Quantum graphs with general vertex coupling: approximation by scaled Schrödinger operators on manifolds

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- Summary and outlook



Quantum graph concept

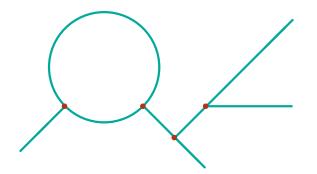
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The concept extends, however, to graphs of arbitrary shape



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 at least a quantum graph is also equivalent to a *microwave network* built of optical cables – see [Hul et al.'04]
- There are structures described by generalized graphs consisting of components of different dimensions
- Now when the microstructures reach molecular size quantum graphs "return" in a sense to their origin!



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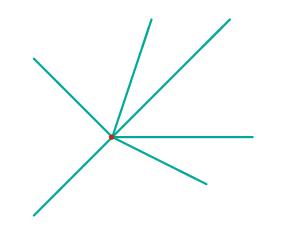
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- Graphs can support also *Dirac operators*, see [Bulla-Trenckler'90], [Bolte-Harrison'03], and also recent applications to *graphene* and its derivates



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- Graphs can support also *Dirac operators*, see [Bulla-Trenckler'90], [Bolte-Harrison'03], and also recent applications to *graphene* and its derivates
- The graph literature is extensive; a good up-to-date reference are proceedings of the last-year semester AGA Programme at INI Cambridge



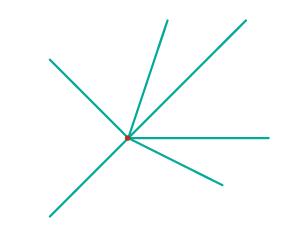
Vertex coupling



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



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

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

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

- 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

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

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

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



Remarks

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

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

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



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The parametrization leads to simple expressions of the quantities such as on-shell scattering matrix for a star graph of n halflines with such a coupling which equals

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

Hence the matrix U describing the coupling can be reconstructed if we know S(k) at a single value of k



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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- $\alpha = 0$ 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



n

Why are vertices interesting?

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

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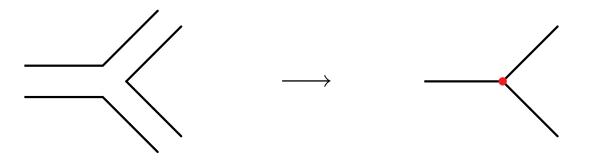
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- A nontrivial vertex coupling can lead to number theoretic properties of graph spectrum [E'96]
- On more practical side, the conductivity of graph nanostructures is controlled typically by external fields, vertex coupling can serve the same purpose
- 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*



A straightforward approximation idea

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

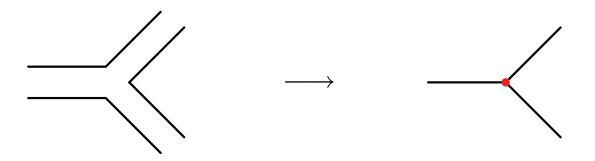


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 after a long effort the Neumann-like case was solved [Freidlin-Wentzell'93], [Freidlin'96], [Saito'01], [Kuchment-Zeng'01], [Rubinstein-Schatzmann'01], [E.-Post'05, 07], [Post'06] giving free b.c. only

 there is a recent progress in *Dirichlet case* [Post'05], [Molchanov-Vainberg'07], [E.-Cacciapuoti'07], [Grieser'07], but a lot of work remains to be done

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resonances on or around thresholds can produce a nontrivial coupling [Grieser'08], [E.-Cacciapuoti'07]

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

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



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Consider next a Riemannian manifold X of dimension $d \ge 2$ 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

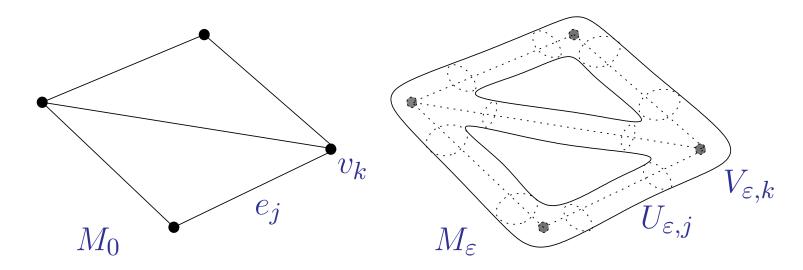
$$q_X(u) := \|\mathrm{d}u\|_X^2 = \int_X |\mathrm{d}u|^2 \mathrm{d}X, \ |\mathrm{d}u|^2 = \sum_{i,j} g^{ij} \partial_i u \, \partial_j \overline{u}$$

The closure of this form is associated with the 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



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In this setting one can prove the following result.

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



Improving the 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, $\Delta_{M_{\varepsilon}} \rightarrow \Delta_{M_0}$ as $\varepsilon \rightarrow 0+$ 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.



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 $\varepsilon \rightarrow 0$ [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

Can one do better?



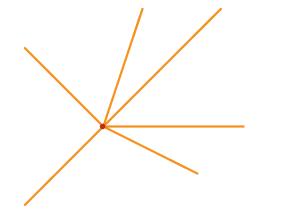
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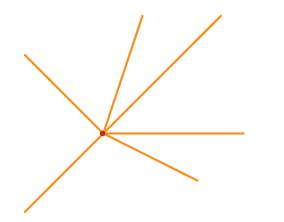


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We make the following assumptions:

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

• δ coupling with a parameter α in the vertex

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



Potential approximation of δ coupling

Suppose that the potential has a shrinking component,

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

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

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



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



Formulation: the graph model

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 $L_2(G) := \bigoplus_{e \in E} L_2(I)_e$, the *decoupled* Sobolev space of order k is defined as

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

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Let $\underline{p} = \{p_e\}_e$ be a vector of $p_e > 0$ for $e \in E$. The Sobolev space associated to 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 $\underline{p} = (1, ..., 1)$ we arrive at the *continuous* Sobolev space $H^1(G) := H^1_p(G)$.



Operators on the graph

We introduce first the (weighted) *free* Hamiltonian Δ_G defined via the quadratic form $\vartheta = \vartheta_G$ given by

 $\mathfrak{d}(f) := \|f'\|_G^2 = \sum_e \|f'_e\|_{I_e}^2 \quad \text{and} \quad dom\mathfrak{d} := \mathsf{H}^1_{\underline{p}}(G)$ for a fixed \underline{p} (we drop the index \underline{p}); form is a closed as related to the Sobolev norm $\|f\|_{\mathsf{H}^1(G)}^2 = \|f'\|_G^2 + \|f\|_G^2$.



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

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

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

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 $g_{\varepsilon,v} = \varepsilon^2 g_v$.



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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

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

with the norm given by

$$||u||_{X_{\varepsilon}}^{2} = \sum_{e \in E} \varepsilon^{d-1} \int_{X_{e}} |u|^{2} \,\mathrm{d}y_{e} \,\mathrm{d}s + \varepsilon^{d} \int_{X_{v}} |u|^{2} \,\mathrm{d}x_{v}$$

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



The function spaces

The Hilbert space of the manifold model is

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

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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 $||u||^2_{H^1(X_{\varepsilon})} = ||du||^2_{X_{\varepsilon}} + ||u||^2_{X_{\varepsilon}}$



The operators

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

$$\mathfrak{d}_{\varepsilon}(u) := \|\mathrm{d}u\|_{X_{\varepsilon}}^{2} = \sum_{e \in E} \varepsilon^{d-1} \int_{X_{e}} \left(|u'(s,y)|^{2} + \frac{1}{\varepsilon^{2}} |\mathrm{d}_{Y_{e}}u|_{h_{e}}^{2} \right) \mathrm{d}y_{e} \,\mathrm{d}s + \varepsilon^{d-2} \int_{X_{v}} |\mathrm{d}u|_{g_{v}}^{2} \,\mathrm{d}x$$

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

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

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

Relative boundedness

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

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

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

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



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I will present here neither the proof nor the constants – cf. [E-Post'08] – 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 $c_{vol}(v) := volX_{v}/vol\partial X_{v}$



Identification maps

Our operators acts in different spaces, namely

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

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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

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

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



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

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

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



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

$$J^{1}f := \varepsilon^{-(d-1)/2} \Big(\bigoplus_{e \in E} (f_{e} \otimes \mathbf{1}_{e}) \oplus f(v) \mathbf{1}_{v} \Big),$$

where $\mathbf{1}_v$ 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 $Jf \in H^1(X_{\varepsilon})$



Let us next introduce the following averaging operators

$$f_v u := f_{X_v} u \, \mathrm{d} x_v \quad \text{and} \quad f_e u(s) := f_{Y_e} u(s, \cdot) \, \mathrm{d} y_e$$

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

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



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

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

where χ_e is a smooth cut-off function such that $\chi_e(0) = 1$ and $\chi_e(\ell_e) = 0$. By construction, $J'_e{}^1 u \in \mathsf{H}^1_p(G)$

$\delta\text{-coupling results}$

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

Theorem [E-Post'08]: We have

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

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

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



$\delta\text{-coupling}$ 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.



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Corollary: For any $\lambda \in \sigma_{disc}(H)$ there exists a family $\{\lambda_{\varepsilon}\}_{\varepsilon}$ with $\lambda_{\varepsilon} \in \sigma_{disc}(H_{\varepsilon})$ 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



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Theorem [E-Post'08]: Assume that *G* is a metric graph and X_{ε} the corresponding approximating manifold. If

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

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 $O(\varepsilon^{1/2})$ -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 illustrate what one can do in the other case we choose the δ'_s -coupling as a generic example



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To illustrate what one can do in the other case we choose the δ'_s -coupling as a generic example

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



A $\delta_{\rm s}'$ star graph

Let $G = I_{v_0}$ be a star graph with the vertex v_0 and $n = \deg v$, $e = 1, \ldots, n$. For simplicity, we leave out weights and assume that all lengths are *finite and equal*, $\ell_e = 1$.



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The operator H^{β} , formally written as $H^{\beta} = \Delta_G + \beta \delta'_{v_0}$, acts as $(H^{\beta}f)_e = -f''_e$ on each edge for f in the domain

$$dom H^{\beta} := \left\{ f \in \mathsf{H}_{\max}^{2}(G) \, \middle| \, \forall e_{1}, e_{2} : f_{e_{1}}'(0) = f_{e_{2}}'(0) =: f'(0), \\ \sum_{e} f_{e}(0) = \beta f'(0), \forall e : f_{e}'(\ell_{e}) = 0 \right\}$$

For the sake of definiteness we imposed here Neumann conditions at the free ends of the edges



A $\delta'_{\rm s}$ star graph, continued

The corresponding quadratic form is given as

$$\begin{split} \mathfrak{h}^{\beta}(f) &= \sum_{e} \|f'_{e}\|^{2} + \frac{1}{\beta} \Big| \sum_{e} f_{e}(0) \Big|^{2}, \qquad dom \mathfrak{h}^{\beta} = \mathsf{H}^{1}_{\max}(G) \\ \text{if } \beta \neq 0 \text{ and} \\ \mathfrak{h}^{\beta}(f) &= \sum_{e} \|f'_{e}\|^{2}, \qquad dom \mathfrak{h}^{\beta} = \{ f \in \mathsf{H}^{1}_{\max}(G) \mid \sum_{e} f_{e}(0) = 0 \} \\ \text{if } \beta &= 0 \end{split}$$



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The corresponding quadratic form is given as

$$\mathfrak{h}^{\beta}(f) = \sum_{e} \left\| f'_{e} \right\|^{2} + \frac{1}{\beta} \left| \sum_{e} f_{e}(0) \right|^{2}, \qquad dom\mathfrak{h}^{\beta} = \mathrm{H}^{1}_{\mathrm{max}}(G)$$
 if $\beta \neq 0$ and

 $\mathfrak{h}^{\beta}(f) = \sum_{e} ||f'_{e}||^{2}, \quad dom\mathfrak{h}^{\beta} = \{ f \in \mathsf{H}^{1}_{\max}(G) \mid \sum_{e} f_{e}(0) = 0 \}$ if $\beta = 0$. The (negative) spectrum of H^{β} is easily found: **Proposition**: If $\beta \geq 0$ then $H^{\beta} \geq 0$. On the other hand, if $\beta < 0$ then H^{β} has exactly one negative eigenvalue $\lambda = -\kappa^{2}$ where κ is the solution of the equation

$$\cosh \kappa + \frac{\beta \kappa}{\deg v} \sinh \kappa = 0$$



Inspiration: the CS approximation

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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]



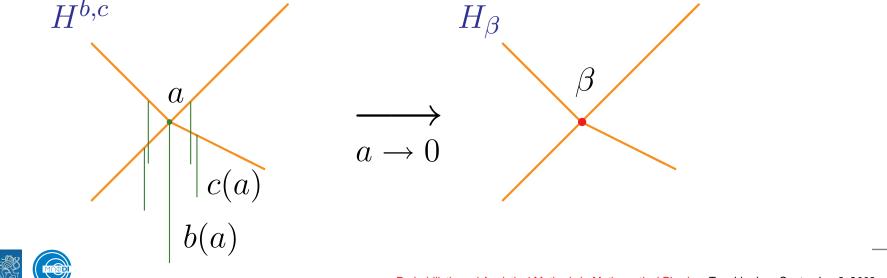
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This suggests the following scheme:



A $\delta_{\rm s}^\prime$ 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

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



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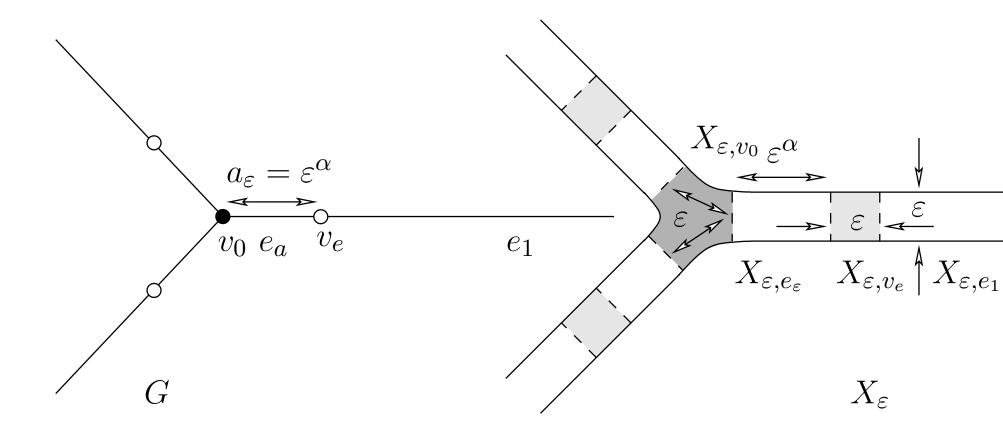
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Theorem [Cheon-E'04]: We have

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

Scheme of the lifting





Lower spectral edge

Proposition: If $\beta < 0$, the spectrum of $H^{\beta,a}$ is uniformly bounded from below as $a \rightarrow 0$: there is C > 0 such that

 $\inf \sigma(H^{\beta,a}) \ge -C \quad \text{as} \quad a \to 0$

If $\beta \ge 0$, on the other hand, then the spectrum of $H^{\beta,a}$ is asymptotically unbounded from below,

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Proposition: If $\beta \ge 0$, the spectrum of H_{ε}^{β} is asymptotically unbounded from below,

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The $\delta_{\rm s}^\prime$ approximation result

Using the same technique as in the δ case, one can prove **Theorem [E-Post'08]**: Assume that $0 < \alpha < 1/13$, then

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

as the radius parameter $\varepsilon \to 0$



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

(ii) The asymptotic lower unboundedness of H_{ε}^{β} and $H^{\beta,\varepsilon}$ for $\beta \geq 0$ is not a contradiction 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 $-\infty$



Beyond δ'_s : a permutation symmetry

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

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

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



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The graph-approximation scheme used for δ'_s generalizes to this case – cf. [E-Turek'06] – one has to employ

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

generically, and other choices of b(a), c(a) for exceptions



Nonsymmetric singular couplings

One naturally asks 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:



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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:* 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



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Using the δ coupling in the centre of Γ we get

$$c_{j}\psi_{j}(0) - c_{k}\psi_{k}(0) + t_{j}\psi_{j}'(0_{+}) - t_{k}\psi_{k}'(0_{+}) = 0, \quad 1 \le j, h \le n,$$
$$\sum_{j=1}^{n} \gamma_{j}\psi_{j}(0) + \sum_{j=1}^{n} \tau_{j}\psi_{j}'(0_{+}) = 0,$$

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



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

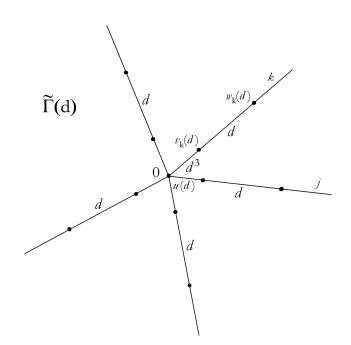
A concrete approximation

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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. \Box

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}



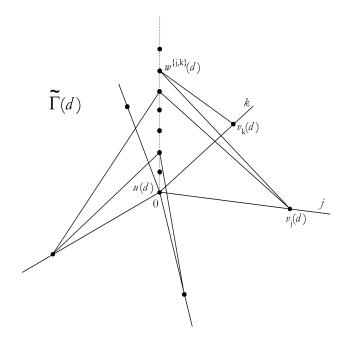
The arrangement, visualization

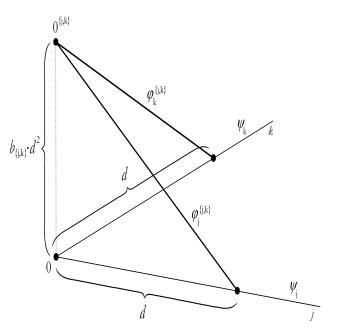
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Choice of the parameters

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



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

and furthermore,

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



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Conjecture: The described approximations converges not only in terms of boundary conditions, but in the norm-resolvent sense as well, and *they can be lifted to appropriate network manifolds*



A general approximation

One can do better. To get a fully general and more elegant construction, the following is needed

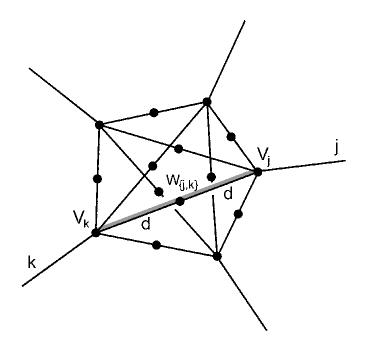
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The convergence result

Now one has to do the following:

- choose δ -couplings properly, similarly as above
- choose vector potential properly, singular as $d \rightarrow 0$



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Theorem [Cheon-E.-Turek'09]: With a proper parameter choice we get the norm-resolvent convergence,

$$||R_d^{\text{star}}(k^2) - R_d^{\text{approx}}(k^2)|| = \mathcal{O}(d^{1/2}) \quad \text{as} \quad d \to 0$$



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Conjecture: The described approximation *can be lifted to the appropriate family of network manifolds*, and moreover, the result will extend to wide class of graphs satisfying uniformity conditions, similar as above



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- Using an elaborate and highly non-generic procedure one can approximate δ'_s -couplings as well
- We have shown how more general coupling can be approximated on graphs and *conjectured* that the procedure can be lifted to manifolds
- One would like to know whether other approximations are possible, for instance, based on geometric properties of the approximating manifolds



The talk was based on

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- [ET07] P.E., O. Turek: Approximations of singular vertex couplings in quantum graphs, *Rev. Math. Phys.* **19** (2007), 571-606
- [CET09] T. Cheon, P.E., O. Turek Approximation of a general singular vertex coupling in quantum graphs, arXiv:0908.2679 [quant-ph]



Thank you for your attention!

