Quantum waveguides: mathematical problems

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Talk overview

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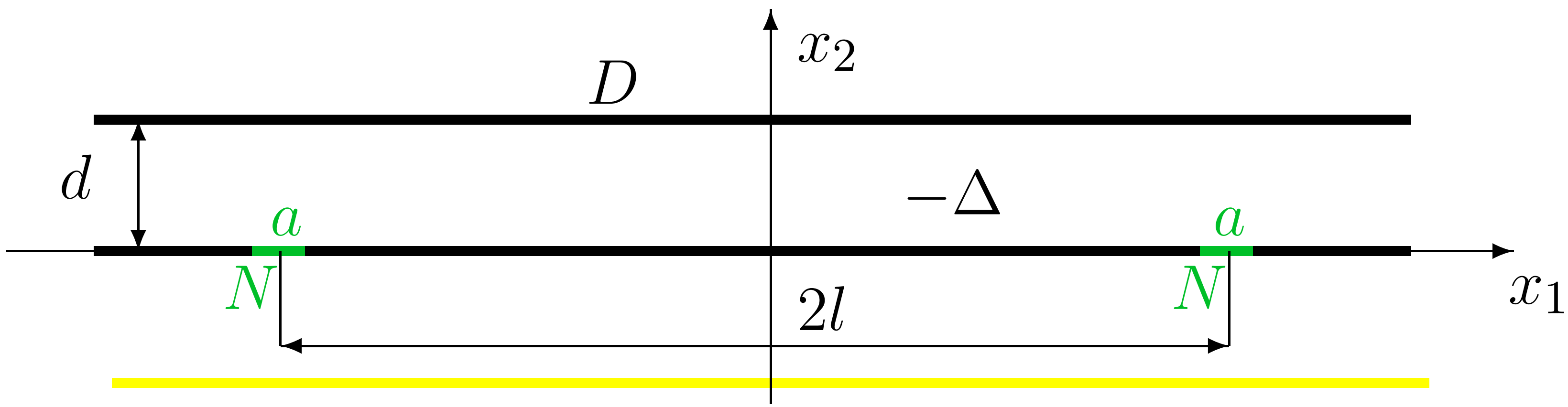
- *Exponential splitting for distant perturbations* physically "obvious", mathematically not at all
- *Squeezing limit of thin graph-like manifolds* where the difficult part still lays ahead
- *An isoperimetric problem for point interactions* or there are still open questions in Euclidean geometry, believe or not

The first problem: distant perturbations

Consider example of a hard-wall (Dirichlet) waveguide with *two Neumann "windows"*:



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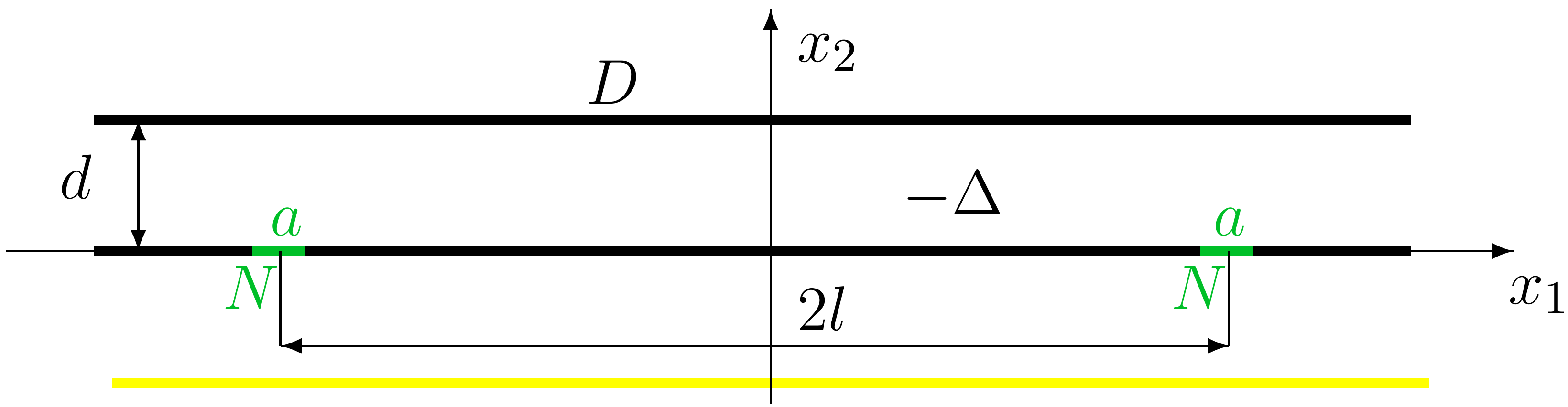

Naturally this can be regarded as a double waveguide with two windows in the common boundary (its nontrivial part)

We call the strip Π, its right and left half $\Pi^{\pm}$, respectively. The Dirichlet part of the boundary is denoted $\Gamma_l(a)$, the Neumann one $\gamma_l(a)$. The Laplacian with the appropriate b.c. is a s-a operator denoted $H_\ell(a)$ which is the main object of our interest

Preliminaries: a single window

Recall a few facts – cf. [E.-Šeba-Tater-Vaněk'96] – about the spectrum of a waveguide with *a single* Neumann window of width a. Call this Hamiltonian $H(a)$. Without loss of generality we may suppose $d = \pi$

- $\sigma_{\mathrm{ess}}(H(a) = [1, \infty)$ and $\sigma_{\mathrm{disc}}(H(a)) \neq \emptyset$ for any $a > 0$

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- There are critical values $0 = a_0 < a_1 < a_2 < \ldots$ for which the system has threshold-resonance solutions ψ^n
- In the limit $x_1 \to \infty$ we have

$$
\begin{aligned}
\psi^n(x) &= \sqrt{\frac{2}{\pi}}\,\sin(x_2) + \beta_n\,\mathrm{e}^{-\sqrt{3}\,x_1}\sin(2x_2) + \mathcal{O}\left(\mathrm{e}^{-\sqrt{8}\,x_1}\right), \\
\psi_j(x) &= \alpha_j(a)\,\mathrm{e}^{-\sqrt{1-\lambda_j(a)}\,x_1}\sin(x_2) + \mathcal{O}\left(\mathrm{e}^{-\sqrt{4-\lambda_j(a)}\,x_1}\right)
\end{aligned}
$$

The non-critical case

Theorem [Borisov-E.'04]: Let $a \in (a_{n-1}, a_n)$ for some $n \in \mathbb{N}$. Then the operator $H_l(a)$ with $d = \pi$ has for any l large enough exactly $2n$ eigenvalues $\lambda_j^{\pm}(l,a)$, $j = 1, \dots, n$, situated in the interval $(\frac{1}{4}, 1)$. Each of them is simple and has the asymptotic expansions

$$\lambda_j^{\pm}(l,a) = \lambda_j(a) \mp \mu_j(a)\, \mathrm{e}^{-2l\sqrt{1-\lambda_j(a)}} + \mathcal{O}\left(\mathrm{e}^{-(4\sqrt{1-\lambda_j(a)}-\sigma)l}\right),$$

as $l \to \infty$ for $j = 1, \dots, n$ with any fixed $\sigma > 0$. The coefficient μ_j is given by

$$\mu_j(a) = \alpha_j(a)^2 \pi \sqrt{1-\lambda_j(a)} = \frac{1}{\pi\sqrt{1-\lambda_j(a)}} \left(\int_{\gamma(a)} \psi_j(x)\, \mathrm{e}^{\sqrt{1-\lambda_j(a)}\, x_1}\, \mathrm{d}x_1 \right)^2,$$

where $\gamma(a)$ denotes the two windows.

The non-critical case, continued

Theorem, continued: The eigenfunctions $\psi_j^{\pm}(x)$ associated with eigenvalues $\lambda_j^{\pm}(l,a)$, $j=1,\dots,n$, are even for $\lambda_j^{+}(l,a)$ and odd for $\lambda_j^{-}(l,a)$. Furthermore, in the halfstrips spaces $W^{2,1}(\Pi^{\pm})$ they can be approximated for $\ell \to \infty$ by

$$\begin{aligned} \psi_j^{+}(x) &= \psi_j(x_1 \mp l, x_2) + \mathcal{O}\left(\mathrm{e}^{-(2\sqrt{1-\lambda_j(a)}-\sigma)l}\right), \\ \psi_j^{-}(x) &= \pm\psi_j(x_1 \mp l, x_2) + \mathcal{O}\left(\mathrm{e}^{-(2\sqrt{1-\lambda_j(a)}-\sigma)l}\right). \end{aligned}$$

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Remark: The case of a general strip width d is obtained easily by scaling, cf. [Borisov-E.'04]; the same applies to the critical case below.

The critical case

Theorem [Borisov-E.'04]: Let $a = a_n$ for some $n \in \mathbb{N}$. Then the operator $H_l(a)$ with $d = \pi$ has for $2n+1$ ev's in $(\frac{1}{4}, 1)$ for l large enough. The first $2n$ of them together with the associated eigenfunctions behave as above, while the last one, $\lambda^+_{n+1}(l, a_n)$, has the asymptotics

$$\lambda^+_{n+1}(l, a_n) = 1 - \mu\, \mathrm{e}^{-4\sqrt{3}\, l} + \mathcal{O}\left(\mathrm{e}^{-2(\sqrt{8}+\sqrt{3})\, l}\right),$$

where

$$\mu = 3\beta_n^4 \pi^2 = \frac{16}{3\pi^2} \left(\int_{\gamma(a_n)} \psi^n(x)\, \mathrm{e}^{\sqrt{3}\, x_1}\, \mathrm{d}x_1 \right)^4 .$$

The critical case, continued

Theorem, continued: The associated eigenfunction ψ_{n+1}^{+} is even w.r.t. x_1 and for any fixed R it can be approximated in the rectangles $\{x : |x_1 \mp l| < R\} \cap \Pi$ for large values of l as

$$\psi_{n+1}^{+}(x) = \psi^{n}(x_1 \mp l, x_2) + \mathcal{O}\left(\mathrm{e}^{-2\sqrt{3}\,l}\right)$$

in the $W^{2,1}$-norm. Moreover, it behaves asymptotically for $x_1 \to \pm\infty$ as

$$\begin{aligned} \psi_{n+1}^{+}(x) &= \sqrt{\frac{2}{\pi}}\,\mathrm{e}^{-\varkappa|x_1|}\sin(x_2) + \mathcal{O}\left(\mathrm{e}^{-\sqrt{3}|x_1|}\right), \\ \varkappa &:= \sqrt{1-\lambda_{n+1}} = \sqrt{\mu}\,\mathrm{e}^{-2\sqrt{3}l} + \mathcal{O}\left(\mathrm{e}^{-2\sqrt{8}l}\right). \end{aligned}$$

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- Next one has to analyze the resolvent of $H_l(a)$, i.e. to solve the equation $-(\Delta + \lambda)u = f$ with the appropriate b.c. for both the *unperturbed* (one-window) and *perturbed* (two-windows) problem; it is sufficient to do that, say, for a compactly supported $f \in L^2(\Pi)$

Scheme of the proof, continued

- In the *unperturbed case* we first solve (v) pure Dirichlet problem in the halfstrip, then we inspect how the solution changes (w) in a fixed rectangle Π_b when the b.c. change to Neumann in the window. Interpolating between v and w we rewrite the problem equivalently as $(I + T_\infty(\lambda))g = f$, where $T_\infty(\lambda)$ is a Fredholm operator on $L^2(\Pi_b)$ expressed in terms of v, w

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- the *threshold-resonance situation* is treated similarly, just the estimates are more complicated $\Box$

Lessons from this example

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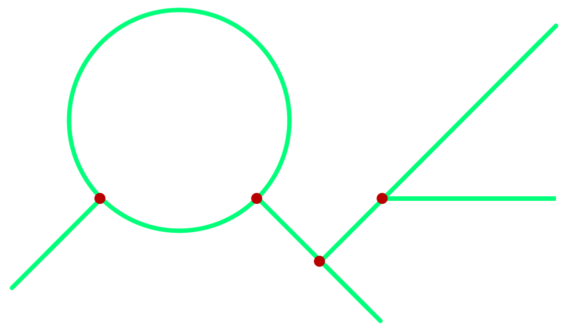
- the result is rather complete including *coefficient values* due to explicit construction which yield the singularities
- similar construction is likely to work for *other QWG* with distant perturbations such as *bends, bulges,* etc.
- At the same time the explicit construction is not simple and has to be done separately in each particular case. *Thus the following question arises:*

  Can one formulate a general result using a quantity which would replace the standard *Agmon metric* in the present situation?

The second problem: quantum graphs

Theoretically, *QM on (metric) graphs* is a natural concept:



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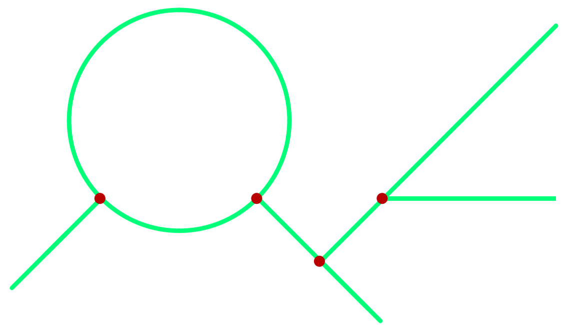

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It appears that it does. First used by Ruedenberg and Scherr in 1953 as a model of aromatic hydrocarbons, the idea became really important 10-15 years ago with the progress of techniques allowing fabrication of *quantum graphs* of semiconductor quantum wires

Recently *carbon nanotubes* became a building material, after branchings were fabricated, and also *microwave network* of optical cables were studied – see [Hul et al.'04]

Remarks on quantum graphs

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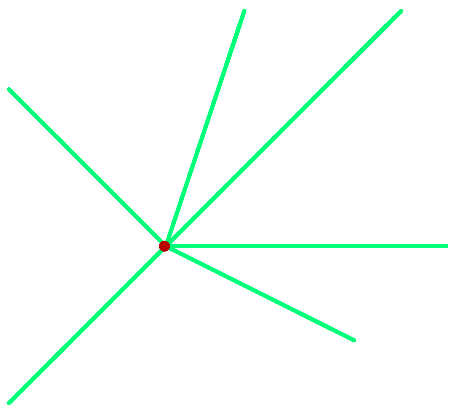
- Graphs can support also *Dirac operators*, see [Bulla-Trenckler'90], although this remains so far a theoretical possibility only.
- The graph literature is extensive; let us refer just to a review [Kuchment'04] and other references in the recent topical issue of *"Waves in Random Media"*

Vertex coupling



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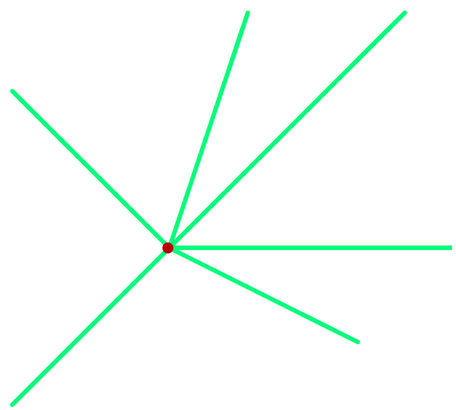

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If we take functions from $\bigoplus_{j=1}^{n} W^{2,2}(\mathbb{R}_+)$ satisfying $\psi_j(0) = \psi_j'(0) = 0,\ \ j = 1, \dots, n$, as the domain, we get a symmetric operator with deficiency indices (n, n). Admissible Hamiltonian has to be chosen among its *s-a extensions* being characterized by n^2 real parameters

Since the operator is second-order, all such extensions are characterized by boundary condition which couple $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$

Vertex coupling parametrization

Universal b.c. were proposed in [Kostrykin-Schrader'99]. They are given by a pair of $n \times n$ matrices A, B such that

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

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Moreover, the obvious non-uniqueness of such a parametrization can be removed:

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

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

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*,

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,, \; j,k = 1,\dots,n\,, \quad \sum_{j=1}^{n} \psi'_j(0) = \alpha\psi(0)$$

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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

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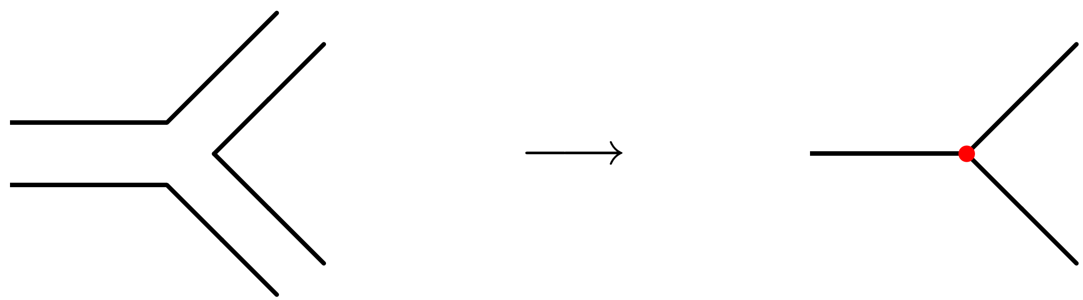
- More recently, the same system has been proposed as a way to realize a *qubit*, with obvious consequences [Tsutsui-Fülöp-Cheon, quant-ph/0404039]
- Recall also that in a rectangular lattice with δ coupling of nonzero α spectrum depends on *number theoretic properties* of model geometric parameters [E.'95,'96a; E.-Gawlista'96]

It seems to be obvious what to do

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



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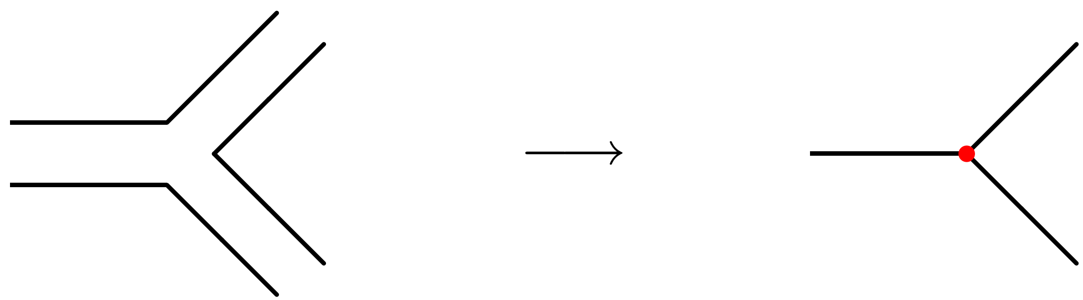

Unfortunately, this is not sufficient because

- 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

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

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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

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

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

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

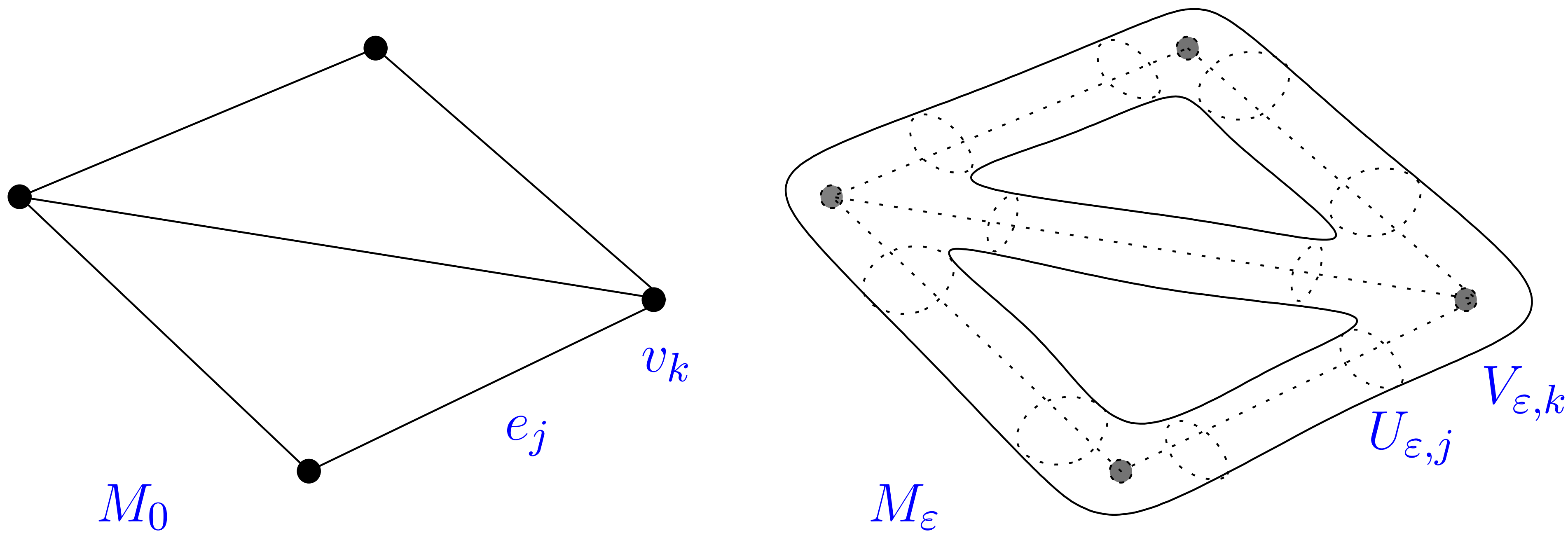
The closure of this form is associated with the s-a operator Δ_X which acts in fixed chart coordinates as

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

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

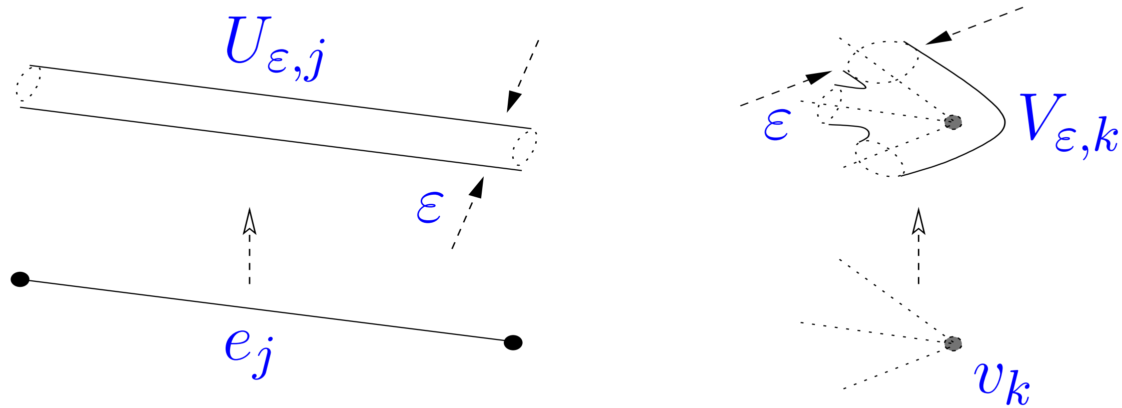
Fat graphs and sleeves: manifolds

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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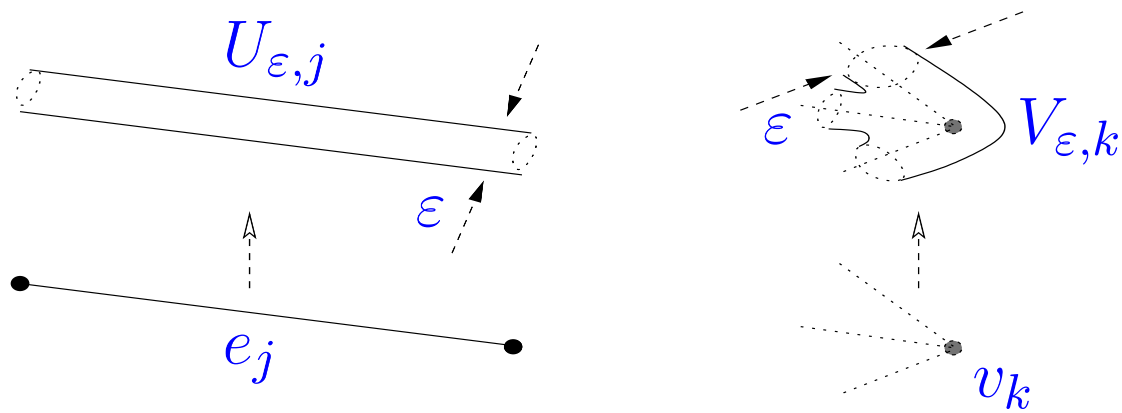

However, M_ε *need not be embedded* in some $\mathbb{R}^d$.

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 $V_{\varepsilon,k} = V_\varepsilon$

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

for all $u \in \mathcal{H}^1(M_\varepsilon)$

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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 $\|u\|^2_{Q,n} := \|u\|^2 + \|Q^{n/2}u\|^2$.

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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

This property allows us to treat manifolds embedded in $\mathbb{R}^d$ (with metric $\tilde{g}_\varepsilon$) using product metric g_ε on the edges

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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'04]: 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 $\square$

A lower bound

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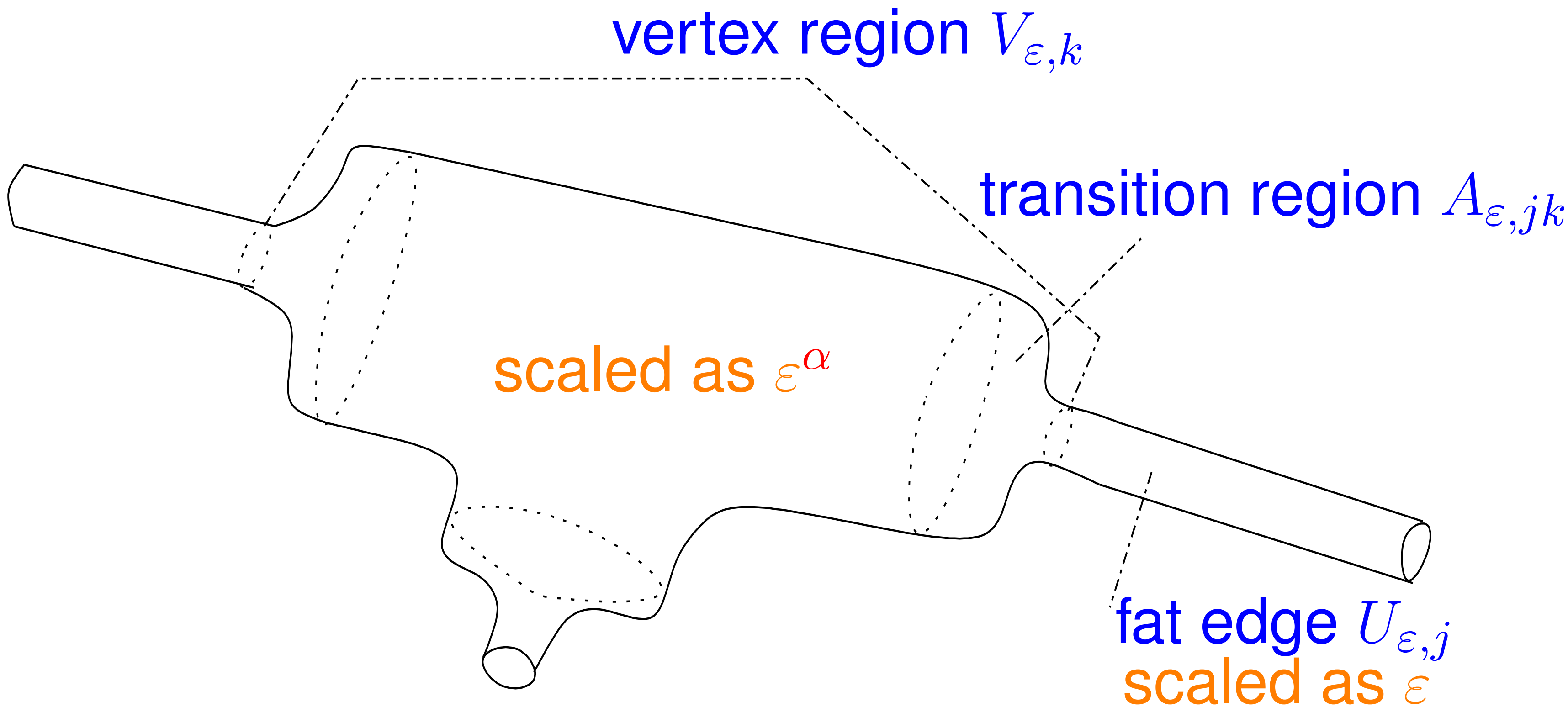
In the borderline case, $\mathrm{vol}_d V_\varepsilon \approx \mathrm{vol}_{d-1}\partial V_\varepsilon$, the ef's should again vary slowly making the integral of $\langle \mathrm{d}\phi, \mathrm{d}u \rangle$ negligible and giving

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

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

  It seems that to get a nontrivial coupling one has to add either *manifold geometry* or *external potentials*

The third topic: isoperimetric problems

This a traditional topic indeed. Recall, e.g., the *Faber-Krahn inequality* for the Dirichlet Laplacian $-\Delta_D^M$ in a compact M: among all regions with a fixed area the ground state is uniquely minimized by the circle,

$$\inf \sigma(-\Delta_D^M) \geq \pi\, j_{0,1}^2\, |M|^{-1}$$

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However, topology is crucial. In various problems with non-simply connected M the ground state is *maximized* by a rotationally symmetric shape:

- a strip of fixed length and width [E.-Harrell-Loss'99]
- a circular obstacle in circular cavity [Harrell-Kröger-Kurata'01]

Point interaction "loops"

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Let us discuss the simplest possible example where the confinement is due to a *closed array of δ potentials*, so the Hamiltonian can be written formally as

$$-\Delta + \tilde{\alpha} \sum_{j+1}^{N} \delta(x - y_j) \quad \text{in } \ L^2(\mathbb{R}^d), \ d = 2, 3\,,$$

where the y_j's are vertices of an *equilateral polygon* $\mathcal{P}_N$

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- where the y_j's are vertices of an *equilateral polygon* $\mathcal{P}_N$
- We ask about extremal properties of a *regular* polygon $\tilde{\mathcal{P}}_N$ of the edge length ℓ, which means planar (trivial if $d=2$) with vertices lying on a circle of radius $\ell\left(2\sin\frac{\pi}{N}\right)^{-1}$

2D point interactions

Fixing the site y and "coupling constant" α we define them by b.c. which change *locally* the domain of $-\Delta$: we require

$$\psi(x) = -\frac{1}{2\pi}\log|x-y|\,L_0(\psi,y) + L_1(\psi,y) + \mathcal{O}(|x-y|)\,,$$

where the generalized b.v. $L_0(\psi,y)$ and $L_1(\psi,y)$ satisfy

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In this way we define our Hamiltonian $-\Delta_{\alpha,\mathcal{P}_N}$ in $L^2(\mathbb{R}^d)$ with N point interactions. We suppose $\sigma_{\mathrm{disc}}\left(-\Delta_{\alpha,\mathcal{P}_N}\right)\neq\emptyset$, i.e.

$$\epsilon_1 \equiv \epsilon_1(\alpha,\mathcal{P}_N) := \inf\sigma\left(-\Delta_{\alpha,\mathcal{P}_N}\right) < 0\,,$$

which is satisfied for any $\alpha\in$ if $d=2$, while in the case $d=3$ it is true below a certain critical value of α – cf. [AGHH'88]

The result

Theorem [E.'04]: Under the stated conditions, $\epsilon_1(\alpha, \mathcal{P}_N)$ is for fixed α and ℓ *locally sharply maximized* by a regular polygon, $\mathcal{P}_N = \tilde{\mathcal{P}}_N$.

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Proof will be reduced to the following geometric problem:

Let $\mathcal{P}_N$ be an equilateral polygon in $\mathbb{R}^d$, $d \geq 2$. Given a fixed integer $m = 2, \dots, [\frac{1}{2}N]$ we denote by $\mathcal{D}_m$ the *sum of lengths of all m-diagonals*, i.e. those jumping over m vertices.

(P_m) The quantity $\mathcal{D}_m$ is, in the set of equilateral polygons $\mathcal{P}_N \subset \mathbb{R}^d$ with a fixed edge length $\ell > 0$, *uniquely maximized* by $\tilde{\mathcal{D}}_m$ referring to the (family of) regular polygon(s) $\tilde{\mathcal{P}}_N$.

Do not believe to find it in Euclidean geometry textbooks :-(

Geometric reformulation

By Krein formula, the spectral condition is reduced to an algebraic problem. Using $k = i\kappa$ with $\kappa > 0$, we find the ev's $-\kappa^2$ from

$$\det \Gamma_k = 0 \qquad \text{with} \qquad (\Gamma_k)_{ij} := (\alpha - \xi^k)\delta_{ij} - (1 - \delta_{ij})g_{ij}^k \,,$$

where $g_{ij}^k := G_k(y_i - y_j)$, or equivalently

$$g_{ij}^k = \begin{cases} \frac{1}{2\pi} K_0(\kappa|y_i - y_j|) & \dots \quad d = 2 \\ \frac{e^{-\kappa|y_i - y_j|}}{4\pi|y_i - y_j|} & \dots \quad d = 3 \end{cases}$$

and the regularized Green's f. at the interaction site is

$$\xi^k = \begin{cases} -\frac{1}{2\pi}\left(\ln\frac{\kappa}{2} + \gamma_{\mathrm{E}}\right) & \dots \quad d = 2 \\ -\frac{\kappa}{4\pi} & \dots \quad d = 3 \end{cases}$$

Geometric reformulation, continued

The ground state refers to point where the lowest ev of $\Gamma_{i\kappa}$ vanishes. Using smoothness and monotonicity of the κ-dependence we have to check that

$$\min \sigma(\Gamma_{i\tilde{\kappa}_1}) < \min \sigma(\tilde{\Gamma}_{i\tilde{\kappa}_1})$$

holds locally for $\mathcal{P}_N \neq \tilde{\mathcal{P}}_N$, where $-\tilde{\kappa}_1^2 := \epsilon_1(\alpha, \tilde{\mathcal{P}}_N)$

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There is a *one-to-one relation* between an ef $c = (c_1, \dots, c_N)$ of $\Gamma_{i\kappa}$ at that pointand the corresponding ef of $-\Delta_{\alpha,\mathcal{P}_N}$ given by $c \leftrightarrow \sum_{j=1}^N c_j G_{i\kappa}(\cdot - y_j)$, up to normalization. In particular, the lowest ev of $\tilde{\Gamma}_{i\tilde{\kappa}_1}$ corresponds to the eigenvector $\tilde{\phi}_1 = N^{-1/2}(1, \dots, 1)$. Hence

$$\min \sigma(\tilde{\Gamma}_{i\tilde{\kappa}_1}) = (\tilde{\phi}_1, \tilde{\Gamma}_{i\tilde{\kappa}_1} \tilde{\phi}_1) = \alpha - \xi^{i\tilde{\kappa}_1} - \frac{2}{N} \sum_{i<j} \tilde{g}_{ij}^{i\tilde{\kappa}_1}$$

Geometric reformulation, continued

On the other hand, we have $\min \sigma(\Gamma_{i\tilde{\kappa}_1}) \le (\tilde{\phi}_1, \Gamma_{i\tilde{\kappa}_1}\tilde{\phi}_1)$, and therefore it is sufficient to check that

$$\sum_{i<j} G_{i\kappa}(y_i - y_j) > \sum_{i<j} G_{i\kappa}(\tilde{y}_i - \tilde{y}_j)$$

holds for *all* $\kappa > 0$ and $\mathcal{P}_N \ne \tilde{\mathcal{P}}_N$.

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holds for *all* $\kappa > 0$ and $\mathcal{P}_N \neq \tilde{\mathcal{P}}_N$. Call $\ell_{ij} := |y_i - y_j|$ and $\tilde\ell_{ij} := |\tilde y_i - \tilde y_j|$ and define $F:\ (\mathbb{R}_+)^{N(N-3)/2} \to \mathbb{R}$ by

$$F(\{\ell_{ij}\}) := \sum_{m=2}^{[N/2]} \sum_{|i-j|=m} \left[G_{i\kappa}(\ell_{ij}) - G_{i\kappa}(\tilde\ell_{ij})\right]\,;$$

Using *convexity* of $G_{i\kappa}(\cdot)$ for a fixed $\kappa > 0$ we get

$$F(\{\ell_{ij}\}) \ge \sum_{m=2}^{[N/2]} \nu_m \left[G_{i\kappa}\left(\frac{1}{\nu_m}\sum_{|i-j|=m} \ell_{ij}\right) - G_{i\kappa}(\tilde\ell_{1,1+m})\right]\,,$$

where ν_n is the number of the appropriate diagonals

Geometric reformulation, continued

Since $G_{i\kappa}(\cdot)$ is monotonously decreasing in $(0,\infty)$, we need

$$\tilde{\ell}_{1,m+1} \geq \frac{1}{\nu_n} \sum_{|i-j|=m} \ell_{ij}$$

with the sharp inequality for at least one m if $\mathcal{P}_N \neq \tilde{\mathcal{P}}_N$.
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The claim is then implied by the following result:

Proposition: The property (P_m) holds *locally* for any $m = 2, \dots, [\frac{1}{2}N]$

Proof

We are looking for constrained local maxima of the function

$$f_m : \ f_m(y_1, \ldots, y_N) = \frac{1}{N} \sum_{i=1}^{N} |y_i - y_{i+m}|$$

with $g_i(y_1, \ldots, y_n) := \ell - |y_i - y_{i+1}| = 0, \ i = 1, \ldots, N$. There are in fact $(N-2)(d-1)-1$ independent variables because $2d-1$ parameters are related to Euclidean transformations

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We are looking for constrained local maxima of the function

$$f_m : \ f_m(y_1, \ldots, y_N) = \frac{1}{N} \sum_{i=1}^{N} |y_i - y_{i+m}|$$

with $g_i(y_1, \ldots, y_n) := \ell - |y_i - y_{i+1}| = 0$, $i = 1, \ldots, N$. There are in fact $(N-2)(d-1) - 1$ independent variables because $2d - 1$ parameters are related to Euclidean transformations

It is straightforward to check that $\nabla_j K_m(y_1, \ldots, y_N)$ vanish for a regular polygon, $K_m := f_m + \sum_{r=1}^{N} \lambda_r g_r$, with the Lagrange multipliers taking the value

$$\lambda = \frac{\sigma_m}{N \Upsilon_m} \quad \text{with} \quad \sigma_m := \frac{\sin^2 \frac{\pi m}{N}}{\sin^2 \frac{\pi}{N}}, \ \Upsilon_m := \ell^{-1} |\tilde{y}_j - \tilde{y}_{j \pm m}|$$

Proof, continued

Negative definiteness of the Hessian needs more computation. A simple estimate then shows that it is sufficient to establish negative definiteness of the form

$$\xi \mapsto S_m[\xi] := \sum_j \left\{ |\xi_j - \xi_{j+m}|^2 - \sigma_m |\xi_j - \xi_{j+1}|^2 \right\}$$

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The two parts can be simultaneously diagonalized; using their ev's one rewrites the condition as the inequality

$$U_{m-1}\left(\cos\frac{\pi}{N}\right) > \left| U_{m-1}\left(\cos\frac{\pi r}{N}\right) \right|, \; r = 2, \dots, m-1\,,$$

for Chebyshev polynomials of the second kind which can be checked directly □

Is the maximum global?

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Proof: Call β_i the "bending angle" at i-th vertex, then the mean length of the 2-diagonals is $M_2 = \frac{2\ell}{N}\sum_{i=1}^{N} \cos\frac{\beta_i}{2}$. Using *strict convexity* of the function $u \mapsto -\cos\frac{u}{2}$ in $(-\pi, \pi)$ together with $\sum_{i=1}^{N} \beta_i = 2\pi w,\ w \in \mathbb{Z}$, we find

$$-\sum_{i=1}^{N} \cos\frac{\beta_i}{2} \geq -N\cos\left(\sum_{i=1}^{N}\frac{\beta_i}{2}\right) = -N\cos\frac{\pi}{N}\ ;$$

the inequality is sharp unless all the β_i's are the same $\square$

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- *Analogues* of the isoperimetric problem: non-symmetric mass distribution, continuous, higher-dimensional, etc.

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[EP04] P.E., O. Post: Convergence of spectra of graph-like thin manifolds, *J. Geom. Phys.*, to appear; `math-ph/0312028`

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for more information see *http://www.ujf.cas.cz/~exner*