal* part

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We devise the following scheme:

- centre of Γ supports a δ coupling with parameter $u(d)$
- at each halfline we place a δ at the distance d from the centre; the parameter $v_j(d)$ will be related to D_{jj}
- the pairs of edges whose indices j, k correspond to nonzero elements of S we join by an additional edge, whose endpoints are the δ's mentioned above, and in the middle of this edge we place δ interaction with a parameter $w_{\{j,k\}}(d)$ related to the value of S_{jk}

The arrangement, visualization

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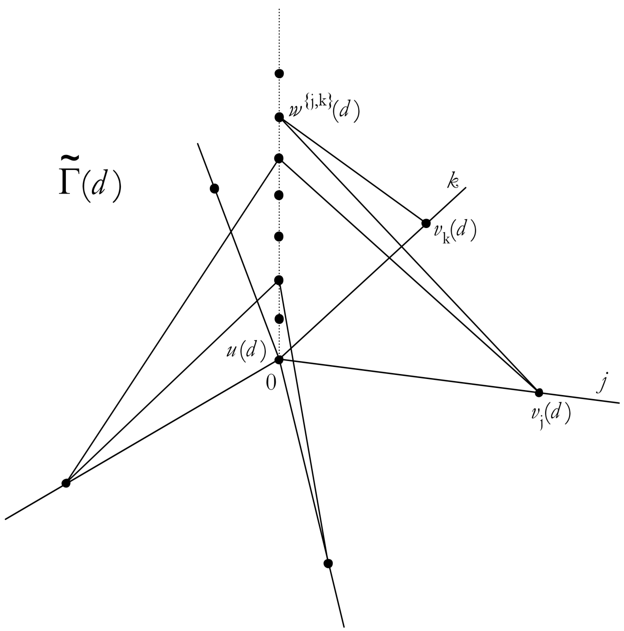

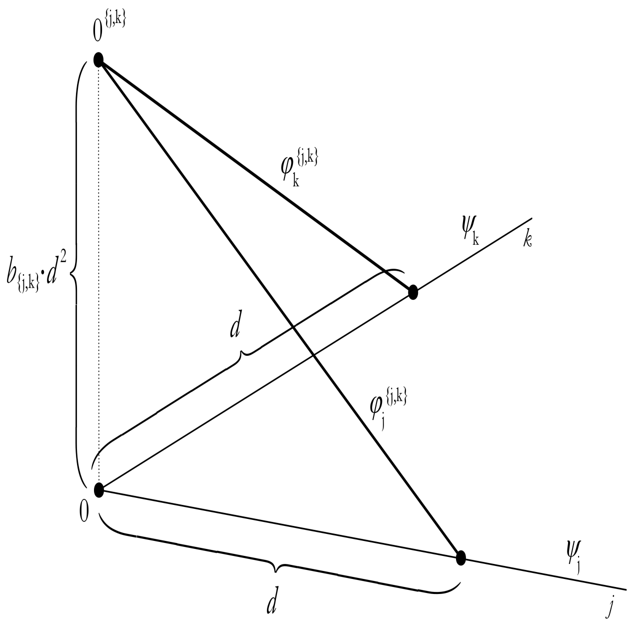

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As before we use the δ conditions and Taylor expansions to write $\psi'_j(d_+)$ through $\psi_j(d)$, $k = 1, ..., n$, and pass to $d \to 0+$

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Denote $N_j := \{k \in \hat{n} :\ S_{jk} \neq 0\}$; then one has to choose

$$v_j(d) := D_j - \frac{\# N_j + 1}{d} - \sum_{k \in N_j} S_{jk}\,,$$

and furthermore,

$$w_{\{j,k\}}(d) := -\frac{1}{S_{jk}} \cdot \frac{1}{d^2} - \frac{2}{d}\,, \qquad u(d) := \frac{1}{d^3} - \frac{n}{d^2}\,.$$

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Conjecture: The described approximation converges again not only in terms of boundary conditions, but in the norm-resolvent sense as well

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- Analogous problems on *generalized graphs* with “edges” of different dimensions, etc.

The talk was based on

[CE04] T. Cheon, P.E.: An approximation to δ' couplings on graphs, *J. Phys. A: Math. Gen.* **A37** (2004), L329-335

[E96] P.E.: Weakly coupled states on branching graphs, *Lett. Math. Phys.* **38** (1996), 313-320

[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

[EP05] P.E., O. Post: Convergence of spectra of graph-like thin manifolds, *J. Geom. Phys.* **54** (2005), 77-115

[EP07] P.E., O. Post: Convergence of resonances on thin branched quantum wave guides, `math-ph/0702075`

[ET06] P.E., O. Turek: Approximations of permutation-symmetric vertex couplings in quantum graphs, *Proc. of the Conf. "Quantum Graphs and Their Applications" (Snowbird 2005)*; AMS "Contemporary Math" Series, vol. 415, pp. 109-120

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