Approximating quantum graphs by Schrödinger operators on thin networks

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Talk overview

- Quantum graph vertex couplings
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- Fat graph approximation idea, Dirichlet and Neumann case
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- Generic Kirchhoff limit in the Neumann case: can one do better?
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- Summary and next challenges
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 $\text{rank}(A, B) = n$, $AB^*\text{ is self-adjoint}$. 

Pavel Exner: Quantum graphs ...
Vertex coupling (if there is a need of a reminder)

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

\[ A = U - I, \quad B = i(U + I) \]
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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 $J$ the $n \times n$ matrix whose all entries are equal to one; then $U = \frac{2}{n+i\alpha} J - I$ corresponds to the standard $\delta$ coupling,

$$
\psi_j(0) = \psi_k(0) =: \psi(0), \ j, k = 1, \ldots, n, \ \sum_{j=1}^{n} \psi_j'(0) = \alpha \psi(0)
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- Similarly, $U = I - \frac{2}{n-i\beta} J$ describes the $\delta'_s$ coupling

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

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].
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- 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
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- 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*:

\[ \text{Diagram showing a branching tube structure.} \]

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.
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Briefly, more on the Dirichlet case

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- The above claim depends energy renormalization one chooses, though. If you blow up the spectrum for a fixed point *separated from thresholds*, i.e.

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- The above claim depends energy renormalization one chooses, though. If you blow up the spectrum for a fixed point *separated from thresholds*, i.e.

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- **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 $e_j \simeq l_j := [0, \ell_j]$, $j \in J$; the respective state Hilbert space is thus $L^2(M_0) := \bigoplus_{j \in J} L^2(l_j)$.

The form $u \mapsto \|u'\|^2_{M_0} := \sum_{j \in J} \|u'\|^2_{l_j}$ with $u \in H^1(M_0)$ is associated with the operator which acts as $-\Delta_{M_0} u = -u''$ and satisfies free b.c.
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The form $u \mapsto \|u'\|_{M_0}^2 := \sum_{j \in J} \|u'\|_{l_j}^2$ with $u \in H^1(M_0)$ 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 $dX$ equal to $(\det g)^{1/2} dx$ in a fixed chart. For $u \in C^\infty_{\text{comp}}(X)$ 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 self-adjoint *Neumann* Laplacian $\Delta_X$ on the $X$. 
Relating the two together

We associate with the graph $M_0$ a family of manifolds $M_\varepsilon$

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

The analysis requires dissection of $M_\varepsilon$ into a union of compact edge and vertex components $U_{\varepsilon,j}$ and $V_{\varepsilon,k}$ with appropriate scaling properties, namely
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 $m := d - 1$
**Eigenvalue convergence**

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- For vertex regions we assume that the manifold $V_{\varepsilon,k}$ is diffeomorphic to an $\varepsilon$-independent manifold $V_k$. 

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.!)
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In this setting one can prove the following result:

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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 $M_\varepsilon$ 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 $\sigma_{\text{disc}}$ and $\sigma_{\text{ess}}$ converge uniformly in a 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,
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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.
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?
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Using exterior complex scaling in the “longitudinal” variable one can prove a convergence result for resonances as $\varepsilon \rightarrow 0$ [E-Post’07]. The same is true for embedded eigenvalues of the graph Laplacian which may remain embedded or become resonances for $\varepsilon > 0$. 

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Hence we have a number of convergence results, however, the limiting operator corresponds always to free b.c. only.
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*Can one do better?*
As a hint, an approximation on graphs

The way out: \textit{replace the Laplacian by suitable Schrödinger operators.}

Look first at the problem on the graph alone
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Look first at the problem on the graph alone

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

- $V_j \in L^1_{\text{loc}}(\mathbb{R}_+), \ j = 1, \ldots, n$
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- \( \delta \) coupling with a parameter \( \alpha \) in the vertex
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We make the following assumptions:

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- $\delta$ coupling with a parameter $\alpha$ in the vertex

Then the operator, denoted as $H_\alpha(V)$, is self-adjoint.
Potential approximation of $\delta$ coupling

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

$$W_{\epsilon,j} := \frac{1}{\epsilon} W_j \left( \frac{x}{\epsilon} \right), \quad j = 1, \ldots, n$$
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Theorem (E’96)

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

$$H_0(V + W_{\varepsilon}) \rightarrow H_\alpha(V)$$

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

$$\alpha := \sum_{j=1}^{n} \int_{0}^{\infty} W_j(x) \, dx.$$
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**Proof:** Analogous to that for $\delta$ interaction on the line. □
A network model of $\delta$ 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 $\ell_e \in (0, \infty]$. 
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The corresponding Hilbert space is $L_2(G) := \bigoplus_{e \in E} L_2(I_e)$, the decoupled Sobolev space of order $k$ is defined as

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

together with its natural norm.
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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

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

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

Pavel Exner: Quantum graphs ... 8th Congress of Romanian Mathematicians Iasi, June 27, 2015
Operators on the graph

We introduce first the (weighted) free Hamiltonian $\Delta_G$ defined via the quadratic form $\mathcal{D} = \mathcal{D}_G$ given by

$$\mathcal{D}(f) := \|f'\|^2_G = \sum_e \|f'_e\|^2_{I_e} \quad \text{and} \quad \text{dom} \mathcal{D} := H^1_p(G)$$

for a fixed $p$ (we drop the index $p$); form is a closed as related to the Sobolev norm $\|f\|^2_{H^1(G)} = \|f'\|^2_G + \|f\|^2_G$.
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Furthermore, the Hamiltonian with $\delta$-coupling of strength $q$ is defined via the quadratic form $\mathcal{h} = \mathcal{h}_{(G,q)}$ given by

$$\mathcal{h}(f) := \|f'\|_G^2 + q(v)|f(v)|^2 \quad \text{and} \quad \text{dom } \mathcal{h} := H^1_p(G)$$

Using standard Sobolev arguments one can show that the $\delta$-coupling is a “small” perturbation of the free operator by estimating the difference $\mathcal{h}(f) - \mathcal{d}(f)$ in various ways.
Manifold model of the “fat” graph

Given $\varepsilon \in (0, \varepsilon_0]$ we associate a $d$-dimensional manifold $X_\varepsilon$ 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 $\varepsilon Y_e$ is a manifold $Y_e$ equipped with metric $h_{\varepsilon,e} := \varepsilon^2 h_e$ and $\varepsilon X_{\varepsilon,v}$ carries the metric $g_{\varepsilon,v} = \varepsilon^2 g_v$. 

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As before, we use the $\varepsilon$-independent coordinates $(s, y) \in X_e = I_e \times Y_e$ and $x \in X_v$, so the radius-type parameter $\varepsilon$ only enters via the Riemannian metric.
Manifold model of the “fat” graph

Given \( \varepsilon \in (0, \varepsilon_0] \) we associate a \( d \)-dimensional manifold \( X_\varepsilon \) 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 \( \varepsilon Y_e \) 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 \( \varepsilon \)-independent coordinates \( (s, y) \in X_e = I_e \times Y_e \) and \( x \in X_v \), so the radius-type parameter \( \varepsilon \) only enters via the Riemannian metric.

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

The Hilbert space of the manifold model is

\[ L_2(X_\varepsilon) = \bigoplus_e \left( L_2(I_e) \otimes L_2(\varepsilon Y_e) \right) \oplus L_2(\varepsilon X_v) \]

with the norm given by

\[ \| u \|_{X_\varepsilon}^2 = \sum_{e \in E} \varepsilon^{d-1} \int_{X_e} |u|^2 dy_e ds + \varepsilon^d \int_{X_v} |u|^2 dx_v \]

where \( dx_e = dy_e ds \) and \( dx_v \) denote the Riemannian volume measures associated to the (unscaled) manifolds \( X_e = I_e \times Y_e \) and \( X_v \), respectively.
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$$\|u\|_{X_\varepsilon}^2 = \sum_{e \in E} \varepsilon^{d-1} \int_{X_e} |u|^2 \, dy_e \, ds + \varepsilon^d \int_{X_v} |u|^2 \, dx_v$$

where $dx_e = dy_e \, ds$ and $dx_v$ denote the Riemannian volume measures associated to the (unscaled) manifolds $X_e = I_e \times Y_e$ and $X_v$, respectively.

Let further $H^1(X_\varepsilon)$ be the Sobolev space of order one, the completion of the space of smooth functions with compact support under the norm

$$\|u\|_{H^1(X_\varepsilon)}^2 = \|d_u\|_{X_\varepsilon}^2 + \|u\|_{X_\varepsilon}^2.$$
The operators

The Laplacian $\Delta_{X_\varepsilon}$ on $X_\varepsilon$ is given via its quadratic form

$$\vartheta_\varepsilon(u) := \|du\|^2_{X_\varepsilon} = \sum_{e \in E} \varepsilon^{d-1} \int_{X_e} \left( |u'(s, y)|^2 + \frac{1}{\varepsilon^2} |dy_e u|_{h_e}^2 \right) dy_e ds + \varepsilon^{d-2} \int_{X_v} |du|_{g_v}^2 dx_v$$

where $u'$ is the *longitudinal* derivative, $u' = \partial_s u$, and $du$ is the exterior derivative of $u$. Again, $\vartheta_\varepsilon$ is closed by definition.
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where $u'$ is the longitudinal derivative, $u' = \partial_s u$, and $du$ is the exterior derivative of $u$. Again, $\vartheta_\varepsilon$ is closed by definition.

Adding a potential, we define the Hamiltonian $H_\varepsilon$ as the operator associated with the form $h_\varepsilon = h(X_\varepsilon, Q_\varepsilon)$ given by

$$h_\varepsilon(u) = \|du\|_{X_\varepsilon}^2 + \langle u, Q_\varepsilon u \rangle_{X_\varepsilon}$$

where $Q_\varepsilon$ 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 $H_\varepsilon$ with respect to the free operator $\Delta_{X_\varepsilon}$.
Relative boundedness

We can prove the relative (form-)boundedness of $H_\varepsilon$ with respect to the free operator $\Delta_{\chi_\varepsilon}$.

Lemma

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

$$|h_\varepsilon(u) - d_\varepsilon(u)| \leq \eta d_\varepsilon(u) + \widetilde{C}_\eta \|u\|_{\chi_\varepsilon}^2$$

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

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

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 $c_{vol}(v) := vol X_v/vol \partial X_v$. 

Pavel Exner: Quantum graphs ...
8th Congress of Romanian Mathematicians
Iasi, June 27, 2015
Identification maps

Our operators acts in different spaces, namely

$$\mathcal{H} := L^2(G), \quad \mathcal{H}^1 := H^1(G), \quad \tilde{\mathcal{H}} := L^2(X_\varepsilon), \quad \tilde{\mathcal{H}}^1 := H^1(X_\varepsilon),$$

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

For further purpose we set

\[ p_e := (\text{vol}_{d-1} Y_e)^{1/2} \quad \text{and} \quad q(\nu) = \int_{X_\nu} Q \, d\nu \]

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

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

where $1_e$ is the normalized eigenfunction of $Y_e$ associated to the lowest (zero) eigenvalue, i.e. $1_e(y) = p_e^{-1}$.
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To relate the Sobolev spaces we need a similar map, $J^1: \mathcal{H}^1 \longrightarrow \tilde{\mathcal{H}}^1$, defined by

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

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

Let us next introduce the following averaging operators

\[ f_v u := \int_{X_v} u \, dx_v \quad \text{and} \quad f_e u(s) := \int_{Y_e} u(s, \cdot) \, dy_e \]

The opposite direction, \( J' : \tilde{\mathcal{H}} \longrightarrow \mathcal{H} \), is given by the adjoint,

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

where \( \chi_e \) is a smooth cut-off function such that \( \chi_e(0) = 1 \) and \( \chi_e(\ell) = 0 \). By construction, \( J'_1 u \in H_1 \).
Identification maps, continued

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Furthermore, we define $J'_{e 1} : \tilde{\mathcal{H}}^1 \longrightarrow \mathcal{H}^1$ by

$$(J'_{e 1} u)(s) := \varepsilon^{(d-1)/2} \left[ \langle 1_e, u_e(s, \cdot) \rangle_{Y_e} + \chi_e(s) p_e \left( f_v u - f_e u(0) \right) \right],$$

where $\chi_e$ is a smooth cut-off function such that $\chi_e(0) = 1$ and $\chi_e(\ell_e) = 0$. By construction, $J'_{e 1} u \in H^1_{p}(G)$. 
δ-coupling results

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

\[ \|J(H - z)^{-1} - (H_\epsilon - z)^{-1}J\| = O(\epsilon^{1/2}) \]

for \( z/\in \left[ \lambda_0, \infty \right) \). The error depends only on parameters listed above.

Moreover, \( \phi(\lambda) = (\lambda - z)^{-1} \) 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.
\( \delta \)-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

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\| J(H - z)^{-1} - (H_\varepsilon - z)^{-1} J \| = O(\varepsilon^{1/2}),
\]

\[
\| J(H - z)^{-1} J' - (H_\varepsilon - z)^{-1} \| = O(\varepsilon^{1/2})
\]

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 \( \sigma(H) \).*
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This result further implies

**Corollary**

*The spectrum of $H_\varepsilon$ converges to the spectrum of $H$ uniformly on any finite energy interval. The same is true for the essential spectrum.*
\( \delta \)-coupling results, continued

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\[ \text{Corollary} \]

*The spectrum of } H_\varepsilon \text{ converges to the spectrum of } H \text{ uniformly on any finite energy interval. The same is true for the essential spectrum.}

and

\[ \text{Corollary} \]

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

\[
\text{Theorem (E-Post'09)}
\]

Assume that $G$ is a metric graph and $X$ ε the corresponding approximating manifold. If

\[
\inf_{v \in V} \lambda_2(v) > 0, \quad \sup_{v \in V} \text{vol } X_v < \infty, \quad \sup_{v \in V} \| Q_{X_v} \|_\infty < \infty, \quad \inf_{e \in E} \lambda_2(e) > 0, \quad \inf_{e \in E} \ell_e > 0,
\]

then the corresponding Hamiltonians $H = \Delta G + \sum_v q(v) \delta v$ and $H_\epsilon = \Delta X_\epsilon + \sum_v \epsilon^{-1} Q_v$ are $O(\epsilon^{-1/2})$-close with the error depending only on the above indicated global constants.
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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 $O(\varepsilon^{1/2})$-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 $\delta$; recall that the latter is the only coupling with functions \textit{continuous} at the vertex.
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To get a more general result let us next consider the $\delta'_s$-coupling and show how it can be approximated by scaled Schrödinger operators.
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The strategy we will employ is the same as above:

- first we work out an approximation on the graph itself
How about other couplings?

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To get a more general result let us next consider the $\delta'_s$-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.
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For years they knew that $\delta'$ 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 $\delta$ interactions
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For years they knew that $\delta'$ 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 $\delta$ interactions

Moreover, the convergence is norm resolvent and gives rise to approximations by regular potentials [Albeverio-Nizhnik’00], [E-Neidhardt-Zagrebnov’01]
In the same spirit one devise an approximation scheme for $\delta'_s$ coupling at a general graph vertex:
A $\delta'_S$ approximation on a star graph

Core of the approximation lies in a suitable, $a$-dependent choice of the parameters of these $\delta$-couplings:

$$H_{\beta,a} := \Delta_G + b(a)\delta v_0 + \sum_{e} c(a)\delta v_e,$$

where

$$b(a) = -\beta a^2,$$

$$c(a) = -\frac{1}{a},$$

which corresponds to the quadratic form

$$h_{\beta,a}(f) := \sum_{e} \|f'e\|_2^2 - \beta a^2 |f(0)|^2 - \frac{1}{a} \sum_{e} |f_e(a)|^2,$$

$$\text{dom } h_a = H^1(G).$$

Theorem (Cheon-E'04)

We have

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

as $a \to 0$ for $z \notin \mathbb{R}$, where $\| \cdot \|$ is the operator norm on $L^2(G)$.

Proof by a direct computation, highly non-generic limit.
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$$\mathcal{H}^{\beta,a}(f) := \sum_e \|f'_e\|^2 - \frac{\beta}{a^2}|f(0)|^2 - \frac{1}{a} \sum_e |f_e(a)|^2, \quad \text{dom } \mathcal{H}^a = H^1(G)$$
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Proof by a direct computation, highly non-generic limit.
Scheme of the lifting

\[ a_\varepsilon = \varepsilon^\alpha \]

\[ v_0 \quad e_a \quad v_e \]

\[ X_\varepsilon, v_0 \quad \varepsilon^\alpha \]

\[ X_\varepsilon, e_e \quad X_\varepsilon, v_e \quad X_\varepsilon, e_1 \]

\[ X_\varepsilon \]
The corresponding $\delta'_S$ approximation result

Using the same technique as in the $\delta$ case, one can prove:

Theorem (E-Post’09)

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

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

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

Remarks:
(i) The value $1/13$ is by all accounts not optimal.
(ii) The operator families $H^\beta_\varepsilon$ and $H^\beta,\varepsilon$ do not have for $\beta \geq 0$ a uniform lower bound (w.r.t. $\varepsilon$).

This does not contradict, however, to the fact that the limit operator $H^\beta$ 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 $H^\beta_\varepsilon$ all have to tend to $-\infty$ as $\varepsilon \to 0$. 

Pavel Exner: Quantum graphs ...
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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].
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The next question is whether the CS-type method – adding properly scaled $\delta$’s on the edges – can work also \textit{without the permutation symmetry}, and which subset of the $n^2$-parameter family it can cover.
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The next question is whether the CS-type method – adding properly scaled $\delta$’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 $\Gamma$ be an $n$-edged star graph and $\Gamma(d)$ obtained by adding a finite number of $\delta$’s at each edge, uniformly in $d$, at the distances $O(d)$ 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 $\delta$ 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 $\delta$ on $j$-th halfline.
Let us *sketch the proof*: one employs Taylor expansion to express boundary values of a $\delta$ 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 $\delta$ on $j$-th halfline.

Using the $\delta$ coupling in the centre of $\Gamma$ we get
\[
c_j \psi_j(0) - c_k \psi_k(0) + t_j \psi'_j(0+) - t_k \psi'_k(0+) = 0, \quad 1 \leq j, h \leq n,
\]
\[
\sum_{j=1}^n \gamma_j \psi_j(0) + \sum_{j=1}^n \tau_j \psi'_j(0+) = 0,
\]
which be written as $A\Psi(0) + B\Psi'(0) = 0$ with coefficients dependent on $2n$ parameters.
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Using the $\delta$ coupling in the centre of $\Gamma$ we get

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$$\sum_{j=1}^{n} \gamma_j\psi_j(0) + \sum_{j=1}^{n} \tau_j\psi'_j(0+) = 0,$$

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 $\delta$'s at each halfline of $\Gamma$. 
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 $\delta$’s at each halfline of $\Gamma$. 

\[ \tilde{\Gamma}(d) \]
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 \( H_{u,v,w}(d) \) converges as \( d \to 0_+ \) in the norm-resolvent sense to some \( H_{\omega,\alpha,\beta} \) depending explicitly on \( 2n \) parameters (notice that, say, \( \alpha_1 \) and \( \beta_1 \) cannot be chosen independently here).
CS-type approximation of star graphs

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**Proof** is rather tedious but straightforward; one has to construct both resolvents and compare them. \( \square \)
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**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.
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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 \( m \leq n \), \( S \in \mathbb{C}^{m,m} \) is a self-adjoint matrix and \( T \in \mathbb{C}^{m,n-m} \), then the relation

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

expresses self-adjoint boundary conditions of the KS-type. Conversely, for any self-adjoint vertex coupling there is an \( m \leq n \) 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 \( S \in \mathbb{C}^{m,m} \).
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**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 $\pm 1$. 
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 $\delta$ 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 $\delta$-coupling to the edges specified below with the parameter $w_j(d)$ at the point $v_j$ for all $j = 1, \ldots, n$. 

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) $j = 1, \ldots, m$, $k \geq m + 1$, and $T_{jk} \neq 0$ (or $j \geq m + 1$, $k = 1, \ldots, m$, and $T_{kj} \neq 0$),

(b) $j, k = 1, \ldots, m$, and $S_{jk} \neq 0$ or ($\exists \ l \geq m + 1$) ($T_{jl} \neq 0 \land T_{kl} \neq 0$).
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  (b) $j, k = 1, \ldots, m$, and $S_{jk} \neq 0$ or $(\exists l \geq m + 1) (T_{jl} \neq 0 \land T_{kl} \neq 0)$. 
At each middle-segment point $v_{\{j,k\}}$ we place a $\delta$ 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 $A_{\{k,j\}}(d)$, and between the points $v_{\{j,k\}}$ and $v_k$ as $A_{\{j,k\}}(d)$. It follows from the continuity that $A_{\{k,j\}}(d) = -A_{\{j,k\}}(d)$ for any pair $\{j,k\}$. 

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The approximation scheme, continued

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• 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 $N_j \subset \{1, \ldots, n\}$ containing indices of all the edges that are joined to the $j$-th one by a connecting segment, i.e.

$$
N_j = \{ k \leq m | S_{jk} \neq 0 \} \cup \{ k \leq m | (\exists l \geq m+1)(T_{jl} \neq 0 \land T_{kl} \neq 0) \}
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\]

We distinguish two cases regarding the indices involved:

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

\[
A_{(j,l)}(d) = \begin{cases} 
\frac{1}{2d} \arg T_{jl} & \text{if} \quad \Re T_{jl} \geq 0, \\
\frac{1}{2d} (\arg T_{jl} - \pi) & \text{if} \quad \Re T_{jl} < 0
\end{cases}
\]
The approximation scheme, continued

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

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

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

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

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

Note that the choice of $v_l(d)$ is not unique; this is related to the fact that for $m = \text{rank } B < n$ the number of coupling parameters is reduced from $n^2$ to at most $n^2 - (n - m)^2$. 
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 $\Re(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl} \overline{T_{kl}}) \geq 0$ 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

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

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

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**Theorem (Cheon-E-Turek'10)**

*In the described setting, the operator family $H^\text{approx}_d$ converges to $H^\text{star}$ in the norm-resolvent sense as $d \to 0$.***
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**Theorem (Cheon-E-Turek'10)**

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

*Remark:* The constructed approximation is certainly *not unique*, note that for $\delta'_s$ 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:
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**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 \( H_\varepsilon \) on an approximating manifold \( X_\varepsilon \) constructed in the above described way such that

\[
\| J R_d^{\text{star}}(z) J^* - R_\varepsilon(z) \| = O(\varepsilon^{\min\{1-13\alpha,\alpha\}/2})
\]

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 $\delta$-couplings at the vertices.

Using a procedure inspired by Cheon and Shigehara we have demonstrated that one can approximate $\delta'$-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 be worked out properly and the universality of the solution remains unclear.

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The talk was based on

It remains to say

Vă mulțumim pentru atenție!