



Constrained quantum dynamics

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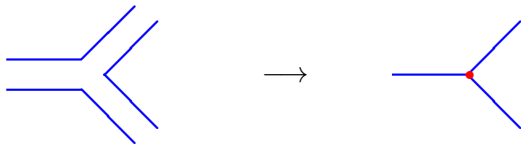
With thanks to all my collaborators

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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



K. Ruedenberg, C.W. Scherr: Free-electron network model for conjugated systems, I. Theory, *J. Chem. Phys.* **21** (1953), 1565–1581.

It looks simple but in fact it is a mathematically quite *hard problem!*

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, $L^2(M_0) := \bigoplus_{j \in J} L^2(I_j)$.

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

Consider next a *Riemannian manifold* X of dimension $d \geq 2$ and the corresponding Hilbert space $L^2(X)$ with the volume element dX equal to $(\det g)^{1/2} dx$ in a fixed chart. For $u \in C_{\text{comp}}^\infty(X)$ 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 operator Δ_X which acts in fixed chart coordinates as

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

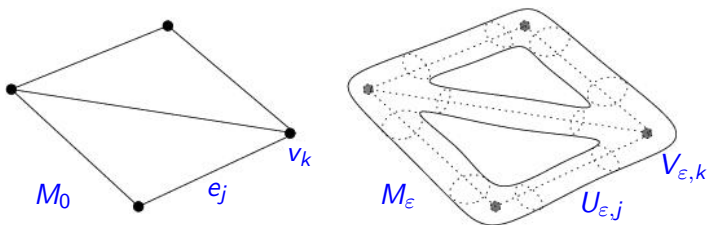
Squeezing a Neumann network



If X is *compact* with a *piecewise smooth boundary*, the form is initially defined on $C^\infty(X)$ and Δ_X is the *Neumann Laplacian* on X .

This formalism allows us to treat '*fat graphs*' and '*sleeves*' on the same footing; what is important is that *lowest 'transverse' eigenfunction* which corresponds to the part of the operator referring to a perpendicular cut of the fattened edge, is in both cases a *constant*.

We associate with graph M_0 a *family of manifolds* M_ϵ as sketched here

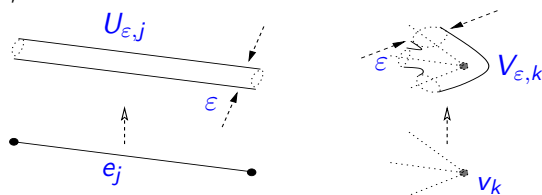


which are all constructed from X by taking a suitable ϵ -*dependent family of metrics*; the advantage of such an approach is that we work with the *intrinsic* geometrical properties only, *no need to embed M into some \mathbb{R}^d* .

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,



- 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 $m := d - 1$ with a metric h ,
- 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 $g_\varepsilon := dx^2 + \varepsilon^2 h(y)$. 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, $\lambda_k(M_\varepsilon) \rightarrow \lambda_k(M_0)$ holds as $\varepsilon \rightarrow 0$.



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

- This convergence concerns the eigenvalues of $-\Delta_{M_\varepsilon}$ associated with the *lowest transverse eigenfunction*, the others escape to infinity.
- We thus get *Kirchhoff conditions*. The same holds more generally when the edge part diameter is *nonconstant*, the limiting graph operator then acts as $u_j \mapsto -\frac{1}{p_j}(p_j u_j)'$.
- The same is true if the vertex region scaling is *slower*, ε^α , with a smooth transition between the two regimes, as long as $\alpha \in (\frac{d-1}{d}, 1)$.
- On the other hand, if the vertex scaling is *too slow*, $\alpha \in [0, \frac{d-1}{d})$, 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



The fact that we get Kirchhoff coupling is not the only problem. The obtained *eigenvalue* convergence for *finite* graphs is in fact a rather weak result. Fortunately, one can do better.

Theorem

Let M_ε be graphlike manifolds associated with a metric graph M_0 , *not necessarily finite*. Under some natural uniformity conditions (see below), $-\Delta_{M_\varepsilon} \rightarrow -\Delta_{M_0}$ as $\varepsilon \rightarrow 0+$ in the *norm-resolvent sense* (with suitable identification), in particular, the σ_{disc} and σ_{ess} converge uniformly in any bounded interval, and *eigenfunctions* converge as well.



O. Post: Spectral convergence of quasi-one-dimensional spaces, *Ann. Henri Poincaré*, **7** (2006), 933–973.



O. Post: *Spectral Analysis on Graph-Like Spaces*, Lecture Notes in Mathematics, vol. 2039, Springer, Berlin 2011.

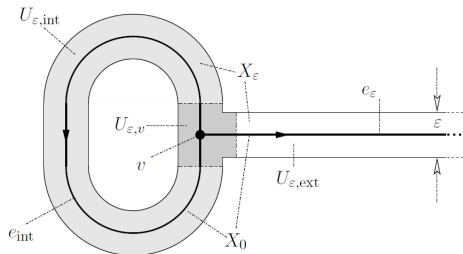
The *natural uniformity conditions* here mean (i) existence of nontrivial bounds on vertex degrees and volumes, edge lengths, and the second Neumann eigenvalues at vertices, (ii) appropriate scaling (analogous to the one described above) of the metrics at the edges and vertices.

More results of this type



The claim looks simple but in fact it is highly nontrivial because we compare here operators acting in *different spaces*; we will mention the used technique briefly a bit later.

Before doing that, let us note that on graphs with semi-infinite 'outer' edges one can investigate *resonances*. What happens with them if the graph is replaced by a family of 'fat' graphs as, for instance, in the *lasso graph* example sketched here?



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

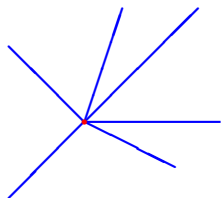


P.E., O. Post: Convergence of resonances on thin branched quantum wave guides, *J. Math. Phys.* **48** (2007), 092104.

Can one get other vertex couplings?



As a hint, let us ask first about an approximation on the graph itself, replacing the *Laplacian* by suitable *Schrödinger operators*.



For the sake of simplicity, consider again a *star graph* with $\mathcal{H} = \bigoplus_{j=1}^n L^2(\mathbb{R}_+)$ and on it Schrödinger operator acting as $\psi_j \mapsto -\psi_j'' + V_j\psi_j$ on the edge components of the wave function

We adopt the following assumptions:

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

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



Suppose that the potential has a shrinking component of the form

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

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 $V_j \in L^1_{\text{loc}}(\mathbb{R}_+)$ 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 $\varepsilon \rightarrow 0+$ in the *norm resolvent sense*, with the coupling parameter $\alpha := \sum_{j=1}^n \int_0^\infty W_j(x) dx$.



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

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

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

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,

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

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

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

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

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 $\|f\|_{H^1(G)}^2 = \|\overline{f'}\|_G^2 + \|f\|_G^2$.

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

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

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

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.

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

$$L_2(X_\varepsilon) = \bigoplus_e (L_2(I_e) \otimes L_2(\varepsilon Y_e)) \oplus L_2(\varepsilon X_v)$$

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.

Note the different scaling in the edge and vertex parts.

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

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

The operators



The Laplacian Δ_{X_ε} on X_ε is associated with the quadratic form

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

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

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

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

where Q_ε is supported only in the vertex region X_v . Inspired by the graph approximation 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}_ε is *relatively form-bounded* with respect to the free form \mathfrak{d}_ε , i.e., there is $\tilde{C}_\eta > 0$ such that

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

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

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*.

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

$$\mathcal{H} := L_2(G), \quad \mathcal{H}^1 := H^1(G), \quad \tilde{\mathcal{H}} := L_2(X_\varepsilon), \quad \tilde{\mathcal{H}}^1 := H^1(X_\varepsilon),$$

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

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

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 $J: \mathcal{H} \rightarrow \tilde{\mathcal{H}}$ between the Hilbert spaces by

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

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

To relate the Sobolev spaces we need a similar map, $J^1: \mathcal{H}^1 \rightarrow \tilde{\mathcal{H}}^1$, which is defined by

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

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

Identification maps: manifold to graph



Let us next introduce the following *averaging operators*:

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

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

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

In the same vein, we define $J'^1 : \tilde{\mathcal{H}}^1 \rightarrow \mathcal{H}^1$ between the Sobolev spaces by

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

where χ_e is a *smooth cut-off function* such that $\chi_e(0) = 1$ and $\chi_e(\ell_e) = 0$. By construction, $J'^1 u \in H_{\underline{p}}^1(G)$, in particular, it belongs to $H^1(G)$ 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 $\varepsilon \rightarrow 0$. If the same can be said about $|\mathfrak{h}(J^1 u, f) - \mathfrak{h}_\varepsilon(u, J^1 f)|$, the forms are *quasi-unitarily equivalent*.

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 $\lambda \rightarrow \infty$ and being continuous in a neighborhood of $\sigma(H)$.

δ -coupling results: consequences of the theorem



Note that the Sobolev map J^1 does not appear in the formulation of the theorem but it is clear that it plays a crucial role in the proof.

The norm resolvent convergence established in the theorem implies:

Corollary

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

and

Corollary

For any $\lambda \in \sigma_{\text{disc}}(H)$ there exists a family $\{\lambda_\varepsilon\}_\varepsilon$ with $\lambda_\varepsilon \in \sigma_{\text{disc}}(H_\varepsilon)$ such that $\lambda_\varepsilon \rightarrow \lambda$ as $\varepsilon \rightarrow 0$, 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

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

holds as $\varepsilon \rightarrow 0$.

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. 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

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

then the corresponding Hamiltonians, 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.

To deal with the others, let us use the same strategy as for δ , namely

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

Note that it is nontrivial even in situations as simple as *approximating the δ' interaction on the line*. For a long time mathematicians believed one cannot do that using *scaled Schrödinger operators*.

Then Cheon and Shigehara proposed a *formal* limiting procedure, and it turned out that it can be adapted into a *norm resolvent* approximation



T. Cheon, T. Shigehara: Realizing discontinuous wave functions with renormalized short-range potentials, *Phys. Lett. A* **243** (1998), 111–116.



S. Albeverio, L. Nizhnik: Approximation of general zero-range potentials, *Ukrainian Math. J.* **52** (2000), 582–589.



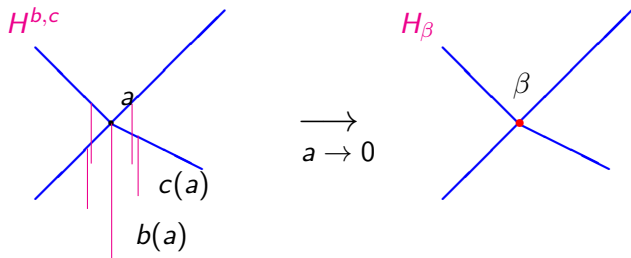
P.E., H. Neidhardt, V.A. Zagrebnev: Potential approximations to δ' : an inverse Klaunder phenomenon with norm-resolvent convergence, *Commun. Math. Phys.* **224** (2001), 593–612.

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:



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

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

Following the idea of Cheon and Shigehara



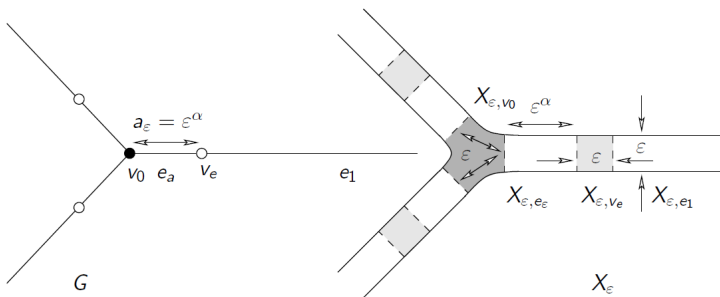
Theorem

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



T. Cheon, P.E.: An approximation to δ' couplings on graphs, *J. Phys. A: Math. Gen.* **37** (2004), L329–L335.

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

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

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

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 $\varepsilon \rightarrow 0$.

How to deal with the general vertex coupling



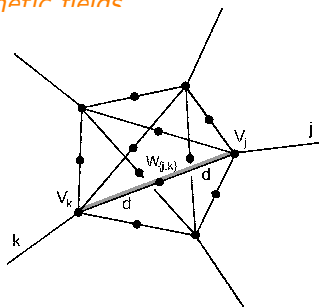
To go beyond these examples, one can try Cheon-Shigehara idea *without the permutation symmetry*; this yields a $2n$ -parameter family.



P.E., O. Turek: Approximations of singular vertex couplings in quantum graphs, *Rev. Math. Phys.* **19** (2007), 571–606.

To get a wider class, however, new ideas are needed. We can, for instance

- *modify the topology locally* adding edges which vanish in the limit. This yields *formally* $A\Psi + B\Psi' = 0$ with *real-valued* matrices A, B with the needed properties, i.e., all *time-reversal invariant* couplings,
- to get *complex* A, B one has to amend the approximating operators with suitably scaled *magnetic fields*



The ST-form of coupling conditions



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

Theorem

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 $S \in \mathbb{C}^{m,m}$.



T. Cheon, P.E., O. Turek: Approximation of a general singular vertex coupling in quantum graphs, *Ann. Phys.* **325** (2010), 548–578.

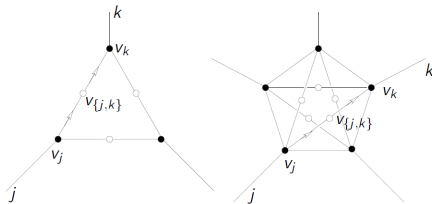
Note that the condition $(U - I)\Psi(0) + i(U + I)\Psi'(0) = 0$ can be split into the Dirichlet, Neumann, and Robin parts related to eigenspaces of U . In the theorem we single out the Dirichlet part referring to eigenvalue -1 .

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.



We number lines of T from 1 to m and the columns from $m + 1$ to n , then

- 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

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

and

$$w_l(d) = \frac{1 - \#N_l + \sum_{h=1}^m \langle T_{hl} \rangle}{d}, \quad w_{\{j,l\}}(d) = \frac{1}{d} \left(-2 + \frac{1}{\langle T_{jl} \rangle} \right)$$

where $\langle c \rangle$ for $c \in \mathbb{C}$ means $\pm|c|$ for $\operatorname{Re} c \geq 0$ and $\operatorname{Re} c < 0$, 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 $n^2 - (n - m)^2$.

The approximation scheme



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 $\text{Re} \left(d \cdot S_{jk} + \sum_{l=m+1}^n T_{jl} \overline{T_{kl}} \right) \geq 0$ and $\mu = 1$ otherwise.

The δ -coupling parameters $w_{\{j,k\}}$ and $w_j(d)$ 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

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

Note that most coefficients behave as $\mathcal{O}(d^{-1})$ when $d \rightarrow 0+$ 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^{star} and H_d^{approx} , as well as their resolvents, $R^{\text{star}}(z)$ and $R_d^{\text{approx}}(z)$, respectively, act on *different spaces*, namely $R^{\text{star}}(z)$ on $L^2(\Gamma)$, while $R_d^{\text{approx}}(k^2)$ acts on the larger space $L^2(\Gamma_d) := L^2(\Gamma \oplus (0, d)^{\sum_{j=1}^n N_j})$.

To be able to compare them, we identify $R^{\text{star}}(z)$ with

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

Theorem

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

The obtained approximation is again *non-generic*; if we violate the elaborate choice of the coefficient functions, ‘almost surely’ we would arrive at the trivial result describing decoupled edges.

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:

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

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

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.

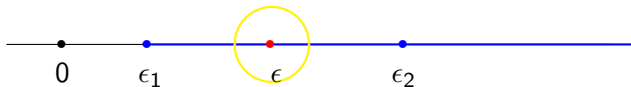
Briefly about the Dirichlet case



We are naturally interested what we can get when a *Dirichlet* network is squeezed, and it appears that the results are *completely different*.

The essential difference comes from the *transverse contribution* to energy: while in the Neumann case it is zero, now it depends on the radius a of the channel and *diverges as $a \rightarrow 0$* . Consequently, the limit needs an *energy renormalization*, in other words, to subtract the divergent term.

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.

Threshold resonances



It is natural to subtract the *threshold energy*, ϵ_1 in the above picture.

Then, however, we are facing a different problem: the limit is *generically trivial* yielding disconnected edges with Dirichlet endpoints. Fortunately, there are situations when the limit is nontrivial; this happens if the operator describing the network has a *resonance at the threshold*.

Let us illustrate this claim on the simplest nontrivial example where there is no branching, just a bent waveguide collapsing onto a *broken line*, i.e. two halflines meeting at a point with a *non-straight angle*.

It is clear that we have to change the channel width and the curvature radius *at the same time*. Should we do the limits consecutively, the $-\frac{1}{4}\gamma(s)^2$ potential would cause trouble, since the curvature of a broken line is proportional to a δ function.

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 $\theta = \int_{\mathbb{R}} \gamma(s) ds$.

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

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

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 be 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

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

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

Energy renormalization



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

$$E_{\varepsilon,n} = \left(\frac{n\pi}{2d\varepsilon^\alpha}\right)^2 \quad \text{with } n = 1, 2, \dots$$

In a straight strip they are *decoupled*. This is not the case when the strip is bent, however, the coupling becomes *weaker* as the strip gets *thin*.

As in the Neumann case, we are interested in the *resolvent convergence*. The resolvent can be written as a *matrix integral operator* with respect to *projections* on the transverse-mode eigenspaces

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

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

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

Threshold resonances



Let us recall what the *threshold* (or zero-energy) *resonance* means for a 1D Schrödinger operator $H = -\frac{d^2}{ds^2} + V(s)$: 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. In particular, if

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

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 $c_2 := -\frac{1}{2} \int_{\mathbb{R}} sV(s)\psi_r(s) ds$ and

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

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 $-\frac{d^2}{ds^2}$. The first one, H^d , describes *Dirichlet-decoupled halflines* which means that its domain is $\mathcal{D}(H^d) := \{f \in H^2(\mathbb{R} \setminus \{0\}) \cap H^1(\mathbb{R}) \mid f(0) = 0\}$.

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

$$\mathcal{D}(H^r) = \left\{ f \in H^2(\mathbb{R} \setminus 0) \mid (c_1 + c_2)f(0^+) = (c_1 - c_2)f(0^-), \right. \\ \left. (c_1 - c_2)f'(0^+) = (c_1 + c_2)f'(0^-) + \frac{\tilde{\lambda}}{c_1 + c_2}f(0^-) \right\} \quad \text{for } c_2 \neq -c_1,$$

$$\mathcal{D}(H^r) = \left\{ f \in H^2(\mathbb{R} \setminus 0) \mid f(0^-) = 0, f'(0^+) = \frac{\tilde{\lambda}}{4c_1^2}f(0^+) \right\} \quad \text{for } c_2 = -c_1,$$

where we put

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

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

$$U := \frac{1}{2(c_1^2 + c_2^2) + i\tilde{\lambda}} \begin{pmatrix} -4c_1c_2 - i\tilde{\lambda} & 2(c_1^2 - c_2^2) \\ 2(c_1^2 - c_2^2) & 4c_1c_2 - i\tilde{\lambda} \end{pmatrix}.$$

The approximation result



In particular, for $\lambda_1 = 0$ the conditions define the *'scale invariant'* point interaction, on the other hand, the *standard δ interaction* of coupling strength $\tilde{\lambda}$ corresponds to $c_1 = 1$ and $c_2 = 0$.

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*:

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

$$\lim_{\varepsilon \rightarrow 0} R_{n,m}^\varepsilon(k^2) = \delta_{n,m} R^d(k^2), \quad k^2 \in \mathbb{C} \setminus \mathbb{R}, \quad \text{Im } k > 0.$$

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

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

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.



- 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.



S. Albeverio, F. Gesztesy, R. Høegh-Krohn, H. Holden: *Solvable Models in Quantum Mechanics*, 2nd edition, AMS Chelsea Publishing, Providence, R.I., 2005.

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



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



G.F. Dell'Antonio, E. Costa: Effective Schrödinger dynamics on ε -thin Dirichlet waveguides via quantum graphs: I. Star-shaped graphs, *J. Phys. A: Math. Theor.* **43** (2010), 474014.

- 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.
- 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.