Approximating quantum graphs by Schrödinger operators on thin networks

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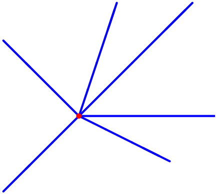
Talk overview

- Quantum graph vertex couplings
- Fat graph approximation idea, Dirichlet and Neumann case
- Generic Kirchhoff limit in the Neumann case: can one do better?
- Scaled potentials on graphs and lifting to fat graphs
- Beyond the δ-coupling case: Cheon & Shigehara idea
- Abandoning permutation symmetry: how many parameters ?
- A general solution in the Neumann case
- Summary and next challenges

Vertex coupling (if there is a need of a reminder)



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

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

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

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

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

Unique form of boundary conditions

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

Proposition (Harmer'00, K-S'00)

Vertex couplings are uniquely characterized by unitary $n \times n$ matrices U such that

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

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

Self-adjointness requires vanishing of the boundary form,

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

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

Examples of vertex coupling

- 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*,

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

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

- $\alpha = 0$ corresponds to the "free motion", the so-called *free boundary conditions* (better name than Kirchhoff)
- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the *δ_s' coupling*

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

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

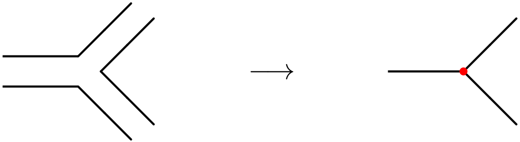
Why are vertices interesting?

Apart of a general interest, there are specific reasons related to various use of such models, for instance:

- The vertex coupling influences spectra of such Hamiltonians. For example, a nontrivial coupling can lead to *number theoretic properties* of graph spectrum – see, e.g., [E'96], [ET'15]
- On more practical side, the conductivity of graph nanostructures is controlled typically by external fields, vertex coupling can serve the same purpose. On does that today for photonic-crystal networks [Chien-Chen-Luan'06, Zhan-Wang'11] and it is only a matter of time to see the same for quantum graphs
- 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 of such a an approach to quantum computing, a modification of *Grover search algorithm* can be found in [Tanaka-Nemoto'10]

A natural approximation idea

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

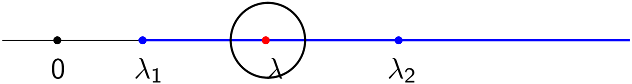


Unfortunately, it is not by far as simple as it looks!

- after a long effort the *Neumann-like case* was solved — see [Freidlin-Wentzell'93], [Freidlin'96], [Saito'01], [Kuchment-Zeng'01], [Rubinstein-Schatzmann'01], [E-Post'05, 07], [Post'06] — giving free b.c. only
- a recent progress in *Dirichlet case*: [Molchanov- Vainberg'07], [Albeverio-Cacciapuoti-Finco'07], [E-Cacciapuoti'07], [Grieser'08], [Dell'Antonio-Costa'10] but a lot remains to be done

Briefly, more on the Dirichlet case

- Here one expects *generically* that the limit *with the energy around the threshold* gives *Dirichlet decoupling*, but there may be *exceptional cases*
- The above claim depends energy renormalization one chooses, though. 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'07]

- resonances *on* or *around thresholds* can produce a nontrivial coupling [E-Cacciapuoti'07], [Grieser'08], [Dell'Antonio-Costa'10], etc.

A brief Neumann case survey

Let first 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 respective state Hilbert space is thus $L^2(M_0) := \bigoplus_{j\in J} L^2(I_j)$.

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.*

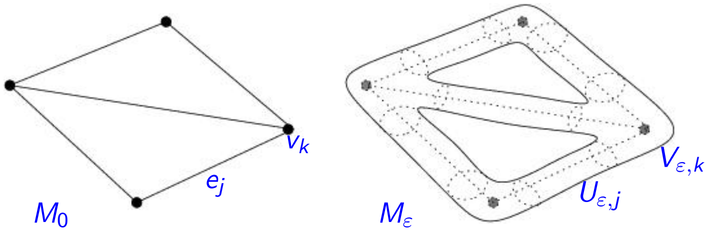
Consider next a Riemannian manifold X of dimension $d \geq 2$ and the corresponding space $L^2(X)$ w.r.t. volume $\mathrm{d}X$ equal to $(\det g)^{1/2}\mathrm{d}x$ in a fixed chart. For $u \in C^\infty_{\mathrm{comp}}(X)$ we set

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

The closure of this form is associated with the self-adjoint *Neumann* Laplacian Δ_X on the X.

Relating the two together

We associate with the graph M_0 a family of manifolds M_ε



which are all constructed from X by taking a suitable *ε-dependent family of metrics*; notice we work here with the *intrinsic* geometrical properties only.

The analysis requires dissection of M_ε into a union of compact edge and vertex components $U_{\varepsilon,j}$ and $V_{\varepsilon,k}$ with appropriate scaling properties, namely

Eigenvalue convergence

- 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

In this setting one can prove the following result:

Theorem (Kuchment-Zeng'01, E-Post'05)

Under the stated assumptions we have $\lambda_k(M_\varepsilon) \to \lambda_k(M_0)$ as $\varepsilon \to 0$ (giving thus free b.c.!)

Improving the convergence

The b.c. are not the only problem. The *ev* convergence for *finite* graphs is a rather weak result. 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.

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.

More results, and what next

For graphs with semi-infinite "outer" edges one often studies *resonances*. What happens with them if the graph is replaced by a family of "fat" graphs?

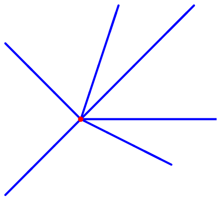
Using *exterior complex scaling* in the "longitudinal" variable one can prove a convergence result for resonances as $\varepsilon \to 0$ [E-Post'07]. The same is true for *embedded eigenvalues* of the graph Laplacian which may remain embedded or become resonances for $\varepsilon > 0$

Hence we have a number of convergence results, however, the limiting operator corresponds always to free b.c. only

Can one do better?

As a hint, an approximation on graphs

The way out: *replace the Laplacian by suitable Schrödinger operators*. Look first at the problem on the graph alone



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

We make the following assumptions:

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

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

Potential approximation of δ coupling

Suppose that the potential has a shrinking component, i.e.

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

Theorem (E'96)

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

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

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

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

A network model of δ coupling: formulation

For simplicity we consider *star graphs*, extension to more general cases is straightforward. Let $G = I_v$ have one vertex v and $\deg v$ adjacent edges of lengths $\ell_e \in (0, \infty]$.

The corresponding Hilbert space is $\mathsf{L}_2(G) := \bigoplus_{e \in E} \mathsf{L}_2(I)_e$, the *decoupled* Sobolev space of order k is defined as

$$\mathsf{H}^k_{\max}(G) := \bigoplus_{e \in E} \mathsf{H}^k(I_e)$$

together with its natural norm.

Let $\underline{p} = \{p_e\}_e$ be a vector of $p_e > 0$ for $e \in E$. The Sobolev space associated to $\underline{p}$ is

$$\mathsf{H}^1_{\underline{p}}(G) := \{\, f \in \mathsf{H}^1_{\max}(G) \,|\, \underline{f} \in \mathbb{C}\underline{p} \,\},$$

where $\underline{f} := \{f_e(0)\}_e$, in particular, if $\underline{p} = (1, \dots, 1)$ we arrive at the *continuous* Sobolev space denoted simply as $\mathsf{H}^1(G) := \mathsf{H}^1_{\underline{p}}(G)$.

Operators on the graph

We introduce first the (weighted) *free* Hamiltonian Δ_G defined via the quadratic form $\mathfrak{d} = \mathfrak{d}_G$ given by

$$\mathfrak{d}(f) := \|f'\|^2_G = \sum_e \|f'_e\|^2_{I_e} \quad \text{and} \quad dom\, \mathfrak{d} := \mathsf{H}^1_{\underline{p}}(G)$$

for a fixed $\underline{p}$ (we drop the index $\underline{p}$); form is a closed as related to the Sobolev norm $\|f\|^2_{\mathsf{H}^1(G)} = \|f'\|^2_G + \|f\|^2_G$.

Furthermore, the Hamiltonian with *δ-coupling of strength q* is defined via the quadratic form $\mathfrak{h} = \mathfrak{h}_{(G,q)}$ given by

$$\mathfrak{h}(f) := \|f'\|^2_G + q(v)|f(v)|^2 \quad \text{and} \quad dom\, \mathfrak{h} := \mathsf{H}^1_{\underline{p}}(G)$$

Using standard Sobolev arguments one can show that the δ-coupling is a "small" perturbation of the free operator by estimating the difference $\mathfrak{h}(f) - \mathfrak{d}(f)$ in various ways.

Manifold model of the "fat" graph

Given $\varepsilon \in (0, \varepsilon_0]$ we associate a d-dimensional manifold X_ε to the graph G as before: to the edge $e \in E$ and the vertex v we ascribe the Riemannian manifolds

$$X_{\varepsilon,e} := I_e \times \varepsilon Y_e \quad \text{and} \quad X_{\varepsilon,v} := \varepsilon X_v,$$

respectively, where εY_e is a manifold Y_e equipped with metric $h_{\varepsilon,e} := \varepsilon^2 h_e$ and $\varepsilon X_{\varepsilon,v}$ carries the metric $g_{\varepsilon,v} = \varepsilon^2 g_v$.

As before, we use the ε-independent coordinates $(s, y) \in X_e = I_e \times Y_e$ and $x \in X_v$, so the radius-type parameter ε only enters via the Riemannian metric

Note that this includes the case of the ε-neighbourhood of an embedded graph $G \subset \mathbb{R}^d$, but only up to a longitudinal error of order of ε. This can be dealt with again using an ε-dependence of the metric in the longitudinal direction.

The function spaces

The Hilbert space of the manifold model is

$$\mathsf{L}_2(X_\varepsilon) = \bigoplus_e \big(\mathsf{L}_2(I_e) \otimes \mathsf{L}_2(\varepsilon Y_e)\big) \oplus \mathsf{L}_2(\varepsilon X_v)$$

with the norm given by

$$\|u\|^2_{X_\varepsilon} = \sum_{e\in E} \varepsilon^{d-1} \int_{X_e} |u|^2 \,\mathrm{d}y_e \,\mathrm{d}s + \varepsilon^d \int_{X_v} |u|^2 \,\mathrm{d}x_v$$

where $\mathrm{d}x_e = \mathrm{d}y_e \,\mathrm{d}s$ and $\mathrm{d}x_v$ denote the Riemannian volume measures associated to the (unscaled) manifolds $X_e = I_e \times Y_e$ and X_v, respectively.

Let further $\mathsf{H}^1(X_\varepsilon)$ be the Sobolev space of order one, the completion of the space of smooth functions with compact support under the norm $\|u\|^2_{\mathsf{H}^1(X_\varepsilon)} = \|\mathrm{d}u\|^2_{X_\varepsilon} + \|u\|^2_{X_\varepsilon}$.

The operators

The Laplacian Δ_{X_ε} on X_ε is given via its quadratic form

$$\mathfrak{d}_\varepsilon(u) := \|\mathrm{d}u\|^2_{X_\varepsilon} = \sum_{e\in E} \varepsilon^{d-1} \int_{X_e} \Big(|u'(s,y)|^2 + \frac{1}{\varepsilon^2} |\mathrm{d}_{Y_e} u|^2_{h_e} \Big) \,\mathrm{d}y_e \,\mathrm{d}s + \varepsilon^{d-2} \int_{X_v} |\,\mathrm{d}u|^2_{g_v} \,\mathrm{d}x_v$$

where u' is the *longitudinal* derivative, $u' = \partial_s u$, and $\mathrm{d}u$ is the exterior derivative of u. Again, $\mathfrak{d}_\varepsilon$ is closed by definition.

Adding a potential, we define the Hamiltonian H_ε as the operator associated with the form $\mathfrak{h}_\varepsilon = \mathfrak{h}_{(X_\varepsilon, Q_\varepsilon)}$ given by

$$\mathfrak{h}_\varepsilon(u) = \|\mathrm{d}u\|^2_{X_\varepsilon} + \langle u, Q_\varepsilon u \rangle_{X_\varepsilon}$$

where Q_ε is supported only in the vertex region X_v. Inspired by the graph approximation, we choose

$$Q_\varepsilon(x) = \frac{1}{\varepsilon} Q(x)$$

where $Q = Q_1$ is a fixed bounded and measurable function on X_v

Relative boundedness

We can prove the relative (form-)boundedness of H_ε with respect to the free operator Δ_{X_ε}.

Lemma

To a given $\eta \in (0,1)$ there exists $\varepsilon_\eta > 0$ such that the form $\mathfrak{h}_\varepsilon$ is relatively form-bounded with respect to the free form $\mathfrak{d}_\varepsilon$, i.e., there is $\widetilde{C}_\eta > 0$ such that

$$|\mathfrak{h}_\varepsilon(u) - \mathfrak{d}_\varepsilon(u)| \leq \eta\, \mathfrak{d}_\varepsilon(u) + \widetilde{C}_\eta \|u\|^2_{X_\varepsilon}$$

whenever $0 < \varepsilon \leq \varepsilon_\eta$ with explicit constants ε_η and $\widetilde{C}_\eta$.

I will present here neither the proof nor the constants – cf. [E-Post'09] – what is important that they we can fully control them in term of the parameters of the model, $\|Q\|_\infty$, minimum edge length $\ell_- := \min_{e\in E} \ell_e$, the second eigenvalue $\lambda_2(v)$ of the Neumann Laplacian on X_v, and the ratio $c_{vol}(v) := vol\, X_v / vol\, \partial X_v$.

Identification maps

Our operators acts in different spaces, namely

$$\mathcal{H} := \mathsf{L}_2(G), \quad \mathcal{H}^1 := \mathsf{H}^1(G), \quad \widetilde{\mathcal{H}} := \mathsf{L}_2(X_\varepsilon), \quad \widetilde{\mathcal{H}}^1 := \mathsf{H}^1(X_\varepsilon),$$

and we thus need first to define quasi-unitary operators to relate the graph and manifold Hamiltonians.

For further purpose we set

$$p_e := (vol_{d-1} Y_e)^{1/2} \quad \text{and} \quad q(v) = \int_{X_v} Q \, \mathrm{d}x_v$$

Recall the graph approximation result and note that the weights p_e will allow us to treat situations when the tube cross sections Y_e are mutually different.

Identification maps, continued

First we define the map $J\colon \mathcal{H} \longrightarrow \widetilde{\mathcal{H}}$ by

$$Jf := \varepsilon^{-(d-1)/2} \bigoplus_{e\in E} (f_e \otimes \mathbb{1}_e) \oplus 0,$$

where $\mathbb{1}_e$ is the normalized eigenfunction of Y_e associated to the lowest (zero) eigenvalue, i.e. $\mathbb{1}_e(y) = p_e^{-1}$.

To relate the Sobolev spaces we need a similar map, $J^1\colon \mathcal{H}^1 \longrightarrow \widetilde{\mathcal{H}}^1$, defined by

$$J^1 f := \varepsilon^{-(d-1)/2} \Big(\bigoplus_{e\in E} (f_e \otimes \mathbb{1}_e) \oplus f(v) 1_v \Big),$$

where 1_v is the constant function on X_v with value 1. The map is well defined; the function $J^1 f$ matches at v along the different components of the manifold, hence $Jf \in \mathrm{H}^1(X_\varepsilon)$.

Identification maps, continued

Let us next introduce the following averaging operators

$$\fint_v u := \fint_{X_v} u \, \mathrm{d}x_v \quad \text{and} \quad \fint_e u(s) := \fint_{Y_e} u(s,\cdot) \, \mathrm{d}y_e$$

The opposite direction, $J' \colon \widetilde{\mathcal{H}} \longrightarrow \mathcal{H}$, is given by the adjoint,

$$(J'u)_e(s) = \varepsilon^{(d-1)/2} \langle \mathbb{1}_e, u_e(s,\cdot) \rangle_{Y_e} = \varepsilon^{(d-1)/2} p_e \fint_e u(s)$$

Furthermore, we define $J'^1 \colon \widetilde{\mathcal{H}}^1 \longrightarrow \mathcal{H}^1$ by

$$(J_e'^1 u)(s) := \varepsilon^{(d-1)/2} \Big[\langle \mathbb{1}_e, u_e(s,\cdot) \rangle_{Y_e} + \chi_e(s) p_e \Big(\fint_v u - \fint_e u(0) \Big) \Big],$$

where χ_e is a smooth cut-off function such that $\chi_e(0) = 1$ and $\chi_e(\ell_e) = 0$. By construction, $J_e'^1 u \in \mathrm{H}^1_{\underline{p}}(G)$.

δ-coupling results

Using properties of the above operators and an abstract convergence result of [Post'06] one can demonstrate the following claims:

Theorem (E-Post'09)

We have

$$\begin{aligned} \|J(H-z)^{-1} - (H_\varepsilon - z)^{-1} J\| &= \mathcal{O}(\varepsilon^{1/2}), \\ \|J(H-z)^{-1} J' - (H_\varepsilon - z)^{-1}\| &= \mathcal{O}(\varepsilon^{1/2}) \end{aligned}$$

for $z \notin [\lambda_0, \infty)$. The error depends only on parameters listed above. Moreover, $\varphi(\lambda) = (\lambda - z)^{-1}$ can be replaced by any measurable, bounded function converging to a constant as $\lambda \to \infty$ and being continuous in a neighbourhood of $\sigma(H)$.

The map J^1 does not appear in the formulation of the theorem but it is important in the proof.

δ-coupling results, continued

This result further implies

Corollary

The spectrum of H_ε converges to the spectrum of H uniformly on any finite energy interval. The same is true for the essential spectrum.

and

Corollary

For any $\lambda \in \sigma_{\rm disc}(H)$ there exists a family $\{\lambda_\varepsilon\}_\varepsilon$ with $\lambda_\varepsilon \in \sigma_{\rm disc}(H_\varepsilon)$ such that $\lambda_\varepsilon \to \lambda$ as $\varepsilon \to 0$, and moreover, the multiplicity is preserved. If λ is a simple eigenvalue with normalized eigenfunction φ, then there exists a family of simple normalized eigenfunctions $\{\varphi_\varepsilon\}_\varepsilon$ of H_ε such that

$$\|J\varphi - \varphi_\varepsilon\|_{X_\varepsilon} \to 0$$

as $\varepsilon \to 0$.

More complicated graphs

So far we have talked for simplicity about the star-shaped graphs only. The same technique of "cutting" the graph and the corresponding manifold into edge and vertex regions works also in the general case. As a result we get

Theorem (E-Post'09)

Assume that G is a metric graph and X_ε the corresponding approximating manifold. If

$$\inf_{v\in V} \lambda_2(v) > 0,\; \sup_{v\in V} \frac{\text{vol}\, X_v}{\text{vol}\, \partial X_v} < \infty,\; \sup_{v\in V} \|Q\restriction_{X_v}\|_\infty < \infty,\; \inf_{e\in E} \lambda_2(e) > 0,\; \inf_{e\in E} \ell_e > 0,$$

then the corresponding Hamiltonians $H = \Delta_G + \sum_v q(v)\delta_v$ and $H_\varepsilon = \Delta_{X_\varepsilon} + \sum_v \varepsilon^{-1} Q_v$ are $\mathcal{O}(\varepsilon^{1/2})$-close with the error depending only on the above indicated global constants.

How about other couplings?

The above scheme does not work for other couplings than δ; recall that the latter is the only coupling with functions *continuous* at the vertex.

To get a more general result let us next consider the δ'_{s}*-coupling* and show how it can be approximated by scaled Schrödinger operators.

The strategy we will employ is the same as above:

- first we work out an approximation on the graph itself
- then we "lift" it to an appropriate family of manifolds

The idea of Cheon and Shigehara

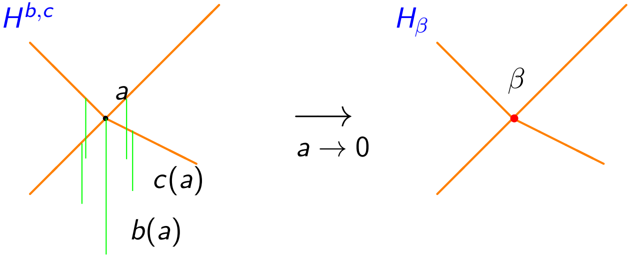
Moral of the following story: mathematicians know a lot of things but sometimes it is useful not to listen to them

For years they knew that δ' on line *cannot* be approximated by scaled potentials – but then a formal argument [Cheon-Shigehara'98] was presented showing how to do using a *nonlinearly* scaled δ interactions

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

Following the idea of Cheon and Shigehara

In the same spirit one devise an approximation scheme for δ'_{s} coupling at a general graph vertex:



A δ_s' approximation on a star graph

Core of the approximation lies in a suitable, *a*-dependent choice of the parameters of these δ-couplings: we put

$$H^{\beta,a} := \Delta_G + b(a)\delta_{v_0} + \sum_e c(a)\delta_{v_e}, \quad b(a) = -\frac{\beta}{a^2}, \quad c(a) = -\frac{1}{a}$$

which corresponds to the quadratic form

$$\mathfrak{h}^{\beta,a}(f) := \sum_e \|f_e'\|^2 - \frac{\beta}{a^2}|f(0)|^2 - \frac{1}{a}\sum_e |f_e(a)|^2, \quad dom\, \mathfrak{h}^a = \mathrm{H}^1(G)$$

Theorem (Cheon-E'04)

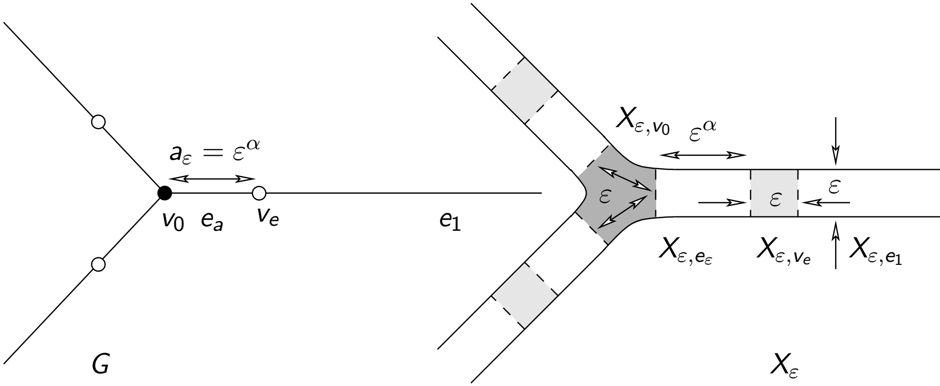
We have

$$\|(H^{\beta,a} - z)^{-1} - (H^{\beta} - z)^{-1}\| = \mathcal{O}(a)$$

as $a \to 0$ for $z \notin \mathbb{R}$, where $\|\cdot\|$ is the operator norm on $\mathrm{L}_2(G)$.

Proof by a direct computation, highly non-generic limit.

Scheme of the lifting



The corresponding δ'_s approximation result

Using the same technique as in the δ case, one can prove:

Theorem (E-Post'09)

Assume that $0 < \alpha < 1/13$, *then*

$$\left\|(H_\varepsilon^\beta - \mathrm{i})^{-1}J - J(H^\beta - \mathrm{i})^{-1}\right\| \to 0$$

as the radius parameter $\varepsilon \to 0$.

Remarks: (i) The value $\frac{1}{13}$ is by all accounts not optimal.

(ii) The operator families H_ε^β and $H^{\beta,\varepsilon}$ do not have for $\beta \geq 0$ a uniform lower bound (w.r.t. ε).

This does not contradict, however, to the fact that the limit operator H^β is non-negative. Note that the spectral convergence holds only for *compact* intervals $I \subset \mathbb{R}$, which means that the negative spectral branches of H_ε^β all have to tend to $-\infty$ as $\varepsilon \to 0$.

Beyond the two examples, first on graphs

It is relatively easy to extend the result to two-parameter set of coupling symmetric w.r.t. interchange of edges – cf. [E-Turek'06].

The next question is whether the CS-type method – adding properly scaled δ's on the edges – can work also *without the permutation symmetry*, and which subset of the n^2-parameter family it can cover.

In general we have the following claim:

Theorem (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:* one employs 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.

Using the δ coupling in the centre of Γ we get

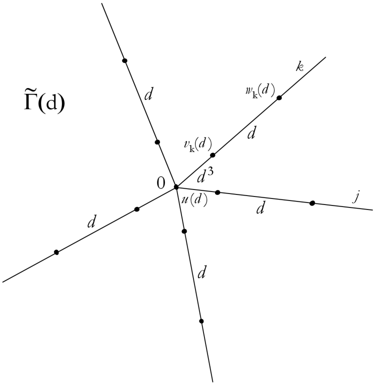
$$\begin{aligned} c_j\psi_j(0) - c_k\psi_k(0) + t_j\psi_j'(0_+) - t_k\psi_k'(0_+) &= 0\,, \quad 1 \le j, h \le n\,, \\ \sum_{j=1}^{n} \gamma_j\psi_j(0) + \sum_{j=1}^{n} \tau_j\psi_j'(0_+) &= 0\,, \end{aligned}$$

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

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

A concrete approximation

The next question is whether a $2n$-parameter approximation can be indeed constructed. Let us investigate a possible way in the arrangement with two δ's at each halfline of Γ.



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).

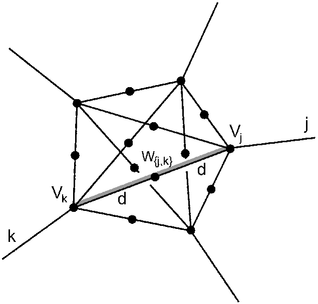
Proof is rather tedious but straightforward; one has to construct both resolvents and compare them. □

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

A universal graph approximation

We introduce two new ideas:

- We *modify the topology locally* adding edges which vanish in the limit. One can check formally – cf. [E-Turek'07] – that it gives $A\Psi + B\Psi' = 0$ with all *real-valued* A, B satisfying KS-conditions, thus all *time-reversal invariant* couplings.
- To get complex A, B one has to amend the approximating operators with suitably scaled *magnetic fields*



The ST-form of coupling conditions

To construct such an approximation we need an auxiliary result:

Theorem (Cheon-E-Turek'10)

Consider a quantum graph vertex of degree n. If $m \le n$, $S \in \mathbb{C}^{m,m}$ is a self-adjoint matrix and $T \in \mathbb{C}^{m,n-m}$, then the relation

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \Psi$$

expresses self-adjoint boundary conditions of the KS-type. Conversely, for any self-adjoint vertex coupling there is an $m \le n$ and a numbering of the edges such that the coupling is described by the KS boundary conditions with uniquely given matrices $T \in \mathbb{C}^{m,n-m}$ and self-adjoint $S \in \mathbb{C}^{m,m}$.

Remark: [Kuchment'04] writes b.c. in terms of eigenspaces of U. Here we single out the one corresponding to ev -1; there is also a symmetric form referring to ev's ± 1.

Some notations

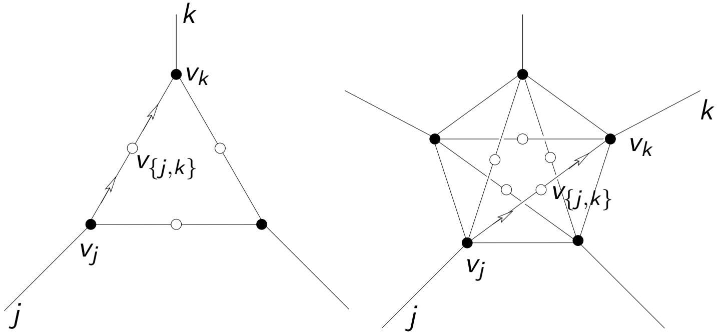


Figure: The approximation scheme for a vertex of degree $n = 3$ and $n = 5$. The inner edges are of length $2d$, some may be missing depending on the choice of the matrices S and T. The arrows symbolise the vector potential. In vertices v_j, $v_{\{j,k\}}$ one places δ interactions of strengths w_j, $w_{\{j,k\}}$, respectively.

The approximation scheme

We adopt the convention: the lines of the matrix T are indexed from 1 to m, the columns from $m+1$ to n.

- Take n halflines, each parametrized by $x \in \mathbb{R}_+$, with the endpoints denoted as v_j, and put a δ-coupling to the edges specified below with the parameter $w_j(d)$ at the point v_j for all $j = 1, \dots, n$.
- Some pairs v_j, v_k, $j \neq k$, of halfline endpoints are connected by edges of length $2d$, and the center of each such joining segment is denoted as $v_{\{j,k\}}$. This happens if one of the following conditions is satisfied:
  (a) $j = 1, \dots, m$, $k \geq m+1$, and $T_{jk} \neq 0$
  (or $j \geq m+1$, $k = 1, \dots, m$, and $T_{kj} \neq 0$),
  (b) $j, k = 1, \dots, m$, and $S_{jk} \neq 0$ or $(\exists l \geq m+1)\,(T_{jl} \neq 0 \wedge T_{kl} \neq 0)$.

The approximation scheme, continued

- At each middle-segment point $v_{\{j,k\}}$ we place a δ interaction with a parameter $w_{\{j,k\}}(d)$. The connecting edges of length $2d$ are considered as consisting of two segments of length d, and on each of them the variable runs from zero at $v_{\{j,k\}}$ to d at the points v_j, v_k.

- On each connecting segment we put a vector potential of constant value between the points v_j and v_k. We denote its strength between the points $v_{\{j,k\}}$ and v_j as $A_{(j,k)}(d)$, and between the points $v_{\{j,k\}}$ and v_k as $A_{(k,j)}(d)$. It follows from the continuity that $A_{(k,j)}(d) = -A_{(j,k)}(d)$ for any pair $\{j, k\}$.

The approximation scheme, continued

The choice of the dependence of $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$ on the parameter d is naturally crucial. We introduce the set $N_j \subset \{1,\dots,n\}$ containing indices of all the edges that are joined to the j-th one by a connecting segment, i.e.

$$\begin{aligned} N_j &= \{k \le m |\, S_{jk} \ne 0\} \cup \{k \le m |\, (\exists l \ge m+1)(T_{jl} \ne 0 \wedge T_{kl} \ne 0)\} \\ &\quad \cup \{k \ge m+1 |\, T_{jk} \ne 0\} \quad \text{for} \quad j \le m \\ N_j &= \{k \le m |\, T_{kj} \ne 0\} \qquad \text{for} \quad j \ge m+1 \end{aligned}$$

We distinguish two cases regarding the indices involved:

Case I. First assume $j = 1,\dots,m$ and $l \in N_j \backslash \{1,\dots,m\}$; then the vector potential may be chosen as

$$A_{(j,l)}(d) = \begin{cases} \frac{1}{2d} \arg\, T_{jl} & \text{if} \quad \mathrm{Re}\, T_{jl} \ge 0\,, \\ \frac{1}{2d} (\arg\, T_{jl} - \pi) & \text{if} \quad \mathrm{Re}\, T_{jl} < 0 \end{cases}$$

The approximation scheme, continued

For the parameters w_l and $w_{\{j,l\}}$ with $l \geq m+1$ we put

$$w_l(d) = \frac{1 - \#N_l + \sum_{h=1}^{m} \langle T_{hl} \rangle}{d} \qquad \forall l \geq m+1\,,$$

$$w_{\{j,l\}}(d) = \frac{1}{d}\left(-2 + \frac{1}{\langle T_{jl} \rangle}\right) \qquad \forall j,l \quad \text{indicated above}\,,$$

where $\langle \cdot \rangle$ for $c \in \mathbb{C}$ means

$$\langle c \rangle = \begin{cases} |c| & \text{if} \quad \mathrm{Re}\, c \geq 0\,, \\ -|c| & \text{if} \quad \mathrm{Re}\, c < 0\,. \end{cases}$$

Note that the choice of $v_l(d)$ is not unique; this is related to the fact that for $m = \mathrm{rank}\, B < n$ the number of coupling parameters is reduced from n^2 to at most $n^2 - (n-m)^2$

The approximation scheme, continued

Case II. Suppose next $j = 1, \ldots, m$ and $k \in N_j \cap \{1, \ldots, m\}$

$$A_{(j,k)}(d) = \frac{1}{2d} \arg \left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl} \overline{T_{kl}} - \mu\pi \right),$$

where $\mu = 0$ if $\mathrm{Re}\left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl} \overline{T_{kl}} \right) \geq 0$ and $\mu = 1$ otherwise. The functions $w_{\{j,k\}}$ are given by

$$w_{\{j,k\}} = -\frac{1}{d} \left(2 + \left\langle d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl} \overline{T_{kl}} \right\rangle^{-1} \right)$$

and $w_j(d)$ for $j = 1, \ldots, m$ by

$$w_j(d) = S_{jj} - \frac{\# N_j}{d} - \sum_{k=1}^{m} \left\langle S_{jk} + \frac{1}{d} \sum_{l=m+1}^{n} T_{jl} \overline{T_{kl}} \right\rangle + \frac{1}{d} \sum_{l=m+1}^{n} (1 + \langle T_{jl} \rangle) \langle T_{jl} \rangle .$$

The graph approximation

The Hamiltonian $H^{\rm star}$ and $H_d^{\rm approx}$ and the corresponding resolvents, $R^{\rm star}(z)$ and $R_d^{\rm approx}(z)$, respectively, act on different spaces: $R^{\rm star}(z)$ on $L^2(\Gamma)$, while $R_d^{\rm approx}(k^2)$ on $L^2(\Gamma_d) := L^2(\Gamma \oplus (0,d)^{\sum_{j=1}^n N_j})$. We identify $R^{\rm star}(z)$ with

$$R_d^{\rm star}(z) = R^{\rm star}(z) \oplus 0\,.$$

Theorem (Cheon-E-Turek'10)

In the described setting, the operator family $H_d^{\rm approx}$ converges to $H^{\rm star}$ in the norm-resolvent sense as $d \to 0$.

Remark: The constructed approximation is certainly *not unique*, note that for $\delta_{\rm s}'$ it differs from the one give in the example above

Complete solution of the Neumann case

Coming to the climax of the story, we have to lift the obtained approximation to tubular Neumann-like manifolds. It is done in the same way as above, with $d = \varepsilon^\alpha$. One has to go through all the estimates which is rather tedious but relatively straightforward. In this way we arrive at the following conclusion:

Theorem (E-Post'13)

Assume that $\Gamma(0)$ is a star graph with vertex condition parametrised by matrices S and T, and let $0 < \alpha < 1/13$. Then there is a Schrödinger operator H_ε on an approximating manifold X_ε constructed in the above described way such that

$$\|JR_d^{\rm star}(z)J^* - R_\varepsilon(z)\| = \mathcal{O}(\varepsilon^{\min\{1-13\alpha,\alpha\}/2})$$

holds true for $z \in \mathbb{C} \setminus \mathbb{R}$, where $R_\varepsilon(z) = (H_\varepsilon - z)^{-1}$.

Summary and next challenges

- We have shown that using families of Schrödinger operators on networks with the "natural" scaling one can approximate quantum-graph Hamiltonians with *δ-couplings* at the vertices.
- Using a procedure inspired by Cheon and Shigehara we have demonstrated that one can approximate *δ'_{s}-couplings* as well.
- Adding local changes in graph topology and properly scaled magnetic fields we have shown that *any self-adjoint coupling* can be approximated by scaled Schrödinger operators on Neumann-type networks.
- One would like to know whether other approximations are possible, for instance, based on geometric properties of the approximating manifolds – cf. [Kuchment-Post, in preparation].
- Contrary to Neumann, the *Dirichlet case* is a big challenge. The approximation principle is understood but it has to to worked out properly and the universality of the solution remains unclear.
- Little is known about the analogous problem for *generalized graphs* with 'edges' of different dimensions.

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- [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
- [ET07] P.E., O. Turek: Approximations of singular vertex couplings in quantum graphs, *Rev. Math. Phys.* **19** (2007), 571-606
- **[CET10]** T. Cheon, P.E., O. Turek Approximation of a general singular vertex coupling in quantum graphs, *Ann. Phys.* **325** (2010), 548-578
- **[EP13]** P.E., O. Post: A general approximation of quantum graph vertex couplings by scaled Schrödinger operators on thin branched manifolds, *CMP* **322** (2013), 207-227
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It remains to say

Vă mulțumim pentru atenție!