Quantum Graphs
and their generalizations

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The minicourse overview

The aim to review some results in the theory of quantum graphs concerning the physical meaning of the model and its generalizations, as well as some spectral and scattering properties:

- *Lecture I*
  The concept of a quantum graph – its history, basic notions, and vertex couplings

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- *Lecture II*
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- *Lecture III*
  Geometric perturbations of quantum graphs. Resonances and their semiclassical behaviour

The minicourse overview, continued

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- *Lecture VI*
  Generalized quantum graphs having “edges” of different dimensions. The physical significance of such models

Quantum graphs

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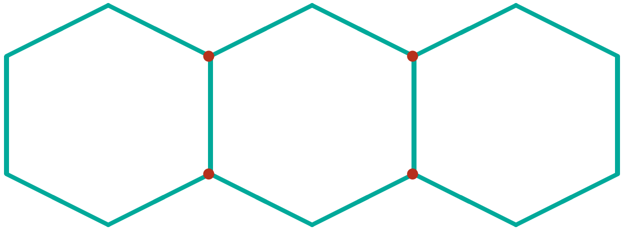


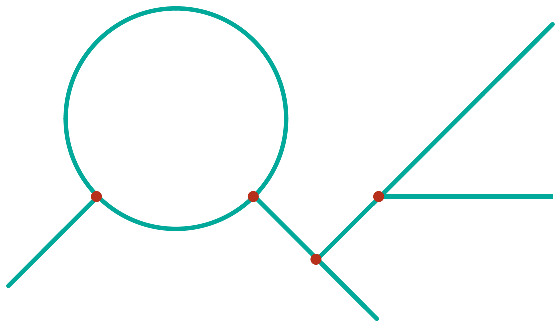
with "Kirchhoff" b.c. in combination with Pauli principle, they reproduced the actual spectra with a $\lesssim 10\%$ accuracy

A caveat: later naive generalizations were less successful

Quantum graph concept

The beauty of theoretical physics resides in permanent oscillation between physical anchoring in reality and mathematical freedom of creating concepts

As a mathematically minded person you can imagine quantum particles confined to a graph of *arbitrary shape*



Hamiltonian: $-\frac{\partial^2}{\partial x_j^2} + v(x_j)$
on graph edges,
boundary conditions at vertices

and, lo and behold, this turns out to be a *practically important* concept – after experimentalists learned in the last 15-20 years to fabricate tiny graph-like structure for which this is a good model

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- Moreover, from the stationary point of view a quantum graph is also equivalent to a *microwave network* built of optical cables – see [Hul et al.'04]
- In addition to graphs one can consider *generalized graphs* which consist of components of different dimensions, modelling things as different as combinations of nanotubes with fullerenes, scanning tunneling microscopy, etc. – we will do that in *Lecture VI*

More remarks

- The vertex coupling is chosen to make the Hamiltonian self-adjoint, or in physical terms, to ensure *probability current conservation*. This is achieved by the method based on s-a extensions which everybody in this audience knows (at least I suppose so)

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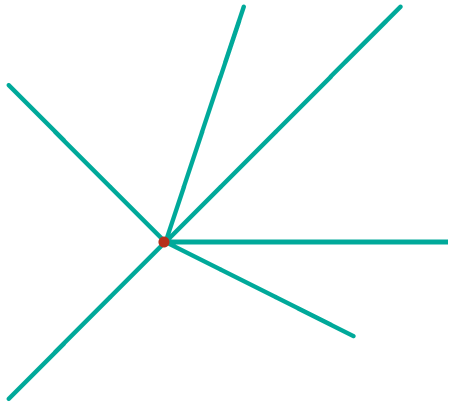
- The graph literature is extensive; a good up-to-date reference are proceedings of the recent semester AGA Programme at INI Cambridge

Wavefunction coupling at vertices



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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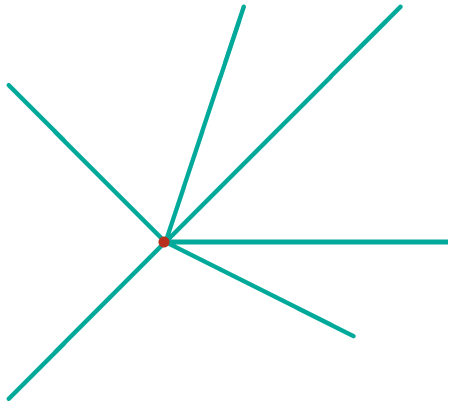

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Since it is second-order, the boundary condition involve $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$ being of the form

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

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

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

Unique boundary conditions

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

Proposition [Harmer'00, K-S'00]: Vertex couplings are uniquely characterized by unitary $n \times n$ matrices U such that

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

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

Self-adjointness requires vanishing of the boundary form,

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

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

Remarks

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

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

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- The *on-shell scattering matrix* for a star graph of n halflines with the considered coupling which equals

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

  giving the *uniqueness of inverse scattering*, $U = S(1)$

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

Further examples

- Another generalization of 1D δ' is the δ' *coupling*:

$$\sum_{j=1}^{n} \psi_j'(0) = 0\,, \quad \psi_j(0)-\psi_k(0) = \frac{\beta}{n}(\psi_j'(0)-\psi_k'(0))\,,\; 1 \le j,k \le n$$

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

$$\begin{aligned} (u-1)(\psi_j(0)-\psi_k(0)) + i(u-1)(\psi_j'(0)-\psi_k'(0)) &= 0 \\ (u-1+nv)\sum_{k=1}^{n}\psi_k(0) + i(u-1+nv)\sum_{k=1}^{n}\psi_k'(0) &= 0 \end{aligned}$$

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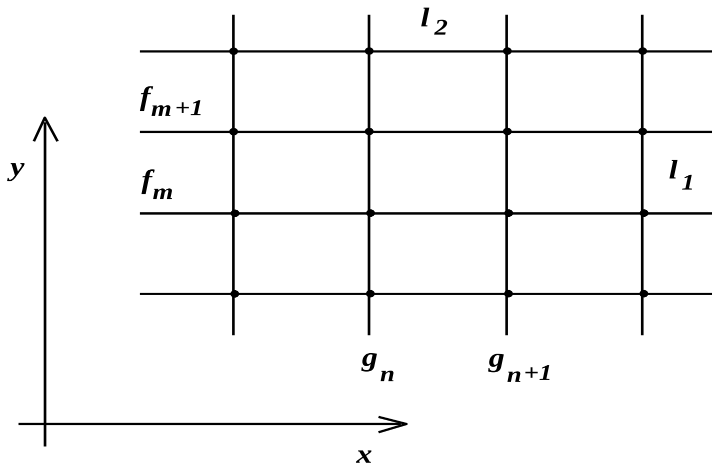
- Recall also that in a rectangular lattice with δ coupling of nonzero α spectrum depends on *number theoretic properties* of model parameters [E.'95]

More on the lattice example

Basic cell is a rectangle of sides ℓ_1, ℓ_2, the δ coupling with parameter α is assumed at every vertex



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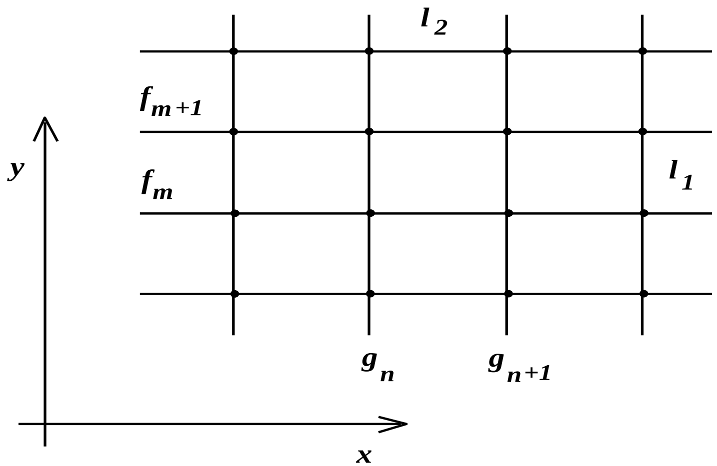

Spectral condition for quasimomentum (θ_1, θ_2) reads

$$\sum_{j=1}^{2} \frac{\cos\theta_j\ell_j - \cos k\ell_j}{\sin k\ell_j} = \frac{\alpha}{2k}$$

Lattice band spectrum

Recall a continued-fraction classification, $\alpha = [a_0, a_1, \ldots]$:

- *"good" irrationals* have $\limsup_j a_j = \infty$ (and full Lebesgue measure)
- *"bad" irrationals* have $\limsup_j a_j < \infty$ (and $\lim_j a_j \neq 0$, of course)

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Theorem [E.’95]: Call $\theta := \ell_2/\ell_1$ and $L := \max\{\ell_1, \ell_2\}$.

(a) If θ is rational or “good” irrational, there are infinitely many gaps for any nonzero α

(b) For a “bad” irrational θ there is $\alpha_0 > 0$ such no gaps open above threshold for $|\alpha| < \alpha_0$

(c) There are infinitely many gaps if $|\alpha|L > \frac{\pi^2}{\sqrt{5}}$

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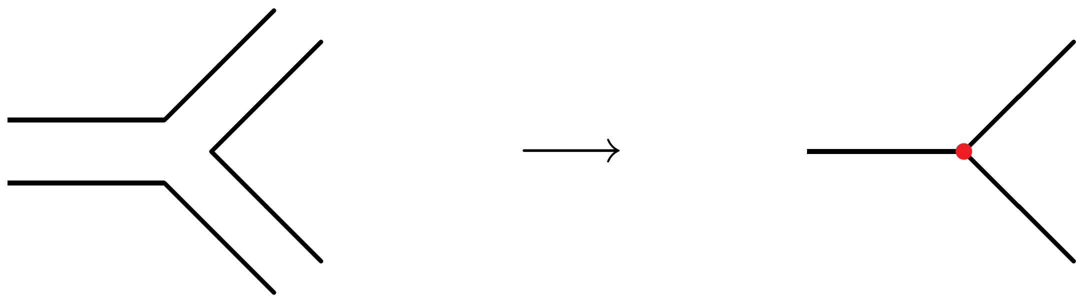
This all illustrates why it is desirable to *understand vertex couplings*. Let us first review the known results

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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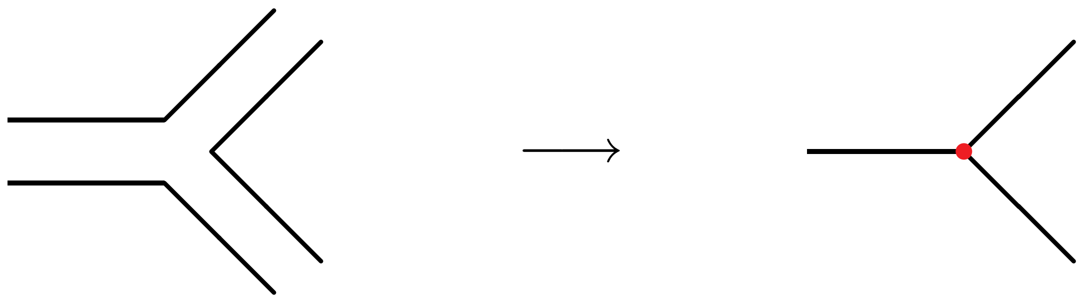

Unfortunately, it is not so simple as it looks because

- 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
- a recent progress in *Dirichlet case*: [Molchanov-Vainberg'07], [E.-Cacciapuoti'07], [Grieser'08], [Dell'Antonio-Costa'10] but a lot remains to be done

First, more on the Dirichlet case

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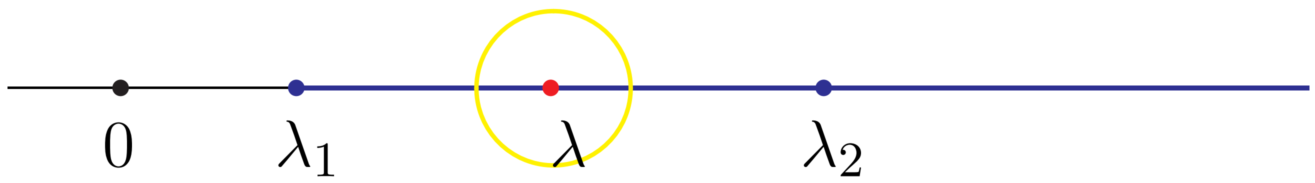

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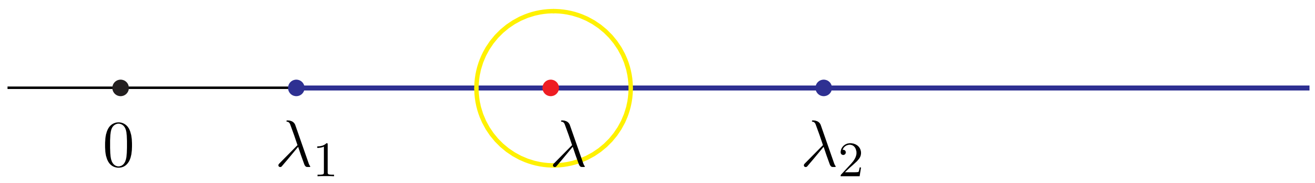

  one gets a nontrivial limit with b.c. fixed by scattering on the "fat star" [Molchanov-Vainberg'07]
- resonances *on* or *around thresholds* can produce a nontrivial coupling [E.-Cacciapuoti'07], [Grieser'08], [Dell'Antonio-Costa'10]

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

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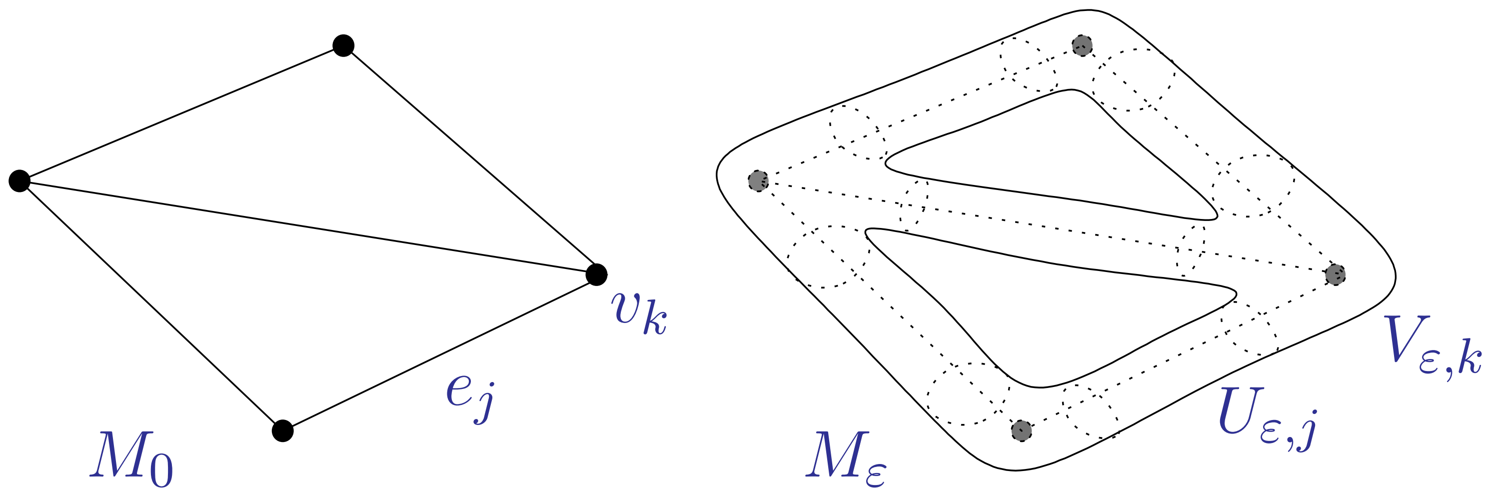
Consider next a Riemannian manifold X of dimension $d \geq 2$ and the corresponding space $L^2(X)$ w.r.t. volume $\mathrm{d}X$ equal to $(\det g)^{1/2}\mathrm{d}x$ in a fixed chart. For $u \in C^\infty_{\mathrm{comp}}(X)$ we set

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

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 $\lambda_k(M_\varepsilon) \to \lambda_k(M_0)$ as $\varepsilon \to 0$ (giving thus free b.c.!)

Improving the convergence

The b.c. are not the only problem. The ev convergence for finite graphs is 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, $\Delta_{M_\varepsilon} \to \Delta_{M_0}$ as $\varepsilon \to 0+$ in the *norm-resolvent sense* (with suitable identification), in particular, the σ_{disc} and σ_{ess} converge uniformly in an bounded interval, and ef's converge as well.

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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 $\varepsilon \to 0$ [E.-Post’07]. The same is true for *embedded eigenvalues* of the graph Laplacian which may remain embedded or become resonances for $\varepsilon > 0$

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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?

Summarizing Lecture I

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- *The quantum graph model* is easy to handle and useful in describing a host of physical phenomena
- *Vertex coupling:* to employ the full potential of the graph model, it is vital to understand the physical meaning of the corresponding boundary conditions
- *"Fat manifold" approximations:* using the simplest geometry only we get free b.c. in the Neumann-like case, partial results known in the Dirichlet case

Some literature to Lecture I

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[Po06] O. Post: Spectral convergence of quasi-one-dimensional spaces, *Ann. Henri Poincaré* **7** (2006), 933-973

Lecture II

How the vertex couplings can be understood in terms of approximations

Lecture overview

- *A strategy:* try first to approximate on the graphs itself and then to“lift” the result to network manifolds

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- *A strategy:* try first to approximate on the graphs itself and then to“lift” the result to network manifolds
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- δ'_s *coupling*: a graph approximation using Cheon-Shigehara idea, then lifting to the manifold
- *More general vertex couplings*: results known on graphs only, in general they require local modifications of the graph topology

Inspiration from graph approximations

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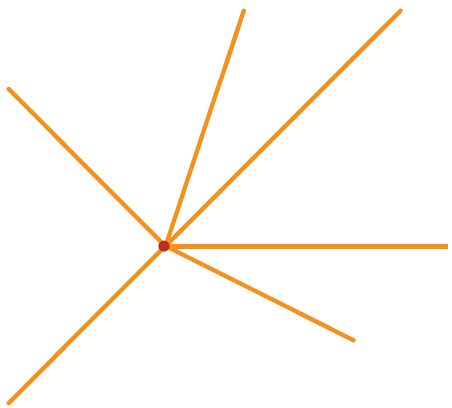

Consider once more *star graph* with $\mathcal{H} = \bigoplus_{j=1}^n L^2(\mathbb{R}_+)$ and Schrödinger operator acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j'' + V_j\psi_j$

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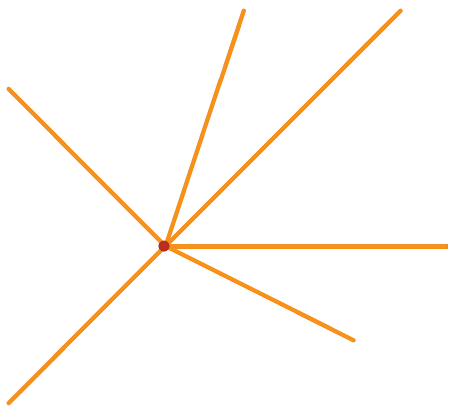

Consider once more *star graph* with $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and Schrödinger operator acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j'' + V_j \psi_j$

We make the following assumptions:

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

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

Potential approximation of δ coupling

Suppose that the potential has a shrinking component,

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

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

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

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. $\square$

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

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

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together with its natural norm.

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

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

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

Operators on the graph

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

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

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

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

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

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

Manifold model of the “fat” graph

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

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

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

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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

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

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 given via its quadratic form

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

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

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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

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

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

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

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

Relative boundedness

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

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

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

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

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

Identification maps

Our operators acts in different spaces, namely

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

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For further purpose we set

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

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

Identification maps, continued

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

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

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

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

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

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

Identification maps, continued

Let us next introduce the following averaging operators

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

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

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

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

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

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

δ-coupling results

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

Theorem [E-Post'09]: We have

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

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

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

δ-coupling results, continued

This result further implies

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

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and

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

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

as $\varepsilon \to 0$.

More complicated graphs

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

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Theorem [E-Post'08]: Assume that G is a metric graph and X_ε the corresponding approximating manifold. If

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

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

How about other couplings?

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

To 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 δ'_s star graph

Let $G = I_{v_0}$ be a star graph with the vertex v_0 and $n = \deg v$, $e = 1, \dots, n$. 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

$$domH^\beta := \Big\{ f \in \mathsf{H}^2_{\max}(G) \,\Big|\, \forall e_1, e_2\colon f'_{e_1}(0) = f'_{e_2}(0) =: f'(0),$$
$$\sum_e f_e(0) = \beta f'(0), \forall e\colon f'_e(\ell_e) = 0 \Big\}$$

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

$$\mathfrak{h}^\beta(f) = \sum_e \|f'_e\|^2 + \frac{1}{\beta}\Big|\sum_e f_e(0)\Big|^2, \qquad dom\,\mathfrak{h}^\beta = \mathsf{H}^1_{\max}(G)$$

if $\beta \neq 0$ and

$$\mathfrak{h}^\beta(f) = \sum_e \|f'_e\|^2, \qquad dom\,\mathfrak{h}^\beta = \{\, f \in \mathsf{H}^1_{\max}(G) \mid \sum_e f_e(0) = 0 \,\}$$

if $\beta = 0$

A δ'_s star graph, continued

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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

Our first task is thus to find an approximation scheme for the δ'_s-coupling on the star graph

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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]

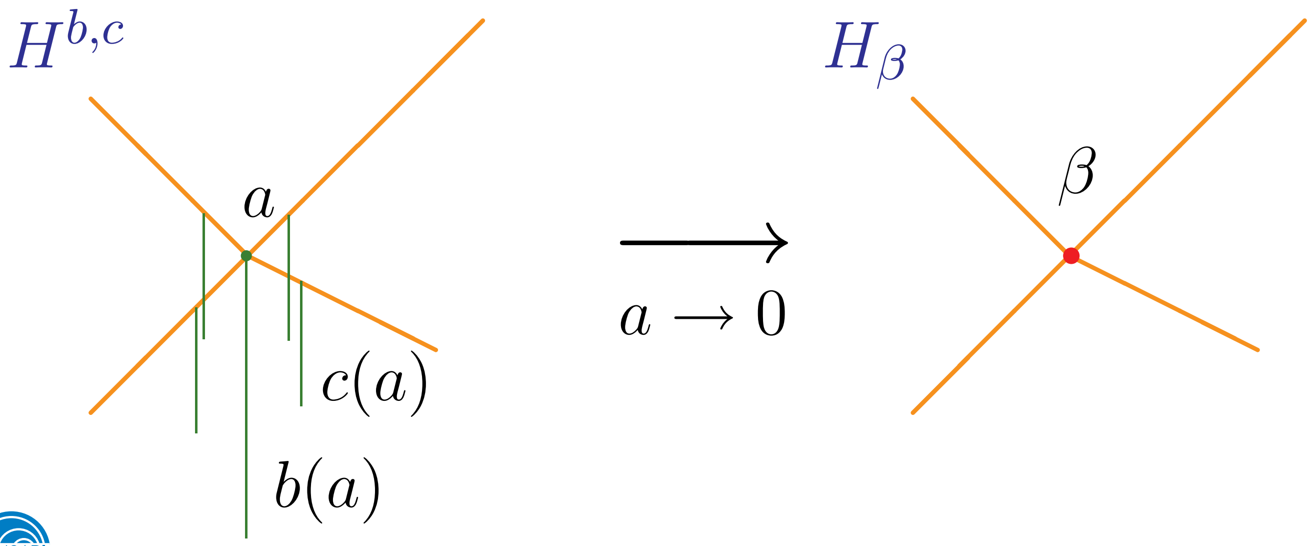
Inspiration: the CS approximation

Our first task is thus to find an approximation scheme for the δ'_s-coupling on the star graph

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]

This suggests the following scheme:



A δ'_s approximation on a star graph

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

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

which corresponds to the quadratic form

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

A δ'_{s} approximation on a star graph

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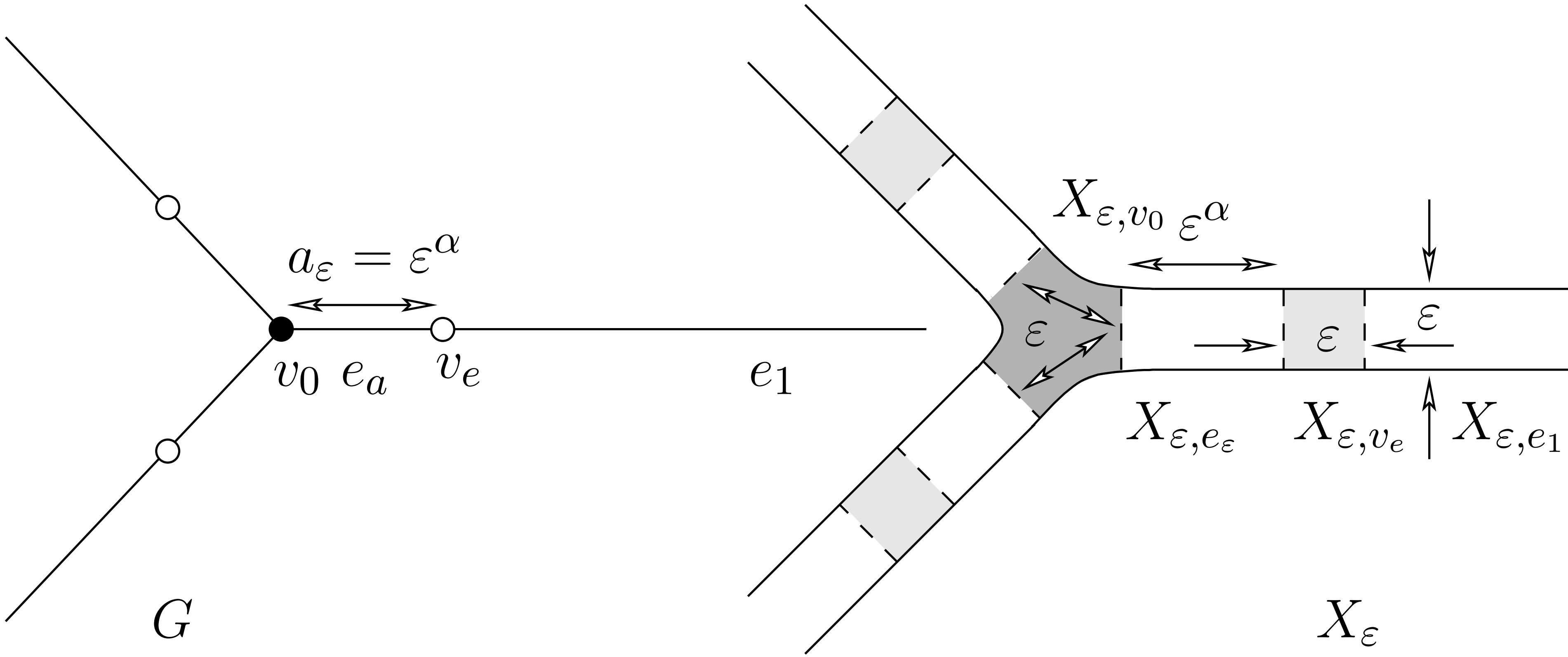
Theorem [Cheon-E'04]: We have

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

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

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 $a \to 0$: there is $C > 0$ such that

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

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

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Proposition: If $\beta \geq 0$, the spectrum of H_ε^β is asymptotically unbounded from below,

$$\inf \sigma(H_\varepsilon^\beta) \to -\infty \quad \text{as} \quad \varepsilon \to 0$$

The δ'_s approximation result

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

Theorem [E-Post'09]: Assume that $0 < \alpha < 1/13$, then

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

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^β_ε 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^β_ε all have to tend to $-\infty$

Proceeding further, so far on graphs

The above results extend to two-parameter set of coupling symmetric w.r.t. interchange of edges – cf. [E-Turek'06].

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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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:

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

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

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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

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

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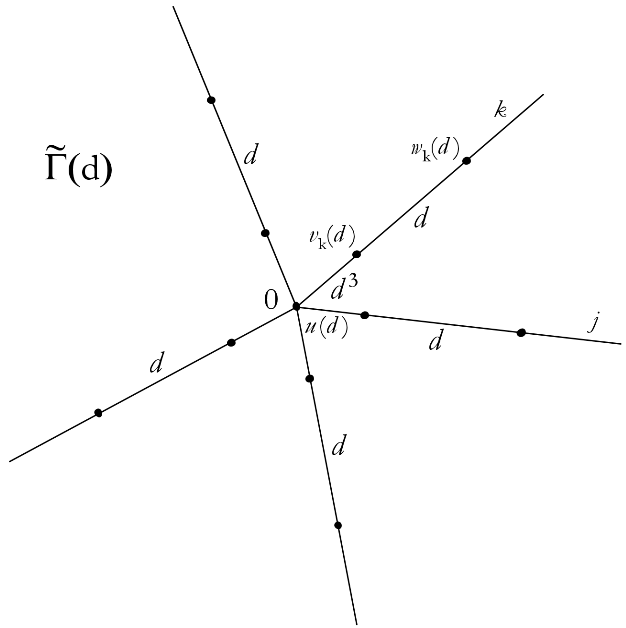

CS-type approximation of star graphs

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. $\square$

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

More general approximations

A more general approximation is obtained if are allowed to add not only vertices, but also *edges* which shrink to the centre of the star graph Γ in the limit

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Remark: The requirement $A, B \in \mathbb{R}^{n,n}$ means that the corresponding coupling is *time-reversal invariant*

More general approximations, contd.

Considerations of [E.-Turek'07] does not provide only an existence result but also a construction of such an approximation. We will not describe it from two reasons:

- it still gives "one half" of the couplings
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More general approximations, contd.

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- it still gives "one half" of the couplings
- it is not particularly elegant

The first deficiency can be resolved by using properly scaled *magnetic fields*, the second one by *leaving out the edges* we do not really need

First we have to introduce, however, an alternative form of the coupling conditions

The ST-form of coupling conditions

Theorem [Cheon-E.-Turek'10]: Consider a quantum graph vertex of degree n. If $m \le n$, $S \in \mathbb{C}^{m,m}$ is a self-adjoint matrix and $T \in \mathbb{C}^{m,n-m}$, then the relation

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

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

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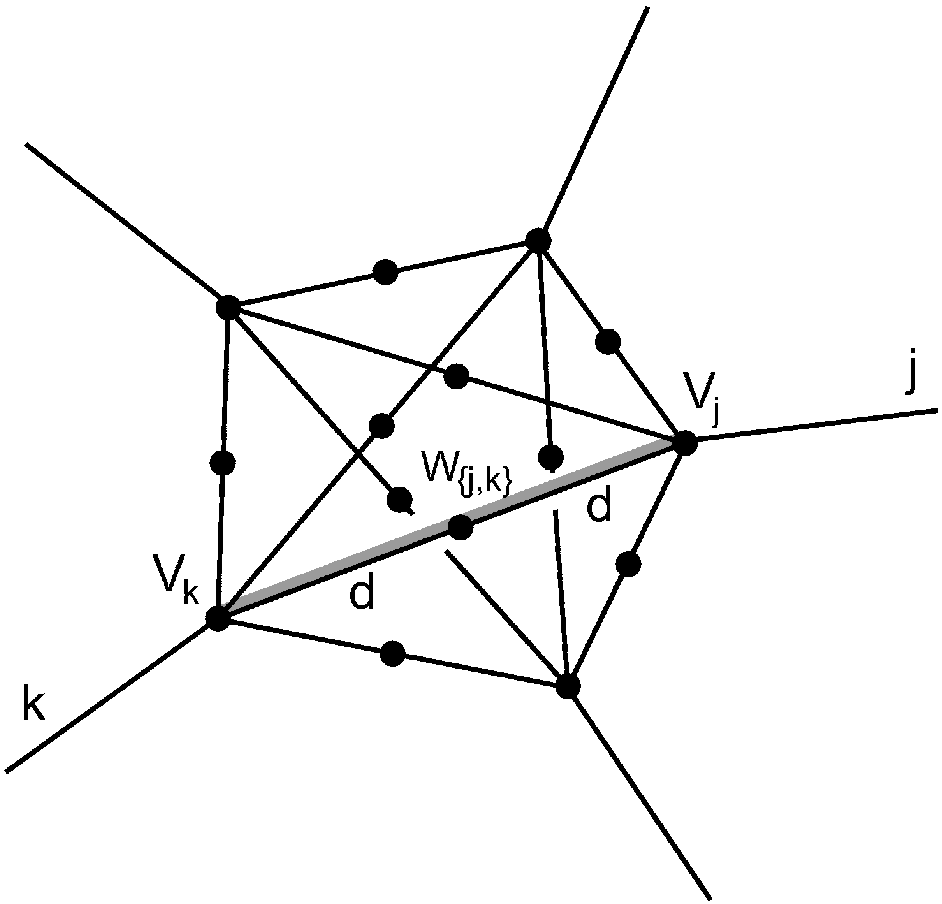
Remark: [Kuchment'04] writes b.c. in terms of eigenspaces of U. Here we single out the one corresponding to ev -1; there is also a symmetrical form referring to ev's ± 1

The approximation scheme, pictorially



All the inner links are of length $2d$, some may be missing. The grey line symbolizes the vector potential $A_{(j,k)}(d)$.

The approximation scheme

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

- Take n halflines, each parametrized by $x \in \mathbb{R}_+$, with the endpoints denoted as V_j, and put a δ-coupling to the edges specified below with the parameter $v_j(d)$ at the point V_j for all $j = 1, \dots, n$.

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- Some pairs $V_j, V_k,\ j \neq k$, of halfline endpoints are connected by edges of length $2d$, and the center of each such joining segment is denoted as $W_{\{j,k\}}$. This happens if one of the following conditions is satisfied:

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

(b) $j, k = 1, \dots, m$, and $S_{jk} \neq 0$ or
$(\,\exists l \geq m+1\,)\,(\,T_{jl} \neq 0 \wedge T_{kl} \neq 0\,)$.

The approximation scheme, continued

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

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

The approximation scheme, continued

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

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

The approximation scheme, continued

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We distinguish two cases regarding the indices involved:
Case I. First assume $j = 1,\dots,m$ and $l \in N_j \backslash \{1,\dots,m\}$; then the vector potential may be chosen as

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

The approximation scheme, continued

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

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

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

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

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

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

The approximation scheme, continued

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

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

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

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

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

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

The result

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

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Theorem [Cheon-E.-Turek'10]: In the described setting, the operator family $H_d^{\rm approx}$ converges to $H^{\rm star}$ in the norm-resolvent sense as $d \to 0$.

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

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Theorem [Cheon-E.-Turek'10]: In the described setting, the operator family H_d^{approx} converges to H^{star} in the norm-resolvent sense as $d \to 0$.

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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Summarizing Lecture II

- The δ *coupling* can be approximated by Neumann-type networks with naturally scaled potentials at the vertex regions
- The δ'_s *coupling* can be approximated using additional potential at the graph edges which move towards the vertex
- *More general couplings* treated so far on the graph level only. Using additional δ interactions one can cover a $2n$ parameter class. Other couplings need a *local change of topology*, to get all the couplings properly scaled *magnetic fields* are needed
- The described graph approximation is conjectured to allow *"lifting"* to Neumann-type network manifolds

Some literature to Lecture II

- [CE04] T. Cheon, P.E.: An approximation to δ' couplings on graphs, *J. Phys. A: Math. Gen.* **A37** (2004), L329-335
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