Approximations of graphs vertices

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Talk overview

- Quantum graphs: a short review

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- Vertex coupling parametrization, examples

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- Heuristic approach: Ruedenberg–Scherr argument
- Squeezing limit using internal geometry
- Scaled potentials on graphs: δ coupling
- Nonlinear scaling: δ' couplings
- Finally, some open questions

Quantum graphs

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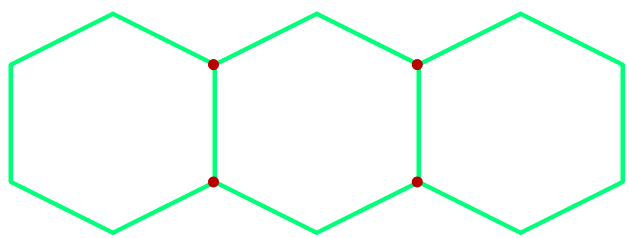
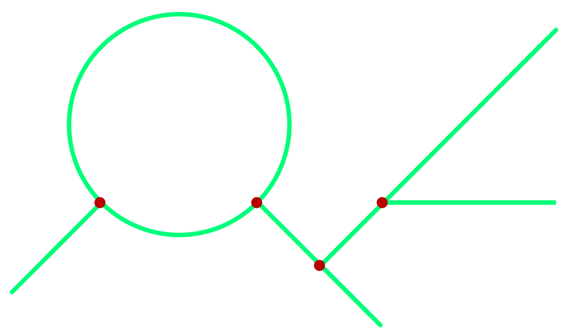


with "Kirchhoff" b.c. in combination with Pauli principle, they reproduced the actual spectra with a $\lesssim 10\%$ accuracy

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 10-15 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.

More remarks

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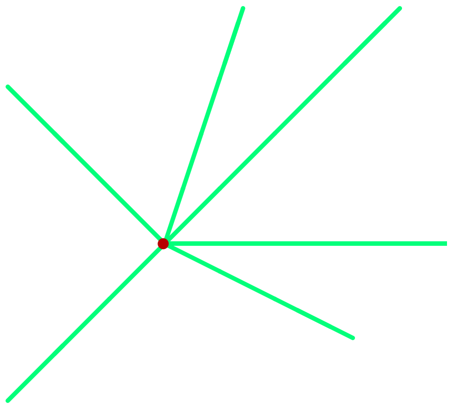
- Graphs can support also *Dirac operators*, see [Bulla-Trenckler'90], although this remains so far a theoretical possibility only.
- The graph literature is extensive; let us refer just to a review [Kuchment'04] and other references in the recent topical issue of *"Waves in Random Media"*

Vertex coupling



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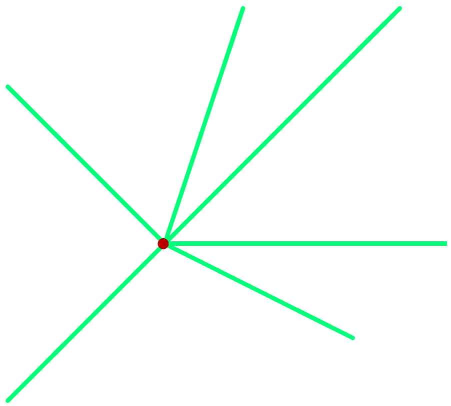

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Since it is second-order, the boundary condition involve $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$ being of the form

$$\Psi'(0) = C\Psi(0) \quad \text{or} \quad \Psi(0) = C\Psi'(0)$$

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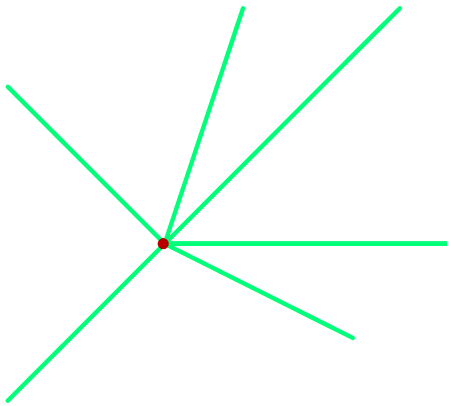

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with a suitable $n \times n$ matrix C parametrizing the coupling.

Disadvantage: Some couplings may be left out if the matrix is singular. One would prefer something analogous to the 1D “universal” condition $\psi(0)\cos\theta + \psi'(0)\sin\theta = 0$

Kostrykin-Schrader b.c.

No coupling is left out if we use the boundary conditions proposed in [Kostrykin-Schrader'99]. They are described by a pair of $n \times n$ matrices A, B such that

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Disadvantage: The matrix pair A, B is naturally not unique

Harmer boundary conditions

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It is obvious that the above A, B have the needed properties. Conversely, to any such A, B there is a $U \in U(n)$ and an invertible C such that $U = C(A - iB)$. Indeed, such a U must satisfy $UU^* = C(BB^* + AA^*)C^*$ since $AB^* = BA^*$ by assumption. The matrix $BB^* + AA^*$ is strictly positive because its null space is

$$\ker A^* \cap \ker B^* = (\mathrm{ran}\, A)^\perp \cap (\mathrm{ran}\, B)^\perp = (\mathrm{ran}\, A \cup \mathrm{ran}\, B)^\perp = \{0\}$$

In particular, it is Hermitean so $C := (BB^* + AA^*)^{-1/2}$ makes sense, it is Hermitean and invertible

A simple derivation of Harmer b.c.

One can modify 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 nonzero ℓ coincide, so the two vectors must be related by an $n \times n$ unitary matrix

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

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

Thus we set $\ell = 1$, which means a choice of the length scale

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

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

To reconstruct U, e.g., it is sufficient to know $S_U(k)$ at a single point where $(k+1)I - (k-1)S_U(k)$ is invertible.

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 *Kirchhoff boundary conditions* (not a well chosen name)
- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the δ_s' *coupling*

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with $\beta \in \mathbb{R}$; for $\beta = \infty$ we get *Neumann* decoupling

Examples: another dual pair

- The "permuted" δ, or δ_p *coupling*:

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

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- The infinite values of α, β refer again to the Dirichlet and Neumann decoupling of the graph edges, respectively
- These examples have all permutation symmetry, hence their U's are linear combinations of symmetric matrices I and $\mathcal{J}$

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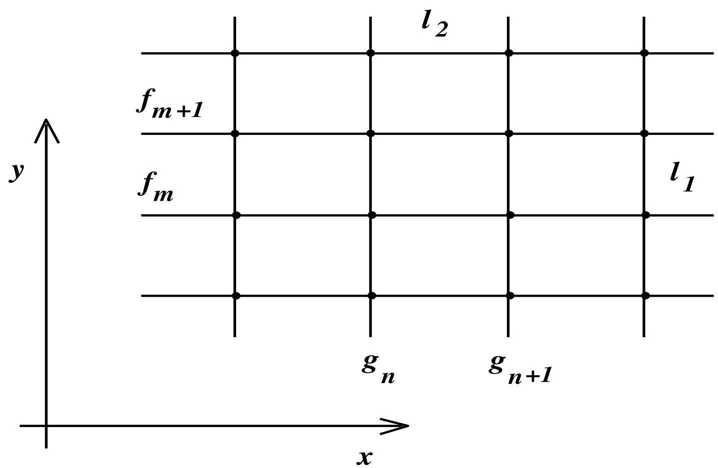
- Recall also that in a rectangular lattice with δ coupling of nonzero α spectrum depends on *number theoretic properties* of model geometric parameters [E.'95,'96a; E.-Gawlista'96]

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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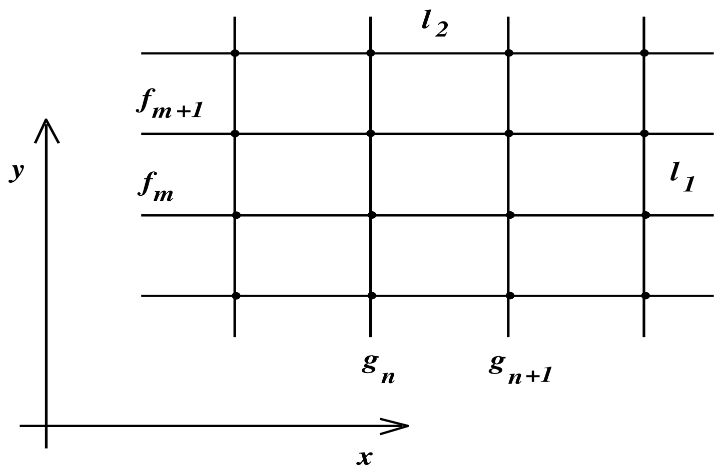

Spectral condition for quasimomentum (θ_1, θ_2) reads

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

Lattice band spectrum

To describe spectral properties of such a system, express the coupling through continued fractions, $\alpha = [a_0, a_1, \dots]$:

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

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Theorem [E.'95,'96a]: 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 $|\alpha| L > \frac{\pi^2}{\sqrt{5}}$

Remarks

- The critical value $\alpha_0 = \frac{\pi^2}{\sqrt{5}}$ is attained, in particular, for *golden mean*, $\frac{1}{2}(1+\sqrt{5}) = [1, 1, 1, \dots]$, i.e. the "worst" irrational

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- Other infinite gap series open at integer multiples of α_0, namely $4, 5, 9, 11, 16, 19, 20, 25, \dots$ which is nothing else than $|m^2 - n^2 - mn|$ with $m, n \in \mathbb{N}$ [E.-Gawlista'96]

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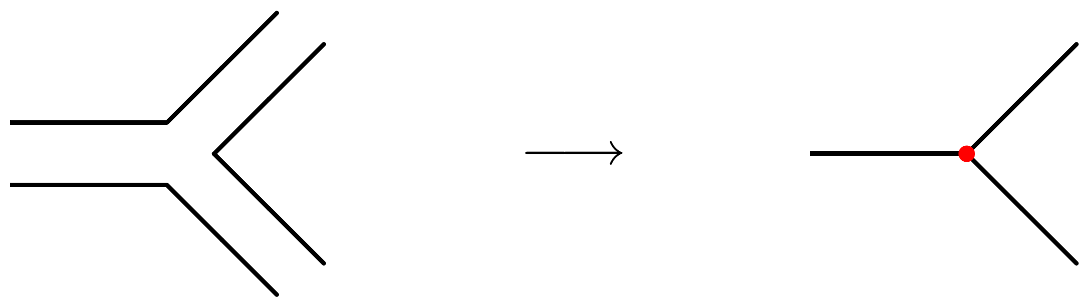
- The above claim can be regarded as *sui generis* counterexample to *Bethe-Sommerfeld conjecture*, of course, if you accept that such a lattice is a 2D system
- These examples – and others – illustrate that it is desirable to understand whether there is a meaningful way *to "construct" vertices with different couplings*

This will be our task in the rest of this talk

So? Any freshman knows what to do

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



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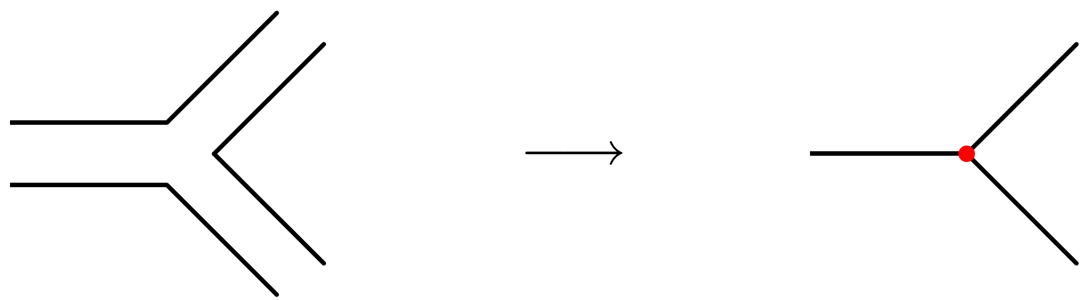

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- after a long effort the Neumann case was solved [Kuchment-Zeng'01, Rubinstein-Schatzmann'01, Saito'01] leading to Kirchhoff b.c. only
- the important *Dirichlet case* is open (and difficult)
- there are interesting situations – remember the *branching nanotubes* mentioned above, etc.

Preliminaries: weighted graphs

Let M_0 be a finite connected graph with vertices v_k, $k \in K$ and edges $e_j \simeq I_j := [0, \ell_j]$, $j \in J$. We add smooth weights $p_j : \, I_j \to \mathbb{R}_+$ so the state Hilbert space is

$$L^2(M_0) := \bigoplus_{j \in J} L^2(I_j, p_j(x)\,\mathrm{d}x)\,;$$

in a similar way Sobolev spaces on M_0 are introduced

Preliminaries: weighted graphs

Let M_0 be a finite connected graph with vertices v_k, $k \in K$ and edges $e_j \simeq I_j := [0, \ell_j]$, $j \in J$. We add smooth weights $p_j : I_j \to \mathbb{R}_+$ so the state Hilbert space is

$$L^2(M_0) := \bigoplus_{j \in J} L^2(I_j, p_j(x)\,\mathrm{d}x)\,;$$

in a similar way Sobolev spaces on M_0 are introduced

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

$$\Delta_{M_0} u = -\frac{1}{p_j(x)} (p_j(x) u_j')'$$

and satisfies (weighted) Kirchhoff b.c.,

$$\sum_{j,\, e_j \text{ meets } v_k} p_j(v_k) u_j'(v_k) = 0$$

Preliminaries: Laplacian on manifolds

Consider 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 s-a operator Δ_X which acts in fixed chart coordinates as

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

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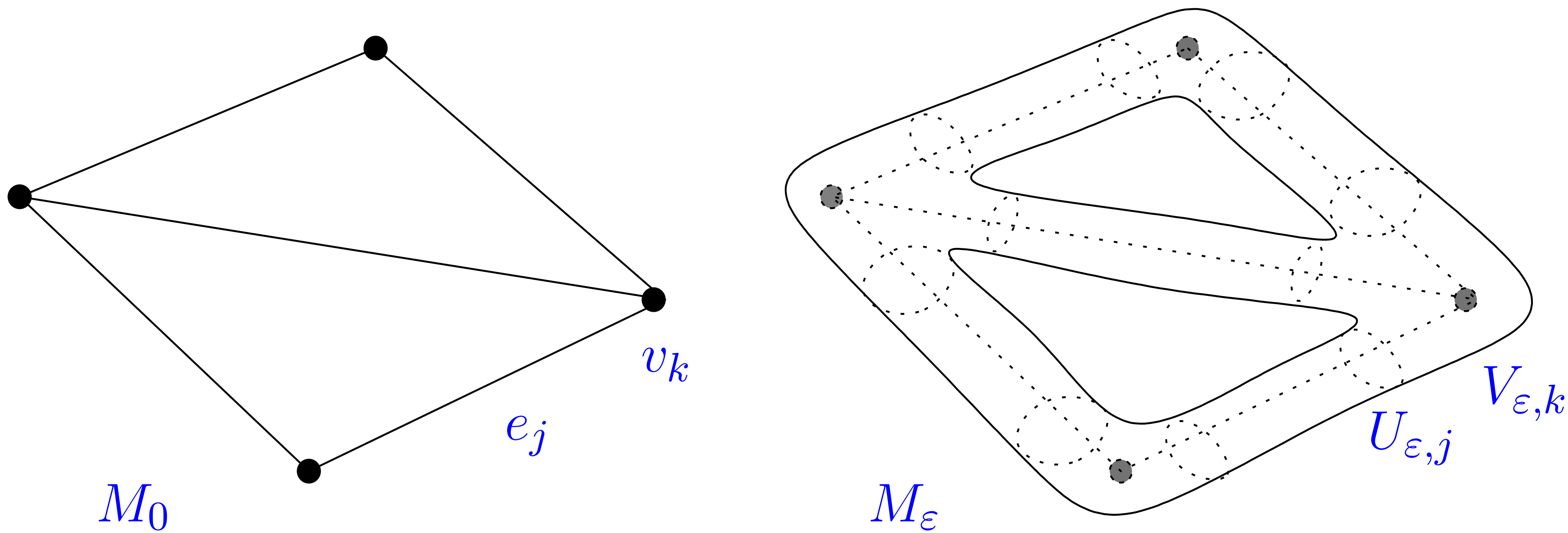
If X is compact with piecewise smooth boundary, one starts from the form defined on $C^\infty(X)$. This yields Δ_X as the *Neumann* Laplacian on X and allows us to treat “fat graphs” and “sleeves” on the same footing

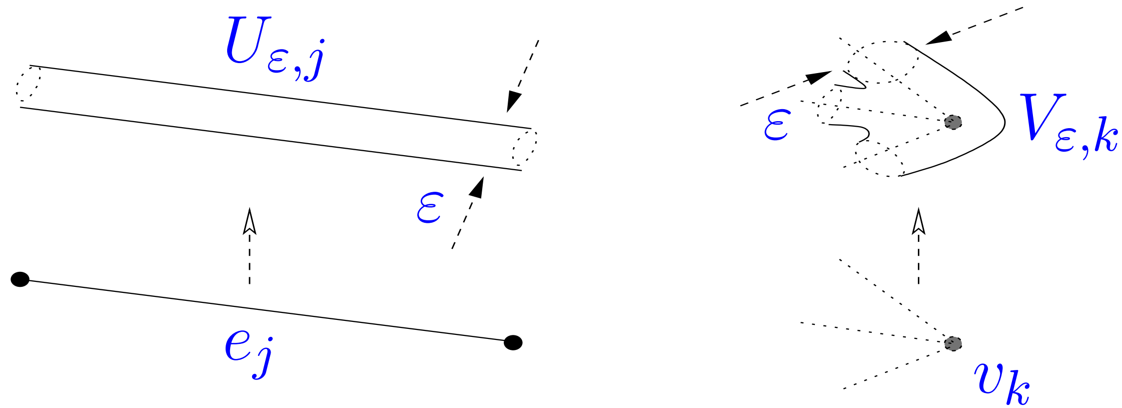
Fat graphs and sleeves: manifolds

We associate with the graph M_0 a family of manifolds M_ε



We suppose that M_ε is a union of compact edge and vertex components $U_{\varepsilon,j}$ and $V_{\varepsilon,k}$ such that their interiors are mutually disjoint for all possible $j \in J$ and $k \in K$

Manifold building blocks



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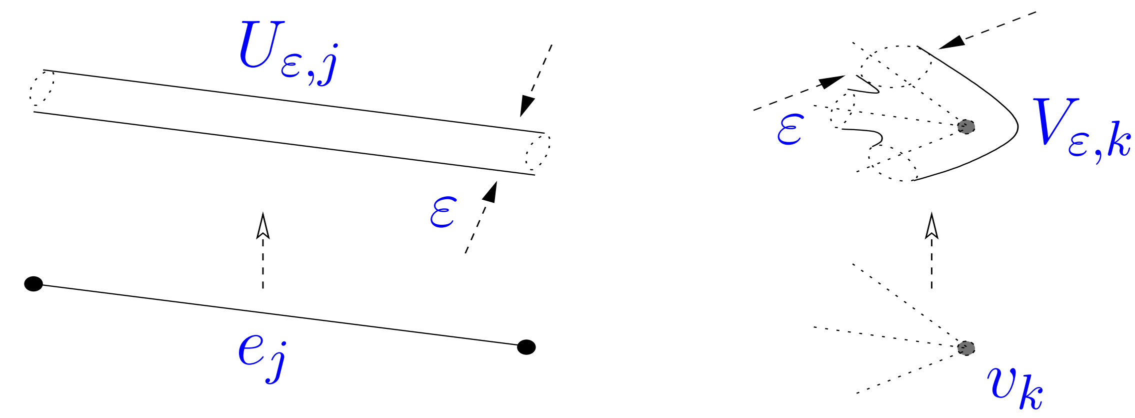

However, M_ε *need not be embedded* in some $\mathbb{R}^d$.

It is convenient to assume that $U_{\varepsilon,j}$ and $V_{\varepsilon,k}$ depend on ε only through their metric:

- 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

Ruedenberg-Scherr argument

For simplicity assume that the radius of $U_{\varepsilon,j}$ does not change, i.e., let $p_j = 1$

Suppose that $\phi = \phi_\varepsilon$ is an ef of Δ_X with the ev $\lambda = \lambda_\varepsilon$. By the Gauss-Green formula we have at the vertex $V_{\varepsilon,k} = V_\varepsilon$

$$\lambda \int_{V_\varepsilon} \phi\,\overline{u}\,\mathrm{d}V_\varepsilon = \int_{V_\varepsilon} \langle \mathrm{d}\phi, \mathrm{d}u \rangle\,\mathrm{d}V_\varepsilon + \int_{\partial V_\varepsilon} \partial_\mathrm{n}\phi\,\overline{u}\,\mathrm{d}\partial V_\varepsilon$$

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Assume that $\lambda_\varepsilon \to \lambda_0$ and $\phi_\varepsilon \to \phi_{0,j}$. Since vertex volume $(\sim \varepsilon^d)$ decays faster than the interface area $(\sim \varepsilon^{d-1})$ only the boundary integral over ∂V_ε survives in the limit $\varepsilon \to 0$ giving thus Kirchhoff boundary conditions

$$0 = \sum_{j \in J_k} \phi'_{0,j}(v_k)$$

Comparison of eigenvalues

Our main tool here will be minimax principle. Suppose that $\mathcal{H}$, $\mathcal{H}'$ are separable Hilbert spaces. We want to compare ev's λ_k and λ_k' of nonnegative operators Q and Q' with purely discrete spectra defined via quadratic forms q and q' on $\mathcal{D} \subset \mathcal{H}$ and $\mathcal{D}' \subset \mathcal{H}'$. Set $\|u\|_{Q,n}^2 := \|u\|^2 + \|Q^{n/2}u\|^2$.

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Lemma: Suppose that $\Phi :\, \mathcal{D} \to \mathcal{D}'$ is a linear map such that there are $n_1, n_2 \geq 0$ and $\delta_1, \delta_2 \geq 0$ such that

$$\|u\|^2 \leq \|\Phi u\|'^2 + \delta_1 \|u\|^2_{Q,n_1}\,, \quad q(u) \geq q'(\Phi u) - \delta_2 \|u\|^2_{Q,n_2}$$

for all $u \in \mathcal{D} \subset \mathcal{D}(Q^{\max\{n_1,n_2\}/2})$. Then to each k there is a positive $\eta_k(\lambda_k, \delta_1, \delta_2)$ which tends to zero as $\delta_1, \delta_2 \to 0$, such that

$$\lambda_k \geq \lambda'_k - \eta_k$$

Thickened edges

Let thus $U = I_j \times F$ with metric g_ε, where cross section F is a compact connected Riemannian manifold of dimension $m = d-1$ with metric h; we assume that $\mathrm{vol}\, F = 1$. We define another metric $\tilde{g}_\varepsilon$ on $U_{\varepsilon,j}$ by

$$\tilde{g}_\varepsilon := \mathrm{d}x^2 + \varepsilon^2 r_j^2(x)\, h(y)\,,$$

where $r_j(x) := (p_j(x))^{1/m}$; they coincide up to $\mathcal{O}(\varepsilon)$ error

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Curved edges: If e_j is a smooth curve in $\mathbb{R}^d$ the metric coming form the embedding contains terms given by the curvature γ of e_j. In the limit $\varepsilon \to 0$ they give rise to effective potential $-\frac{1}{4}\gamma^2$. This effect is well known; for simplicity we assume that the *edges are straight*

Eigenvalue convergence

Theorem [E.-Post'03]: Under the stated assumptions $\lambda_k(M_\varepsilon) \to \lambda_k(M_0)$ as $\varepsilon \to 0$

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Proof is based on two-sided estimates. The upper one is easier and reads

Proposition: $\lambda_k(M_\varepsilon) \le \lambda_k(M_0) + o(1)$ as $\varepsilon \to 0$

To prove it one one defines $\Phi_\varepsilon :\ L^2(M_0) \to L^2(M_\varepsilon)$ by

$$\Phi_\varepsilon u(z) := \begin{cases} \varepsilon^{-m/2} u(v_k) & \text{if } z \in V_k \\ \varepsilon^{-m/2} u_j(x) & \text{if } z = (x,y) \in U_j \end{cases}$$

for any $u \in \mathcal{H}^1(M_0)$, i.e. multiplication by a constant function in transverse direction. It is checked directly that the above lemma applies $\square$

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Here one uses *averaging*:

$$N_j u(x) := \int_F u(x,\cdot)\,\mathrm{d}F\,, \quad C_k u := \frac{1}{\mathrm{vol}\,V_k}\int_{V_k} u\,\mathrm{d}V_k$$

to build the comparison map by *interpolation*:

$$(\Psi_\varepsilon)_j(x) := \varepsilon^{m/2}(N_j u(x) + \rho(x)(C_k u - N_j u(x)))$$

with a suitable ρ smoothly interpolating between zero and one. But a series of estimates one checks that Ψ_ε satisfies again assumptions of the lemma $\square$

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In this way the theorem is proved. However, the limiting operator corresponds to *Kirchhoff b.c. only*

Once more heuristics à la R-S

Trying to get other b.c., consider again the formula

$$\lambda \int_{V_\varepsilon} \phi\,\overline{u}\,\mathrm{d}V_\varepsilon = \int_{V_\varepsilon} \langle \mathrm{d}\phi, \mathrm{d}u \rangle\,\mathrm{d}V_\varepsilon + \int_{\partial V_\varepsilon} \partial_{\mathrm{n}}\phi\,\overline{u}\,\mathrm{d}\partial V_\varepsilon$$

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If the vertex volume decays slower than $\mathrm{vol}_{d-1}\partial V_\varepsilon$, the integrals over V_ε dominate. Normalized ef's are nearly vanishing on V_ε on the scale on $U_{\varepsilon,j}$; this suggests *Dirichlet decoupling* plus extra zero modes at vertices

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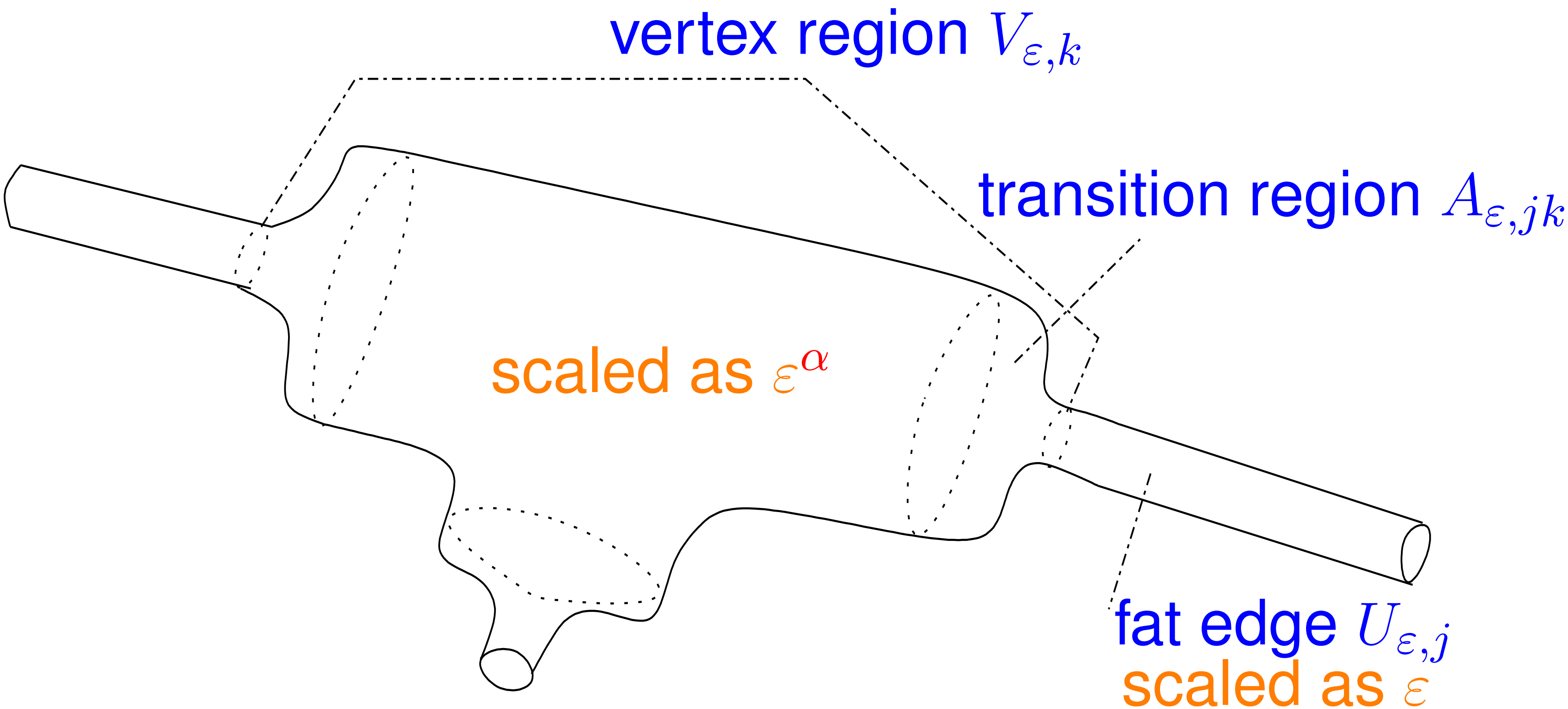
In the borderline case, $\mathrm{vol}_d V_\varepsilon \approx \mathrm{vol}_{d-1}\partial V_\varepsilon$, the ef's should again vary slowly making the integral of $\langle \mathrm{d}\phi, \mathrm{d}u \rangle$ negligible and giving

$$\lambda_0 \phi_0(v_k) = \sum_{j\in J_k} \phi'_{0,j}(v_k)$$

Hence, try a more general scaling

Furthermore, one can try to do the same using *different scaling* of the *edge* and *vertex* regions. Some technical assumptions needed, e.g., the bottlenecks must be “simple”



Two-speed scaling limit

Let vertices scale as ε^{α}. In a similar way (just more complicated) we find that

- if $\alpha \in (1-d^{-1}, 1]$ the result is as above: the ev's at the spectrum bottom converge the graph Laplacian with *Kirchhoff b.c.*, i.e. continuity and

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$$\sum_{\text{edges meeting at } v_k} u_j'(v_k) = 0\,;$$

- if $\alpha \in (0, 1-d^{-1})$ the "limiting" Hilbert space is $L^2(M_0) \oplus \mathbb{C}^K$, where K is $\#$ of vertices, and the "limiting" operator acts as *Dirichlet Laplacian* at each edge and as zero on $\mathbb{C}^K$

Two-speed scaling limit

- if $\alpha = 1 - d^{-1}$, Hilbert space is the same but the limiting operator is given by quadratic form $q_0(u) := \sum_j \|u'_j\|^2_{I_j}$, the domain of which consists of $u = \{\{u_j\}_{j \in J}, \{u_k\}_{k \in K}\}$ such that $u \in H^1(M_0) \oplus \mathbb{C}^K$ and the *edge and vertex parts are coupled* by $(\mathrm{vol}\,(V_k^-)^{1/2} u_j(v_k) = u_k$

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- finally, if vertex regions do not scale at all, $\alpha = 0$, the manifold components decouple in the limit again,

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- Hence such a straightforward limiting procedure *does not help* us to justify choice of appropriate s-a extension

A remedy: one has to add either *manifold geometry* or *external potentials*

Potential approximation

Let us look what we can achieve with potential families *on the graph alone*

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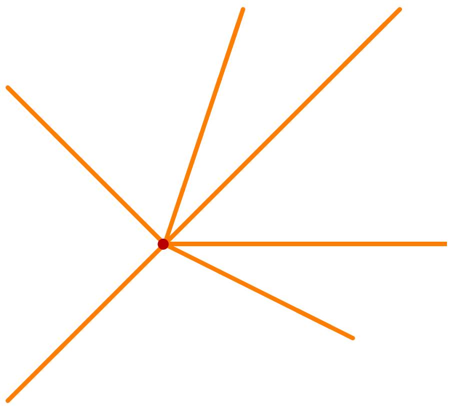

Consider again a *star graph* with $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and Schrödinger operator acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j'' + V_j\psi_j$

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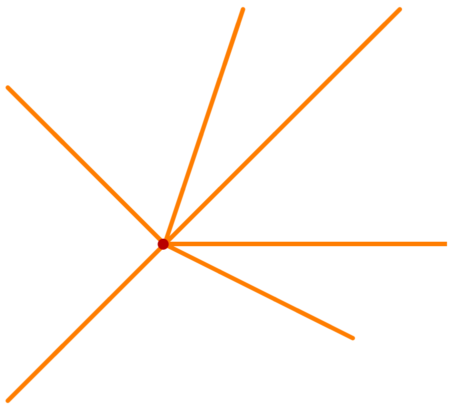

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We make the following assumptions:

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

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

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

Remarks

- Also Birman-Schwinger analysis generalizes easily:

  Theorem [E.'96b]: Let $V_j \in L^1(\mathbb{R}_+, (1+|x|)\mathrm{d}x)$, $j = 1, \dots, n$. Then $H_0(\lambda V)$ has for all small enough $\lambda > 0$ a single negative ev $\epsilon(\lambda) = -\kappa(\lambda)^2$ *iff*

$$\int_0^\infty V_j(x)\,\mathrm{d}x \le 0$$

In that case, its asymptotic behavior is given by

$$\begin{aligned}\kappa(\lambda) &= -\frac{\lambda}{n}\sum_{j=1}^{n}\int_0^\infty V_j(x)\,\mathrm{d}x - \frac{\lambda^2}{2n}\Bigg\{\sum_{j=1}^{n}\int_0^\infty\int_0^\infty V_j(x)|x-y|V_j(y)\,\mathrm{d}x\,\mathrm{d}y \\ &+ \sum_{j,\ell=1}^{n}\left(\frac{2}{n}-\delta_{j\ell}\right)\int_0^\infty\int_0^\infty V_j(x)(x+y)V_\ell(y)\,\mathrm{d}x\,\mathrm{d}y\Bigg\} + \mathcal{O}(\lambda^3)\end{aligned}$$

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$$\left. + \sum_{j,\ell=1}^{n} \left(\frac{2}{n} - \delta_{j\ell} \right) \int_0^\infty \int_0^\infty V_j(x)(x+y)V_\ell(y)\,\mathrm{d}x\,\mathrm{d}y \right\} + \mathcal{O}(\lambda^3)$$

- A Seto-Klaus-Newton bound on $\#\sigma_{\mathrm{disc}}(H_0(\lambda V))$ can be obtained in a similar way

CS-type approximation

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Inspiration: Recall that δ' on the line can be approximated by δ's scaled in a *nonlinear* way [Cheon-Shigehara'98]

Moreover, the convergence is *norm resolvent* and gives rise to approximations by *regular potentials* [Albeverio-Nizhnik'00], [E.-Neidhardt-Zagrebnov'01]

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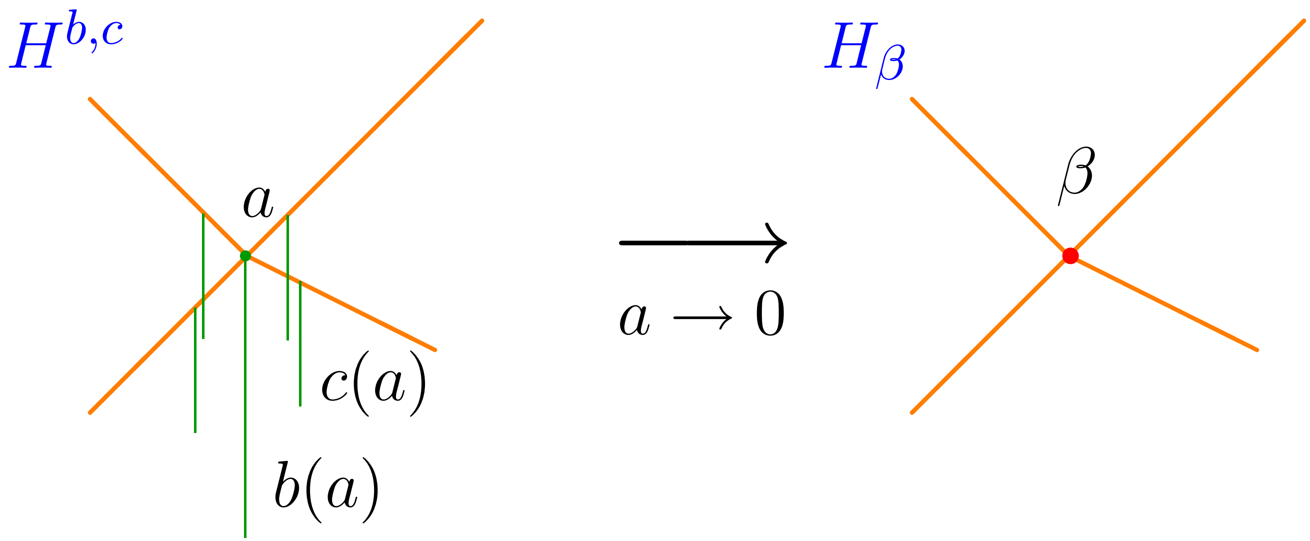
This suggests the following scheme:



Permutation symmetry

The problem simplifies due to symmetry. Each of the Hamiltonians H_β and $H^{b,c}(a)$ decomposes into a nontrivial part which acts on the *one-dimensional subspace* of $\mathcal{H} = \bigoplus_{j=1}^n L^2(\mathbb{R}_+)$ consisting of functions symmetric with respect to permutations, $\psi_j(x) = \psi_k(x)$ for all j, k, and the $(n-1)$-dimensional part corresponding to *Dirichlet* and *Neumann condition* at the central vertex for the δ and δ'_s coupling, respectively

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Notice that the matrices corresponding to these coupling, $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ and $U = I - \frac{2}{n-i\beta}\mathcal{J}$, have each one simple eigenvalue and another one equal to ∓ 1, respectively, of multiplicity $n-1$

Heuristic argument

In the symmetric sector we can drop the indices. The boundary values at $x = 0$ and $x = a$ are related by

$$\psi(a) = \psi(0) + a\psi'(0) + \mathcal{O}(a^2)\,, \quad \psi'(a-) = \psi'(0+) + \mathcal{O}(a)\,,$$
$$\psi'(a+) = \psi'(a-) + c\psi(a)\,, \quad \psi'(0+) = b\psi(0)$$

Eliminating $\psi(0)$ and $\psi'(0+)$ from here, we get in the leading order the relation $B(a)\psi(a) = \psi'(a+)$, where

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Hence $\beta\psi'(0+) = n\psi(0)$, is achieved as $a \to 0+$ if we choose

$$b(a) := -\frac{\beta}{na^2}\,, \qquad c(a) := -\frac{1}{a}$$

Heuristic argument

In the orthogonal complement we again drop the index, because the operators act in the same way on all the linear combinations of $\sum_{j=1}^{n} d_j\psi_j(x)$ with $\sum_{j=1}^{n} d_j = 0$. The b.c. at origin is now replaced by $\psi(0) = 0$

Heuristic argument

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Eliminating then the boundary values at $x = 0$ we get in the leading order the relation $\psi'(a+) = (c + a^{-1})\psi(a) + \mathcal{O}(a)$. The right-hand side vanishes if we choose again

$$b(a) := -\frac{\beta}{na^2}\,, \quad c(a) := -\frac{1}{a}$$

giving Neumann condition, $\psi'(0+) = 0$, in the limit

δ'_s approximation

Theorem [Cheon-E.'04]: $H^{b,c}(a) \to H_\beta$ as $a \to 0+$ in the norm-resolvent sense provided b, c are chosen as

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Proof: By symmetry the task is reduces to a pair of halfline problems. Consider first the one with Dirichlet condition at the origin, so the free Green's function at energy k^2 is $G_k(x,y) = \frac{\sin kx_<}{k}\, \mathrm{e}^{ikx_>}$ for $x, y \geq 0$

The Green's function of the operator with the δ interaction at $x = a$ is obtained easily by Krein's formula

$$G_k^c(x,y) = G_k(x,y) + \frac{G_k(x,a)G_k(a,y)}{-c^{-1} - G_k(a,a)}$$

Proof

The Neumann Green's function is $G_k^N(x,y) = \frac{\cos kx_<}{k}\, \mathrm{e}^{ikx_>}$; the two have to converge to each other for some $k^2 \in \mathbb{C}$.

Choose $k = i\kappa$ with $\kappa > 0$, then the denominator is nonzero for a small enough. It is sufficient to compute the difference in the case when neither of the arguments is smaller than a; for definiteness suppose that $a \le x \le y$; then

$$G_{i\kappa}^c(x,y) - G_{i\kappa}^N(x,y) = \frac{\mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y}}{\kappa} \left[-1 + \frac{\sinh^2 \kappa a}{-\kappa c^{-1} - \mathrm{e}^{-\kappa x} \sinh^2 \kappa a} \right]$$

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If $c = -a^{-1}$ the last term is $1 + \mathcal{O}(a)$ for $a \to 0+$, so

$$\lim_{a\to 0+} G_{i\kappa}^c(x,y) = G_{i\kappa}^N(x,y)$$

holds for all $x, y > 0$

Proof

Consider next δ coupling at the origin using the same values of parameters, $k = i\kappa$ and $a \leq x \leq y$. We need the following two Green's functions,

$$G^b_{i\kappa}(x,y) = \frac{\mathrm{e}^{-\kappa y}}{\kappa(b+\kappa)} \left(b \sinh \kappa x + \kappa \cosh \kappa x\right),$$

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The first of them determines the full approximating Green's function by Krein's formula,

$$G^{b,c}_k(x,y) = G^b_k(x,y) + \frac{G^b_k(x,a)G^b_k(a,y)}{-c^{-1} - G^b_k(a,a)}$$

Proof

$$G^{b,c}_{i\kappa}(x,y) - G^{\beta}_{i\kappa}(x,y) = \frac{\mathrm{e}^{-\kappa y}}{\kappa}\left[\frac{b\sinh\kappa x + \kappa\cosh\kappa x}{b+\kappa}\right.$$

$$\left. + \frac{\frac{\mathrm{e}^{-\kappa x}}{(b+\kappa)^2}(b\sinh\kappa x + \kappa\cosh\kappa x)^2}{\kappa a - \frac{\mathrm{e}^{-\kappa a}}{b+\kappa}(b\sinh\kappa x + \kappa\cosh\kappa x)} - \frac{n\sinh\kappa x + \beta\kappa\cosh\kappa x}{n+\beta\kappa}\right]$$

Proof

$$G^{b,c}_{i\kappa}(x,y) - G^{\beta}_{i\kappa}(x,y) = \frac{e^{-\kappa y}}{\kappa}\left[\frac{b\sinh\kappa x+\kappa\cosh\kappa x}{b+\kappa}\right.$$

$$\left. + \frac{\frac{e^{-\kappa x}}{(b+\kappa)^2}(b\sinh\kappa x+\kappa\cosh\kappa x)^2}{\kappa a - \frac{e^{-\kappa a}}{b+\kappa}(b\sinh\kappa x+\kappa\cosh\kappa x)} - \frac{n\sinh\kappa x+\beta\kappa\cosh\kappa x}{n+\beta\kappa}\right]$$

The first term tends to $\sinh\kappa x$ as $a\to 0+$, while the third one is independent of a, so their sum in the limit gives $-\frac{\beta\kappa\, e^{-\kappa x}}{n+\beta\kappa}$. Next we take the middle term without the factor $e^{-\kappa x}$ and expand the numerator and denominator to the second power in a; this together gives

$$\lim_{a\to 0+} G^{b,c}_{i\kappa}(x,y) = G^{\beta}_{i\kappa}(x,y)\,, \quad x,y>0$$

Finally, the pointwise convergence implies convergence of the resolvents in the HS-norm $\square$

δ' approximation

In a similar way one can approximate the δ' coupling Hamiltonian $\tilde{H}_\beta$ on the star graph

Let the approximating operator $\tilde{H}^{b,c}$ be as above with the central δ replaced by δ_p with coupling strength $b(a)$

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Theorem [Cheon-E.'04]: $\tilde{H}^{b,c}(a) \to \tilde{H}_\beta$ as $a \to 0+$ in the norm-resolvent sense provided b, c are chosen as

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- Analogous problems on *generalized graphs* with "edges" of different dimensions, etc.

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[CE04] T. Cheon, P.E.: An approximation to δ' couplings on graphs, *J. Phys. A: Math. Gen.*, to appear; `quant-ph/0404136`

[E95] P.E.: Lattice Kronig–Penney models, *Phys. Rev. Lett.***75** (1995), 3503-3506

[E96a] P.E.: Contact interactions on graph superlattices, *J. Phys.* **A29** (1996), 87-102

[EG96] P.E., R. Gawlista: Band spectra of rectangular graph superlattices, *Phys. Rev.* **B53** (1996), 7275-7286

[E96b] P.E.: Weakly coupled states on branching graphs, *Lett. Math. Phys.* **38** (1996), 313-320

[ENZ01] P.E., H. Neidhardt, V.A. Zagrebnov: Potential approximations to δ': an inverse Klauder phenomenon with norm-resolvent convergence, *Commun. Math. Phys.* **224** (2001), 593-612

[EP03] P.E., O. Post: Convergence of spectra of graph-like thin manifolds, `math-ph/0312028`

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