Constrained quantum dynamics

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With thanks to all my collaborators

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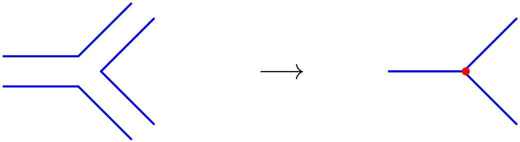
Meaning of the vertex coupling

Let us return to the question how to choose the way in which wave functions in the graph vertices. We have mentioned the natural idea to look into *free motion in a network collapsing to the graph*, symbolically



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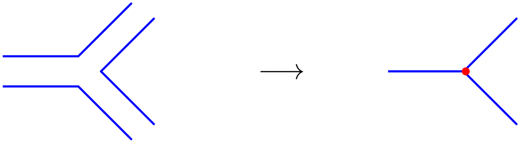

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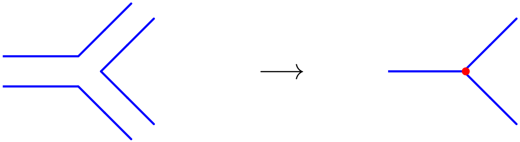

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First of all, the answer depends on which sort of boundary the network has. Ruedenberg and Scherr assumed that it is *Neumann*, and finally, around the turn of the century, mathematicians addressed this case, e.g.

P. Kuchment, H. Zeng: Convergence of spectra of mesoscopic systems collapsing onto a graph, *J. Math. Anal. Appl.* **258** (2001), 671–700.

J. Rubinstein, M. Schatzman: Variational problems on multiply connected thin strips, I. Basic estimates and convergence of the Laplacian spectrum, *Arch. Rat. Mech. Anal.* **160** (2001), 271–308.

Y. Saito: The limiting equation for Neumann Laplacians on shrinking domains, *Electron. J. Differ. Eq.* **31** (2000), 1–25.

Squeezing a Neumann network

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 the orthogonal sum of L^2 spaces on the edges, $L^2(M_0) := \bigoplus_{j\in J} L^2(I_j)$.

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

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

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

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The closure of this form is associated with the self-adjoint operator Δ_X which acts in fixed chart coordinates as

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

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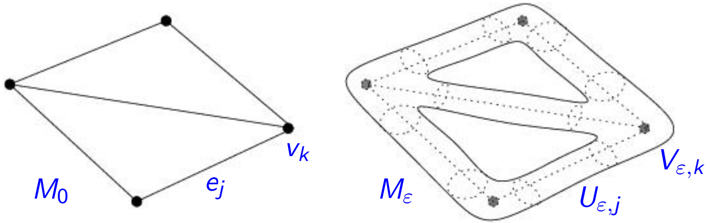

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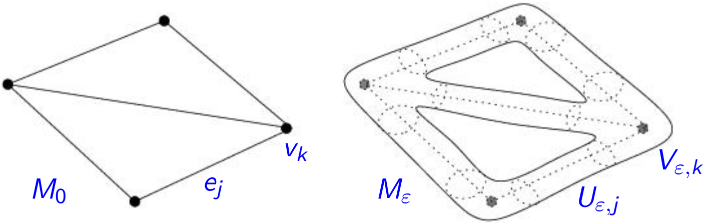
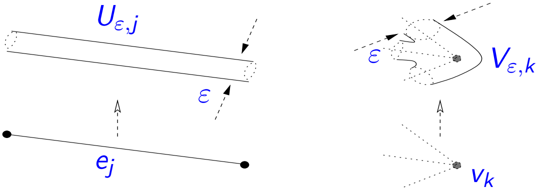


which are all constructed from X by taking a suitable *ε-dependent family of metrics*; the advantage of such an approach is that we work with the *intrinsic* geometrical properties only, *no need to embed M into some $\mathbb{R}^d$*.

Construction of the approximation

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



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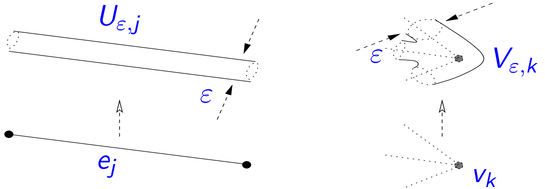

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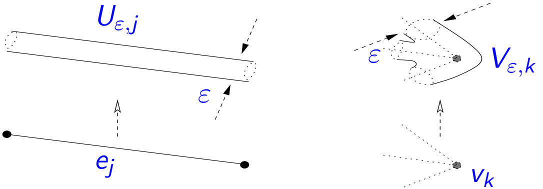

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- for *vertex regions* we assume that the manifold $V_{\varepsilon,k}$ is *diffeomorphic* to an *ε-independent manifold* V_k,
- there is a *technical issue*: we have to replace the product metric on by a modified one given by $g_\varepsilon := \mathrm{d}x^2 + \varepsilon^2 h(y)$. The two coincide up to an $\mathcal{O}(\varepsilon)$ error, of course, the reason is that the length of the edge part changes during the squeezing,

Eigenvalue convergence

In this setting one can prove the convergence in the following sense:

Theorem

Under the stated assumptions, $\lambda_k(M_\varepsilon) \to \lambda_k(M_0)$ *holds as* $\varepsilon \to 0$.

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- On the other hand, if the vertex scaling is *too slow*, $\alpha \in \left[0, \frac{d-1}{d}\right)$, the result is the family of *disconnected edges* with *Dirichlet endpoints*. In the critical case, $\alpha = \frac{d-1}{d}$, we get something like a δ coupling but with the *energy-dependent* coupling constant.

Improving the convergence

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More results of this type

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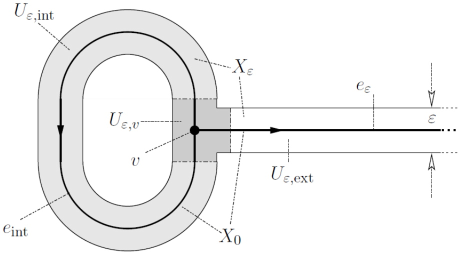

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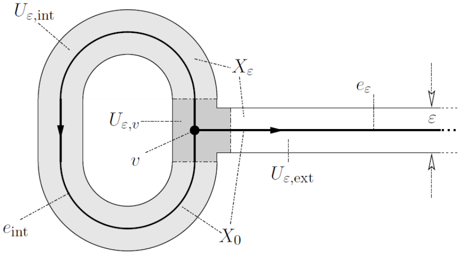

Using *exterior complex scaling* in the 'longitudinal' variable one can prove a convergence result for resonances in the limit $\varepsilon \to 0$; the same is true for *embedded eigenvalues* of the graph Laplacian which may either remain embedded or become resonances for $\varepsilon > 0$.

P.E., O. Post: Convergence of resonances on thin branched quantum wave guides, *J. Math. Phys.* **48** (2007), 092104.

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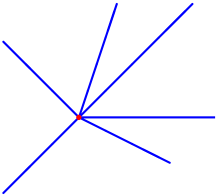

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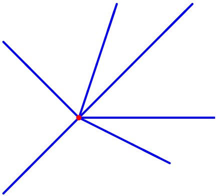

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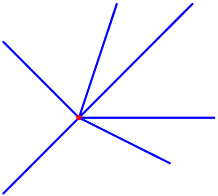

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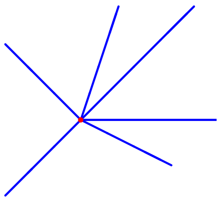

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Then the operator, denoted as $H_\alpha(V)$, is *self-adjoint* as the potential terms in the boundary form obviously cancel.

Potential approximation of a δ coupling

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By an argument analogous to that used in the situation when one approximates the δ function on line by a family of regular functions, one can prove the following result:

Theorem

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* $\alpha := \sum_{j=1}^n \int_0^\infty W_j(x)\,\mathrm{d}x$.

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

A network model of δ coupling: formulation

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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.

A network model of δ coupling: formulation

For simplicity, we will consider *star graphs*; extension to more general cases will be straightforward. Let thus $G = I_v$ 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 the subset with prescribed behavior at the, origin,

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

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 (in general, weighted) *free* Hamiltonian Δ_G as the self-adjoint operator associated with the 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 $\underline{p}$ (from now on, we drop the weight index $\underline{p}$); the form is closed being related to the Sobolev norm $\|f\|^2_{\mathsf{H}^1(G)} = \|f'\|^2_G + \|f\|^2_G$.

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

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

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where the point potential $q(v)$ is what was a while ago denoted as α.

Using standard Sobolev arguments one can show that the δ-coupling is a *'small' perturbation* of the free operator by estimating the difference $\mathfrak{h}(f) - \mathfrak{d}(f)$ of the two forms in various ways in terms $\mathfrak{d}(f)$, $\mathfrak{h}(f)$ and $\|f\|_G^2$.

Manifold model of the 'fat' graph

Given the *radius-type parameter* $\varepsilon \in (0, \varepsilon_0]$ we associate a d-dimensional manifold X_ε to the graph G in the same way 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 the symbol for the manifold Y_e equipped with metric $h_{\varepsilon,e} := \varepsilon^2 h_e$, and similarly, $\varepsilon X_{\varepsilon,v}$ carries the metric $g_{\varepsilon,v} = \varepsilon^2 g_v$.

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As before, we use the *ε-independent coordinates* in the 'dissected' parts of the manifold, $(s, y) \in X_e = I_e \times Y_e$ and $x \in X_v$, so the 'squeezing' parameter ε only enters the argument via the Riemannian metric.

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As before again, we have to deal with the fact such an ε-neighborhood of an embedded graph $G \subset \mathbb{R}^d$ requires a *correction* due to the *error* of the edge length of order of ε, but this can be covered an *ε-dependence of the metric* in the longitudinal direction.

The function spaces on the manifold

We do the same *surgery* as above, cutting the manifold into the edge and vertex part; then the Hilbert space of the manifold model can be written as

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

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.

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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 associated with the 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, the form $\mathfrak{d}_\varepsilon$ is closed by definition.

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Adding a potential, we define the Hamiltonian H_ε as the self-adjoint 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 discussed above, we choose

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

where $Q = Q_1$ is a *fixed bounded and measurable function on X_v* (the ε^{-1} factor in the argument is not missing, it is hidden in the scaled metric!).

Relative boundedness

As in the graphs case, one can prove the relative (form-)boundedness of H_ε with respect to the free operator Δ_{X_ε}, that is, the following claim:

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*

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

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

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

I am not going to present the expressions of the constants involved; what is important that they we can fully control them in term of the *parameters of the model*, namely $\|Q\|_\infty$, the 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

The difficult part of the argument comes from the fact that we want to compare operators acting in *different spaces*.

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To be concrete, we consider on the graph and the manifold the following pairs of spaces,

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

respectively, and we thus need, first of all, to define operators relating the graph and manifold Hamiltonians; we will require them to be *quasi-unitary* in the sense made precise below.

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respectively, and we thus need, first of all, to define operators relating the graph and manifold Hamiltonians; we will require them to be *quasi-unitary* in the sense made precise below.

I have noted that we can cover situations where the tube cross sections Y_e are mutually different. With this fact in mind we set

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

in the case we are most interested in when all the Y_e's are the same we may put all these weights to $p_e = 1$.

Identification maps: graph to manifold

First we define the map $J\colon \mathcal{H} \longrightarrow \widetilde{\mathcal{H}}$ *between the Hilbert spaces* 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* (namely, zero) *eigenvalue*, in other words, $1\!\!\!-_e(y) = p_e^{-1}$.

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To relate the *Sobolev spaces* we need a similar map, $J^1\colon \mathcal{H}^1 \longrightarrow \widetilde{\mathcal{H}}^1$, which is 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 the vertex region X_v having value 1. This map is *well defined*; note that the function $J^1 f$ matches at v along the different components of the manifold, hence we have $Jf \in \mathrm{H}^1(X_\varepsilon)$.

Identification maps: manifold to graph

Let us next introduce the following *averaging operators*:

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

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They allow us to express the map in the opposite direction, $J' \colon \widetilde{\mathcal{H}} \longrightarrow \mathcal{H}$, from the manifold to the graphs, given by the *adjoint to J*,

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

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In the same vein, we define $J'^1 \colon \widetilde{\mathcal{H}}^1 \longrightarrow \mathcal{H}^1$ between the Sobolev spaces 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, $J_e'^1 u \in \mathrm{H}^1_{\underline{p}}(G)$, in particular, it belongs to $\mathrm{H}^1(G)$ in the case of identical edge profiles we are most interested in.

δ-coupling results

The above maps are not unitary, of course, but they are *quasi-unitary* in the sense that norms of $Jf - J^1 f$ and $J^* u - J'^1 u$ are small in terms of Sobolev norms of f and u and vanish as $\varepsilon \to 0$

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This concept leads to an *abstract convergence result*, the idea of which belongs to Olaf Post; in the present context it yields the following result:

Theorem

We have

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

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

for $z \notin [\lambda_0, \infty)$. The error depends only on the 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 neighborhood of $\sigma(H)$.

δ-coupling results: consequences of the theorem

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The norm resolvent convergence established in the theorem implies:

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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

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

holds as $\varepsilon \to 0$.

More complicated graphs

We choose star graphs to explain the approximation. However, the nature of the construction has a *local character*; the same technique of ‘dissecting’ the graph and the corresponding manifold into a family of edge and vertex regions also works in the general case

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We choose star graphs to explain the approximation. However, the nature of the construction has a *local character*; the same technique of ‘dissecting’ the graph and the corresponding manifold into a family of edge and vertex regions also works in the general case. In this way one can prove the following result:

Theorem

Assume that G is a (possibly infinite, but locally finite) metric graph and X_ε the corresponding approximating manifold. If

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

then the corresponding Hamiltonians, i.e. $H = \Delta_G + \sum_v q(v)\delta_v$ 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.

P.E., O. Post: Approximation of quantum graph vertex couplings by scaled Schrödinger operators on thin branched manifolds, *J. Phys. A: Math. Theor.* **42** (2009), 415305.

How about the other couplings?

The above scheme does not work for other couplings than δ – still a small subset in the family of all self-adjoint ones – recall that the δ is the only coupling with functions *continuous* at the vertex.

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T. Cheon, T. Shigehara: Realizing discontinuous wave functions with renormalized short-range potentials, *Phys. Lett.* **A243** (1998), 111–116.

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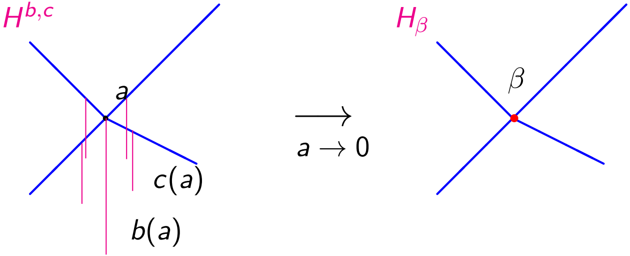
The convergence is a rather *subtle effect* here, in the fifth order only!

Following the idea of Cheon and Shigehara

In a similar way one can approximate the δ'_s *coupling* at the vertex of a star graphs; the scheme of the approximation is the following:



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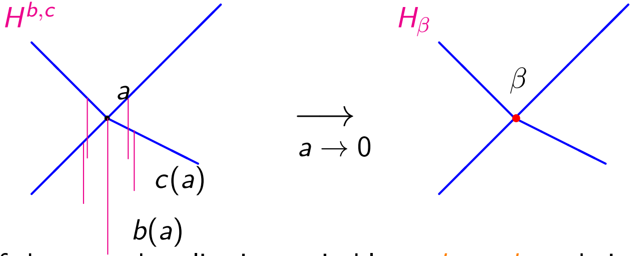

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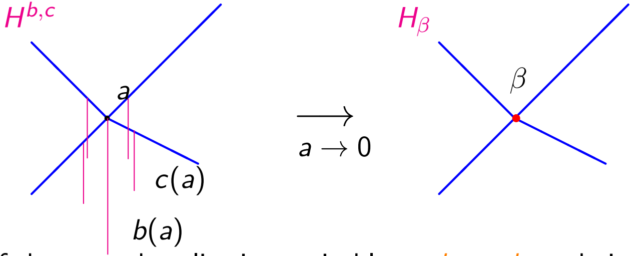

Core of the procedure lies in a suitable, *a-dependent* choice of the parameters of these δ-couplings: we put

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

which corresponds to the quadratic form

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

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Theorem

$\|(H^{\beta,a} - z)^{-1} - (H^{\beta} - z)^{-1}\| = \mathcal{O}(a)$ *holds as* $a \to 0$ *for any* $z \notin \mathbb{R}$.

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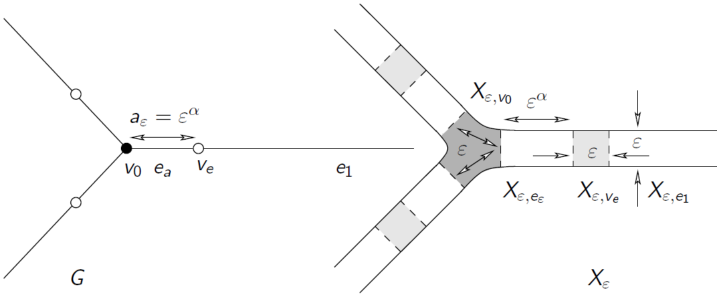
In the next step, we lift this approximation to manifolds as sketched here:



The corresponding δ'_{s} approximation result

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

Theorem

Fix $\alpha \in \left(0, \frac{1}{13}\right)$*, then with* $b(a_\varepsilon)$, $c(a_\varepsilon)$ *as in [Cheon-E'04, loc.cit.] we have*

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

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

(ii) The operator families H_ε^β and H^{β, a_ε} do not have for $\beta \geq 0$ a uniform lower bound with respect to the parameter ε.

This does not contradict, however, to the fact that the limiting operator H^β is *non-negative* for $\beta \geq 0$. 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 $\varepsilon \to 0$.

How to deal with the general vertex coupling

To go beyond these examples, one can try Cheon-Shigehara idea *without the permutation symmetry*; this yields a $2n$-*parameter family*.

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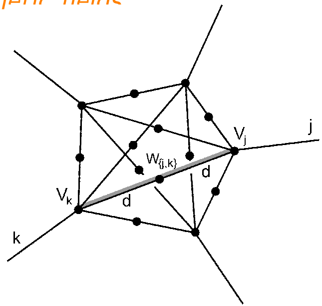

The ST-form of coupling conditions

To make use of these ideas, one has to cast the vertex coupling written as $A\Psi + B\Psi' = 0$ into a suitable form, namely:

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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

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

expresses self-adjoint boundary conditions. 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 above 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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Note that the condition $(U - I)\Psi(0) + i(U + I)\Psi'(0) = 0$ can be split into the Dirichlet, Neumann, and Robin parts related to eigenspaces of U. In the theorem we single out the Dirichlet part referring to eigenvalue -1.

Some notations

Let me show the result – without going into much technical details – mentioning some notations first.

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 symbolize the *vector potential*. In vertices v_j, $v_{\{j,k\}}$ one places δ interactions of strengths w_j, $w_{\{j,k\}}$, respectively.

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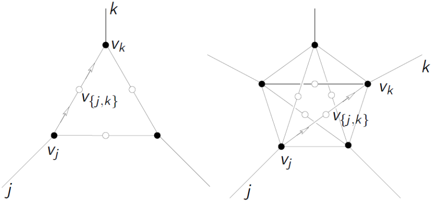

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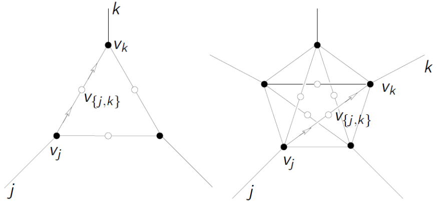

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- the *δ-coupling* of strength $w_j(d)$ is imposed at the points v_j,
- vertices $v_j, v_k,\ j \neq k$ are connected by edges of length $2d$ with the center $v_{\{j,k\}}$ provided (a) $T_{jk} \neq 0$, and (b) either $S_{jk} \neq 0$ or there is an l such that $T_{jl} \neq 0 \wedge T_{kl} \neq 0$; on them we have *vector potential* $A_{(j,k)}(d)$ and at their center *δ-interaction* of strength $w_{\{j,k\}}(d)$

The approximation scheme

The choice of the functions $v_j(\cdot)$, $w_{\{j,k\}}(\cdot)$ and $A_{(j,k)}(\cdot)$ is, of course, crucial. We by N_j the index set of the vertices *connected to v_j*. We distinguish two cases:

Case I: edges connecting the Robin and Dirichlet part. Then we choose

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

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where $\langle c \rangle$ for $c \in \mathbb{C}$ means $\pm|c|$ for $\mathrm{Re}\, c \geq 0$ and $\mathrm{Re}\, c < 0$, respectively.

In fact the choice of $v_l(d)$ is not unique; this is related to the fact that for $m < n$ the number of coupling parameters is reduced from the 'full value' n^2 to at most $n^2 - (n-m)^2$.

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Case II: edges connecting 'Robin' vertices. In this situation we choose

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

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.

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

and

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

Note that most coefficients behave as $\mathcal{O}(d^{-1})$ when $d \to 0+$ but $w_{\{j,k\}}$ may have *stronger singularity*, $\mathcal{O}(d^{-2})$, if the sum in the bracket vanishes.

The convergence

We must take into account, that the Hamiltonians, $H^{\rm star}$ and $H_d^{\rm approx}$, as well as their resolvents, $R^{\rm star}(z)$ and $R_d^{\rm approx}(z)$, respectively, act on *different spaces*, namely $R^{\rm star}(z)$ on $L^2(\Gamma)$, while $R_d^{\rm approx}(k^2)$ acts on the larger space $L^2(\Gamma_d) := L^2(\Gamma \oplus (0,d)^{\sum_{j=1}^n N_j})$.

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At the same time, the described approximation is certainly *not unique*, note that for δ'_{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

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 magnetic Schrödinger operator H_ε on an approximating manifold X_ε constructed in the above described way such that

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

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

P.E., O. Post: A general approximation of quantum graph vertex couplings by scaled Schrödinger operators on thin branched manifolds, *Commun. Math. Phys.* **322** (2013), 207–227.

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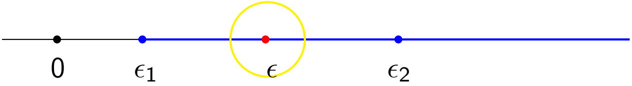
This can be done in different ways. For instance, if you blow up the spectrum from a fixed point *separated from thresholds*, pictorially



one gets a nontrivial limit with the matching conditions fixed by scattering on the 'fat star'. However, the resulting operator is *unbounded from below* and does not fit into our quantum graph picture.

S. Molchanov, B. Vainberg: Scattering solutions in networks of thin fibers, *Comm. Math. Phys.* **273** (2007), 533–559.

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We know that a bent waveguide has always a nontrivial discrete spectrum and note that by *increasing the bending angle* one can produce more eigenvalues, in particular, there are configuration when the eigenvalue is 'emerging from the continuum', i.e. the singularity is *at the threshold*.

The bent waveguide

The operator to consider is *Dirichlet Laplacian* on the bent strip,

$$\Omega := \{(x,y) \in \mathbb{R}^2 :\, x = \Gamma_1(s) - u\Gamma_2'(s), y = \Gamma_2(s) + u\Gamma_1'(s), s \in \mathbb{R}, u \in (-a,a)\}$$

built over a curve Γ determined by its signed curvature γ. We suppose that $\gamma(\cdot)$ is *smooth* outside a compact, and that apart from a bounded part of it, the strip is *straight*. Recall that the total *bending angle* of such a strip is $\theta = \int_{\mathbb{R}} \gamma(s)\,\mathrm{d}s$.

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Now we assume now that the strip changes its shape and width in dependence on the parameter $\varepsilon\in(0,1]$ as

$$\gamma_\varepsilon(s) := \frac{\sqrt{\lambda(\varepsilon)}}{\varepsilon}\,\gamma\Big(\frac{s}{\varepsilon}\Big) \quad \text{and} \quad a_\varepsilon := \varepsilon^\alpha a \quad \text{with} \;\; \alpha>1,$$

where $\lambda(\varepsilon)$ is a fixed function, real and positive; by assumption the width shrinks faster than the curvature radius

The bent waveguide

The operator to consider is *Dirichlet Laplacian* on the bent strip,

$$\Omega := \{(x,y) \in \mathbb{R}^2 :\, x = \Gamma_1(s) - u\Gamma_2'(s), y = \Gamma_2(s) + u\Gamma_1'(s), s \in \mathbb{R}, u \in (-a,a)\}$$

built over a curve Γ determined by its signed curvature γ. We suppose that $\gamma(\cdot)$ is *smooth* outside a compact, and that apart from a bounded part of it, the strip is *straight*. Recall that the total *bending angle* of such a strip is $\theta = \int_{\mathbb{R}} \gamma(s)\, \mathrm{d}s$.

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where $\lambda(\varepsilon)$ is a fixed function, real and positive; by assumption the width shrinks faster than the curvature radius. In particular, the simplest choice $\lambda(\varepsilon) = 1$ means that the bending angle is preserved.

S.A. Albeverio, C. Cacciapuoti, D. Finco: Coupling in the singular limit of thin quantum waveguides, *J. Math. Phys.* **48** (2007), 032103.

The bent waveguide

Let us be slightly more general and suppose the function to analytic near the origin, with the expansion

$$\lambda(\varepsilon) = 1 + \lambda_1 \varepsilon + \mathcal{O}(\varepsilon^2).$$

which means the strip is *'wiggling'*, its bending angle being

$$\theta_\varepsilon = \int_{\mathbb{R}} \gamma_\varepsilon(s)\, \mathrm{d}s = \theta\sqrt{\lambda(\varepsilon)} = \theta\left(1 + \frac{1}{2}\lambda_1\varepsilon\right) + \mathcal{O}(\varepsilon^2).$$

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We may again pass to the unitarily equivalent operator on a *straight strip*,

$$H_\varepsilon = -\frac{\partial}{\partial s}\frac{1}{(1+\varepsilon^{\alpha-1}u\sqrt{\lambda(\varepsilon)}\gamma(\frac{s}{\varepsilon}))^2}\frac{\partial}{\partial s} - \frac{1}{\varepsilon^{2\alpha}}\frac{\partial^2}{\partial u^2} + \frac{1}{\varepsilon^2}V_\varepsilon(s,u)$$

with the effective potential $V_\varepsilon(s,u)$ given by

$$V_\varepsilon(s,u) = -\frac{\lambda(\varepsilon)\gamma(\frac{s}{\varepsilon})^2}{4(1+\varepsilon^{\alpha-1}u\sqrt{\lambda(\varepsilon)}\gamma(\frac{s}{\varepsilon}))^2} + \frac{\varepsilon^{\alpha-1}u\sqrt{\lambda(\varepsilon)}\gamma''(\frac{s}{\varepsilon})}{2(1+\varepsilon^{\alpha-1}u\sqrt{\lambda(\varepsilon)}\gamma(\frac{s}{\varepsilon}))^3} - \frac{5}{4}\frac{\varepsilon^{2\alpha-2}u^2\lambda(\varepsilon)\gamma'(\frac{s}{\varepsilon})^2}{(1+\varepsilon^{\alpha-1}u\sqrt{\lambda(\varepsilon)}\gamma(\frac{s}{\varepsilon}))^4}$$

and $\mathcal{D}(H_\varepsilon) = \{\psi \in L^2(\Omega_0) \,|\, \psi \in C^\infty(\Omega_0),\ \psi(s,\pm d) = 0,\ H_\varepsilon\psi \in L^2(\Omega_0)\}$.

Energy renomalization

Consider the *transverse modes*, i.e. normalized solutions $\varphi_n(u)$ to $-\varepsilon^{-2\alpha}\varphi_n''(u) = E_{\varepsilon,n}\varphi_n(u)$ satisfying $\varphi_n(\pm\varepsilon^\alpha d) = 0$; the corresponding eigenvalues $E_{\varepsilon,n}$ are

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We take the energy *renormalized* by the corresponding *threshold value*

$$\bar{R}^\varepsilon_{n,m}(k^2, s, s') := \int_{-d}^{d}\int_{-d}^{d} \mathrm{d}u\,\mathrm{d}u'\,\varphi_n(u)(H_\varepsilon - k^2 - E_{\varepsilon,m})^{-1}(s, u, s', u')\varphi_m(u').$$

The operators $\bar{R}^\varepsilon_{n,m}(k^2)$ are bounded operator-valued analytic functions of k^2 for all $k^2 \in \mathbb{C}\setminus\mathbb{R}$ and $\mathrm{Im}\,k > 0$.

Threshold resonances

Let us recall what the *threshold* (or zero-energy) *resonance* means for a 1D Schrödinger operator $H = -\frac{\mathrm{d}^2}{\mathrm{d}s^2} + V(s)$: we use this term if there is a function $\psi_r \in L^\infty(\mathbb{R}) \setminus L^2(\mathbb{R})$ solving the equation $H\psi_r = 0$ in the sense of distributions

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$$\int_{\mathbb{R}} V(s)\,\mathrm{d}s \neq 0 \quad \text{and} \quad \mathrm{e}^{a|\cdot|} V \in L^1(\mathbb{R})$$

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for some $a > 0$, then exactly one of the following situations can occur:

- *Case I:* H has no zero energy resonance
- *Case II:* there is such a resonance; then ψ_r can be chosen *real* and the numbers $c_2 := -\frac{1}{2}\int_{\mathbb{R}} sV(s)\psi_r(s)\,\mathrm{d}s$ and

$$c_1 = \left[\int_{\mathbb{R}} V(s)\,\mathrm{d}s\right]^{-1} \int_{\mathbb{R}}\int_{\mathbb{R}} V(s)\frac{|s-s'|}{2}V(s')\psi_r(s')\,\mathrm{d}s\,\mathrm{d}s'$$

cannot not vanish simultaneously.

D. Bollé, F. Gesztesy, S.F.J. Wilk: A complete treatment of low energy scattering in one dimension, *J. Operator Theory* **13** (1985), 3–32.

Point interactions

We distinguish two types operators on line referring to the symbol $-\frac{\mathrm{d}^2}{\mathrm{d}s^2}$. The first one, H^d, describes *Dirichlet-decoupled halflines* which means that its domain is $\mathcal{D}(H^d) := \{f \in H^2(\mathbb{R} \setminus \{0\}) \cap H^1(\mathbb{R}) |\, f(0) = 0\}$.

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The other is a *point-interaction Hamiltonian* H^r the domain of which is

$$\mathcal{D}(H^r) = \Big\{ f \in H^2(\mathbb{R}\setminus 0) |\, (c_1 + c_2) f(0^+) = (c_1 - c_2) f(0^-),$$

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where we put

$$\tilde{\lambda} := \lambda_1 \int_{\mathbb{R}} V(s) \psi_r(s)^2 \, \mathrm{d}s.$$

The operators H^r obviously depend on *two real parameters* and their matching conditions can be written using 2×2 unitary matrices

$$U := \frac{1}{2(c_1^2 + c_2^2) + i\tilde{\lambda}} \begin{pmatrix} -4c_1 c_2 - i\tilde{\lambda} & 2(c_1^2 - c_2^2) \\ 2(c_1^2 - c_2^2) & 4c_1 c_2 - i\tilde{\lambda} \end{pmatrix}.$$

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Theorem

Let the curve C_ε have no self-intersections, γ be piecewise C^2 with a compact support, and γ', γ'' bounded. Assume further that $\alpha > \frac{5}{2}$, then we have the following approximation results in the norm-resolvent sense:

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(i) If $-\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \frac{1}{4}\gamma^2(s)$ has no zero energy resonance, then

$$\lim_{\varepsilon\to 0} R^\varepsilon_{n,m}(k^2) = \delta_{n,m} R^d(k^2), \quad k^2 \in \mathbb{C}\backslash\mathbb{R},\ \ \mathrm{Im}\, k > 0.$$

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(ii) On the other hand, if there is such a resonance, then

$$\lim_{\varepsilon\to 0} R^{\varepsilon}_{n,m}(k^2) = \delta_{n,m} R^r(k^2), \quad k^2 \in \rho(H^r),\ \operatorname{Im} k > 0,$$

where c_1, c_2 and $\tilde\lambda$ are defined as above with $V(s) := -\frac{1}{4}\gamma^2(s)$.

C. Cacciapuoti, P.E.: Nontrivial edge coupling from a Dirichlet network squeezing: the case of a bent waveguide, *J. Phys. A: Math. Theor.* **40** (2007) F511–F523.

Remarks

- Approximations using *threshold resonances* are also used in other situations. Recall *point interactions* in dimensions *two and three*, known alternatively as *Fermi pseudopotentials*. If you want to approximate them by scaled potentials, you have to employ – in contrast to dimension one – Schrödinger operators having a zero-energy resonance, otherwise the limit becomes trivial.

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- Approximation of vertex coupling in case of *branched Dirichlet networks* follows the same idea: one has to used properly scaled operators exhibiting threshold resonances

D. Grieser: Spectra of graph neighborhoods and scattering, *Proc. London Math. Soc.* **97** (2008), 718–752.

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- While the mechanism on which the approximation in the Dirichlet case is clear, we are *far from a complete understanding* at the level achieved with Neumann networks. There is a lot of room here for your activity.

What to bring home from Lecture II

- The multitude of vertex couplings that preserve the probability current is not a mathematical artefact. We have various ways to give *physical meaning* to them; one of them is to regard such graphs as *squeezing limits* of the appropriate networks.

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- A simple physical idea may raise question that mathematically hard, but on the other hand, it can sometimes inspire question of interest for mathematics itself.
- For Neuman-type network we have a complete solution allowing us to *approximate any self-adjoint vertex coupling*.
- For Dirichlet networks, on the other hand, we gave now a clear understinf the mechanism of the squeezing approximation based on threshold resonances, which gives rise to limit *of a non-generic type*. Particular cases are worked out but a complete solution is in this case so far missing.