Approximations *for* and *by* quantum graph Hamiltonians

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Talk overview

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- Vertex coupling parametrization, a reminder: what it is and why it is interesting

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- Emergence of global structures in large graphs

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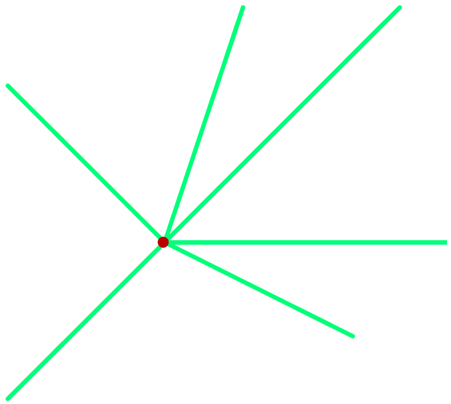
- *etc., etc.* Let us thus go straight *in medias res*

Vertex coupling



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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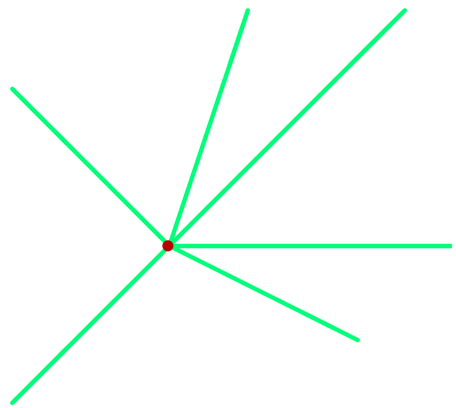

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Since it is second-order, the boundary condition involve $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$ being of the form

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

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

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

HFT boundary conditions

The non-uniqueness of K-S b.c. can be removed:

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

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

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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

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

The choice $\ell = 1$ just fixes 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

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

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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- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the δ_s' *coupling*

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

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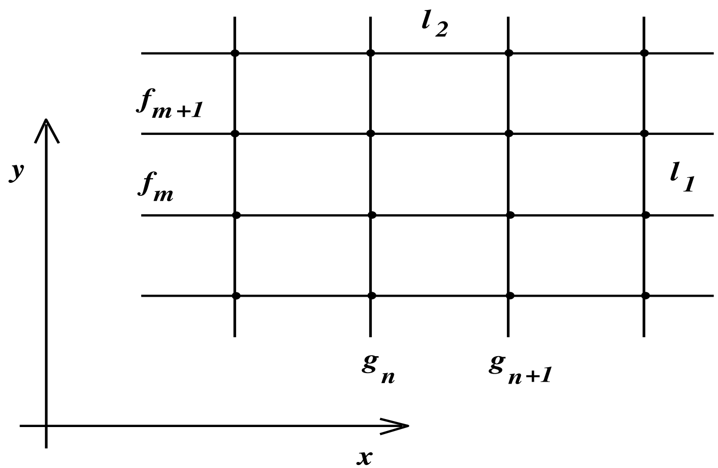
- Recall also that in a rectangular lattice with δ coupling of nonzero α spectrum depends on *number theoretic properties* of model parameters [E.'95]

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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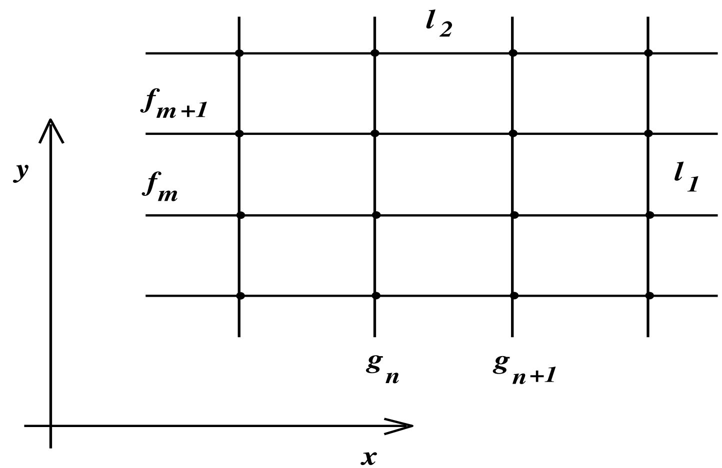

Spectral condition for quasimomentum (θ_1, θ_2) reads

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

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 $|\alpha| < \alpha_0$

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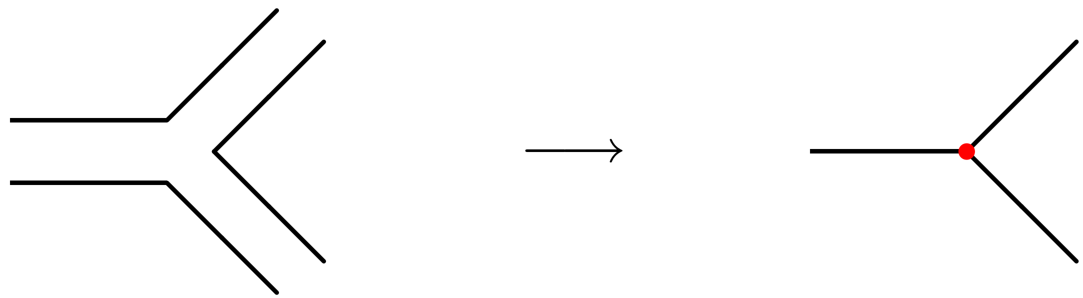
This all illustrates why we seek a meaningful way *to "construct" different vertex couplings*. It will be our next task

A head-on approach

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



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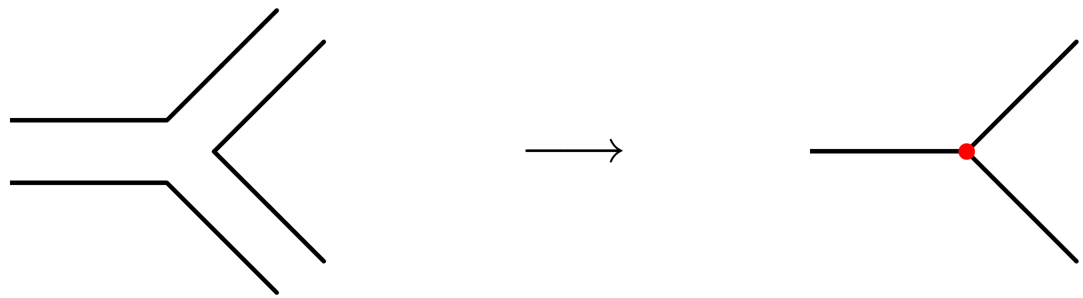

Unfortunately, it is not so simple as it looks because

- after a long effort the Neumann-like case was solved [Kuchment-Zeng'01], [Rubinstein-Schatzmann'01], [Saito'01], [E.-Post'05] leading to free b.c. only
- the important *Dirichlet case* is open (and difficult), apart of the (not so intriguing) case leading to full decoupling of graph edges [Post'05], [Grieser'05]?

Recall the Neumann-like case

The simplest situation in [KZ'01, EP'05] (weights left out)

Let M_0 be a finite connected graph with vertices v_k, $k \in K$ and edges $e_j \simeq I_j := [0, \ell_j]$, $j \in J$; the state Hilbert space is

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

and in a similar way Sobolev spaces on M_0 are introduced

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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 $-\Delta_{M_0} u = -u''_j$ and satisfies free b.c.,

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

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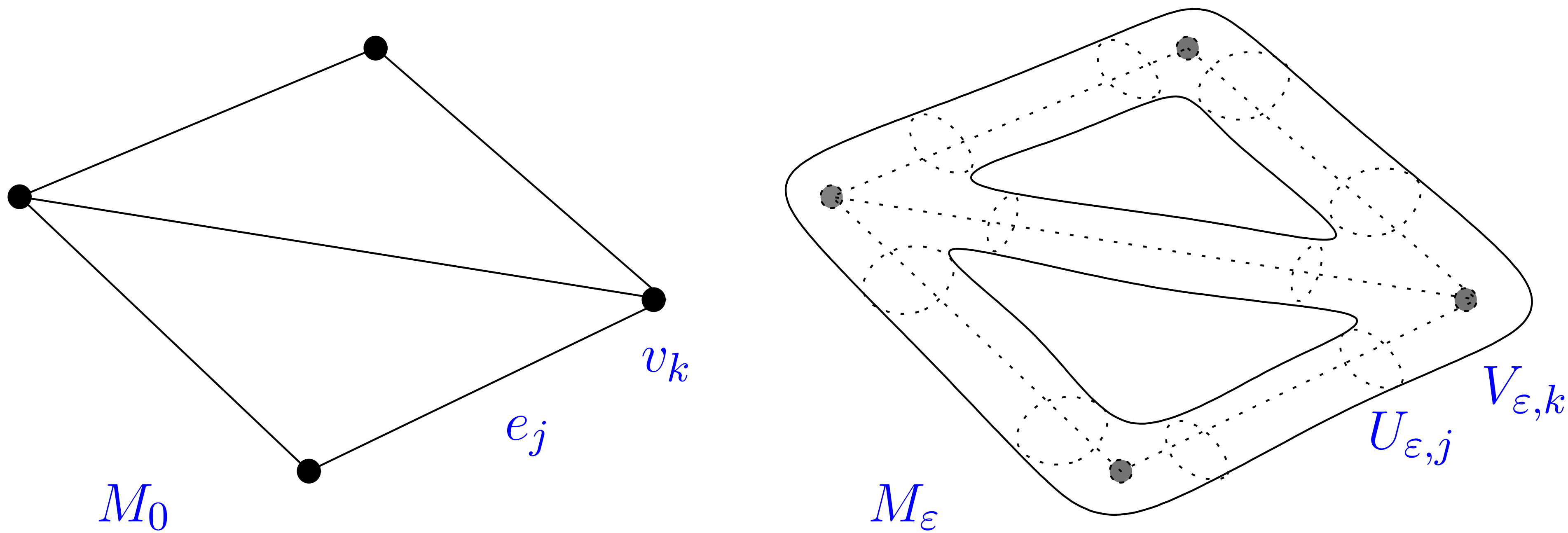
If X is compact with piecewise smooth boundary, one starts from the form defined on $C^\infty(X)$. This yields $-\Delta_X$ as the *Neumann* Laplacian on X and allows us in this way to treat “fat graphs” and “sleeves” on the same footing

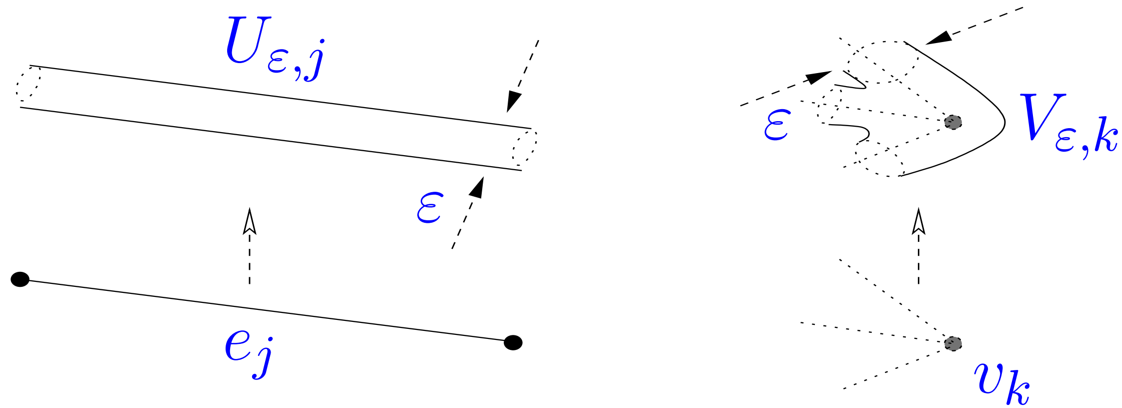
Fat graphs and sleeves: manifolds

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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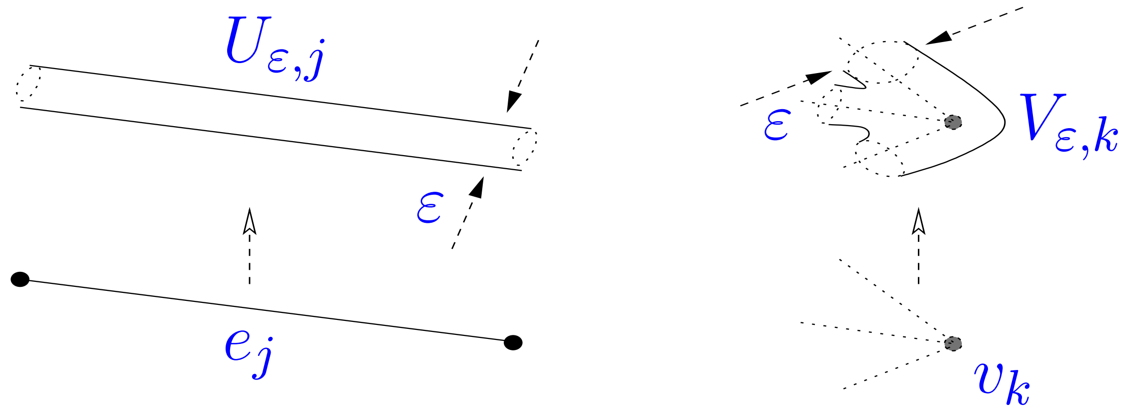

However, M_ε *need not be embedded* in some $\mathbb{R}^d$.

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

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 an $\eta_k(\lambda_k, \delta_1, \delta_2) > 0$ which tends to zero as $\delta_1, \delta_2 \to 0$, such that

$$\lambda_k \geq \lambda_k' - \eta_k$$

Eigenvalue convergence

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

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

the two metrics coincide up to an $\mathcal{O}(\varepsilon)$ 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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The sought result now looks as follows.

Theorem [E.-Post'05]: Under the stated assumptions $\lambda_k(M_\varepsilon) \to \lambda_k(M_0)$ as $\varepsilon \to 0$ (giving thus free b.c.!)

Sketch of the proof

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

To prove it apply the lemma to $\Phi_\varepsilon : \ L^2(M_0) \to L^2(M_\varepsilon)$,

$$\Phi_\varepsilon u(z) := \begin{cases} \varepsilon^{-m/2} u(v_k) & \text{if } z \in V_k \\ \varepsilon^{-m/2} u_j(x) & \text{if } z = (x,y) \in U_j \end{cases} \qquad \text{for } u \in \mathcal{H}^1(M_0)$$

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Proof again by the lemma. Here one uses *averaging*:

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

to build the comparison map by *interpolation*:

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

with a smooth ρ interpolating between zero and one

More general b.c.? Recall RS argument

[Ruedenberg-Scher'53] used the heuristic argument:

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

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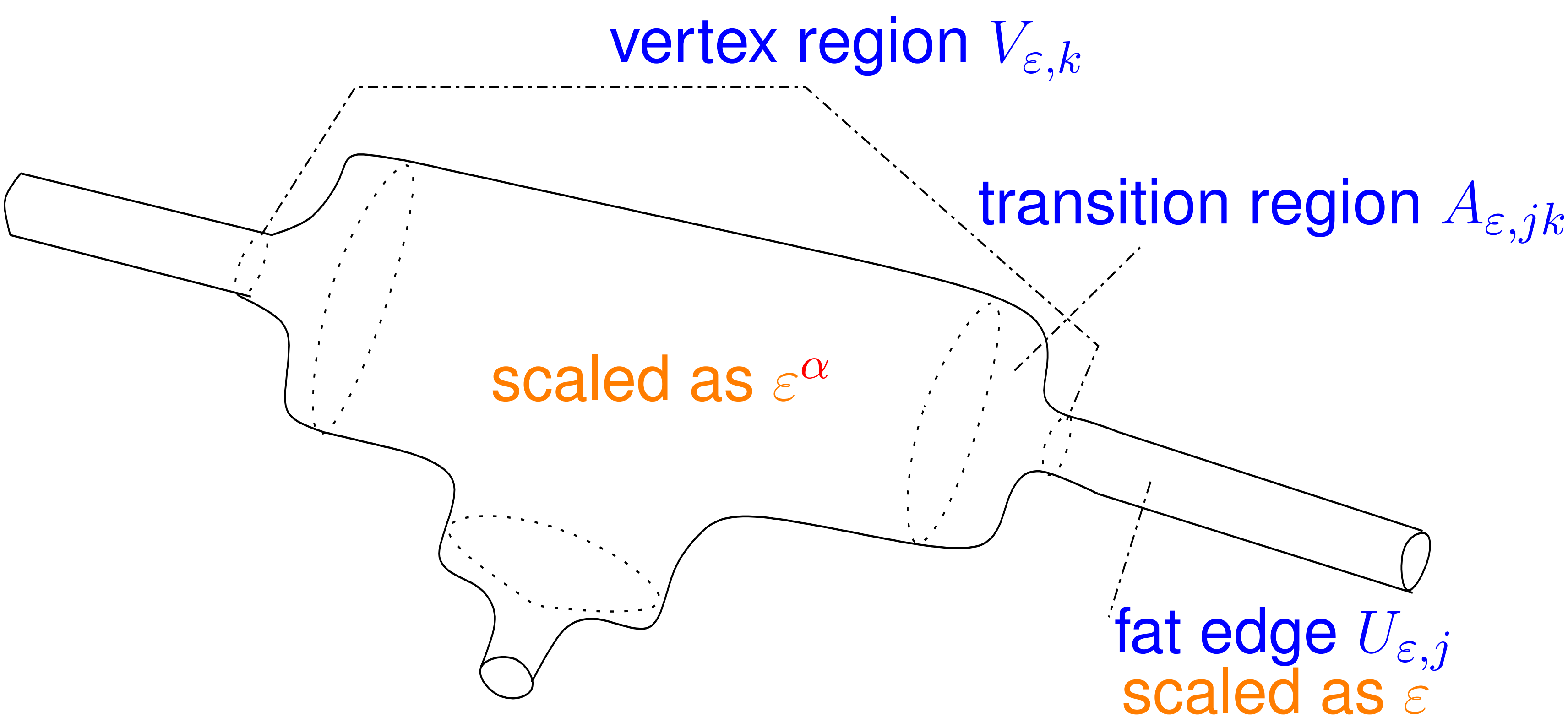
A way out could thus be to use *different* scaling rates of edges and vertices. Of a particular interest is the borderline case, $\mathrm{vol}_d V_\varepsilon \approx \mathrm{vol}_{d-1} \partial V_\varepsilon$, when the integral of $\langle \mathrm{d}\phi, \mathrm{d}u \rangle$ is expected to be negligible and we hope to obtain

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

Scaling with a power α

Let us try to do the same properly 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}. Using the comparison lemma again (just more in a more complicated way) 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 *free b.c.*, i.e. continuity and

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- 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 $\mathbb{C}^K$

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- 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,

$$\bigoplus_{j\in J} \Delta^{\mathrm{D}}_{I_j} \oplus \bigoplus_{k\in K} \Delta_{V_{0,k}}$$

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$$\bigoplus_{j\in J} \Delta^{\mathrm{D}}_{I_j} \oplus \bigoplus_{k\in K} \Delta_{V_{0,k}}$$

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

  Hence the scaling trick does not work: one has to add either *manifold geometry* or *external potentials*

Potential approximation

A more modest goal: let us look what we can achieve with potential families *on the graph alone*

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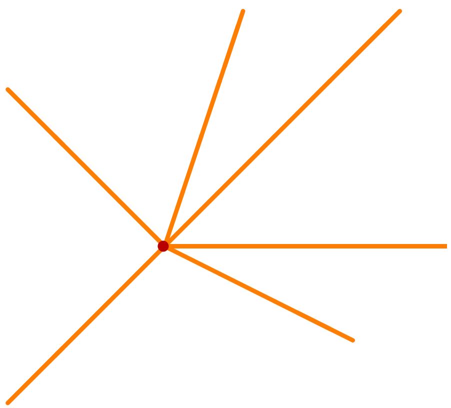

Consider once more *star graph* with $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and Schrödinger operator acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j'' + V_j\psi_j$

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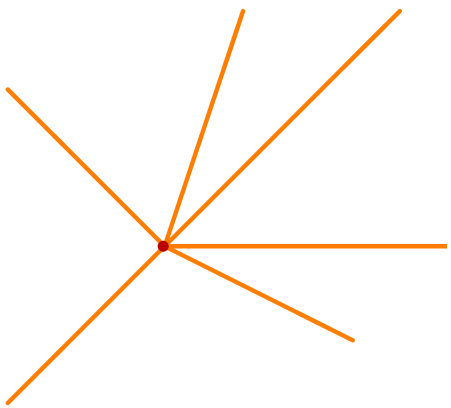

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We make the following assumptions:

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

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

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

More singular couplings

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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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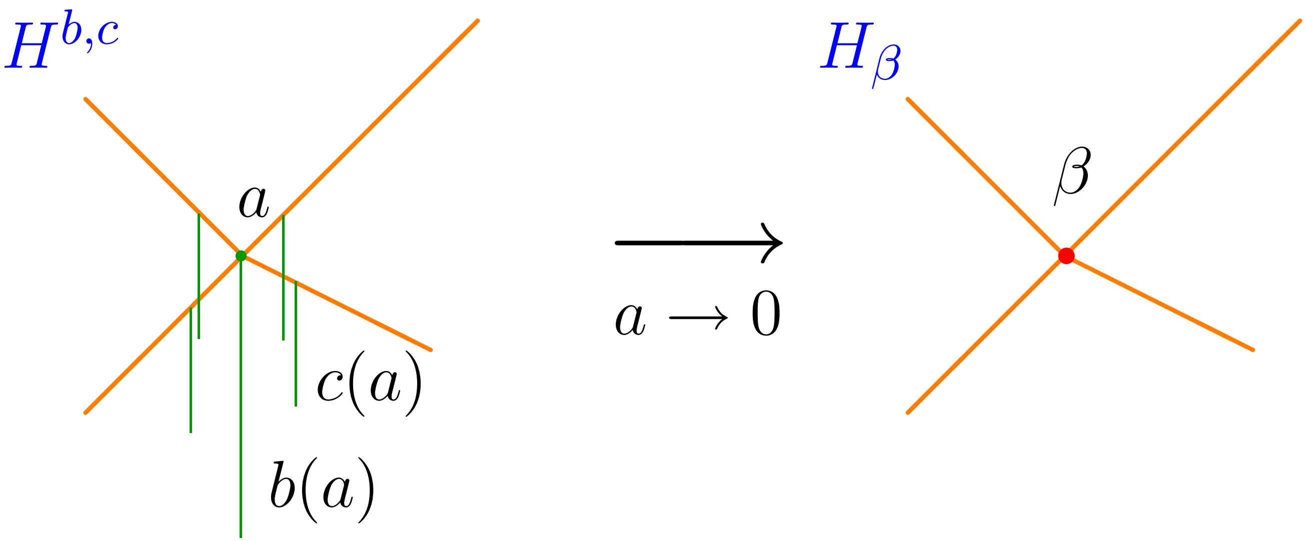
This suggests the following scheme:



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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Remark: Similar approximation can be worked out also for the other couplings mentioned above – cf. [E.-Turek'05]. For the permutation symmetric ones, e.g., one has

$$b(a) := \frac{in}{a^2}\left(\frac{u-1+nv}{u+1+nv} + \frac{u-1}{u+1}\right)^{-1}, \quad c(a) := -\frac{1}{a} - i\frac{u-1}{u+1}$$

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Let us now address the opposite question. Suppose we study a *large* quantum graph asking ourselves whether

- *global structures* may emerge
- graph families can approximate a “continuous” *system described by a suitable PDE*
- such structures are similar to *something really existing in the nature*

A preliminary: some needed notions

- $\mathcal{V} = \{\mathcal{X}_j : j \in I\}$ and $\mathcal{L} = \{\mathcal{L}_{jn} : (j,n) \in I_{\mathcal{L}} \subset I \times I\}$; we may suppose one *edge* between a pair of *vertices*

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- on $\mathcal{L}_{nj} \equiv [0, \ell_{jn}]$ (the right end identified with $\mathcal{X}_j$) we introduce solutions to $-f'' + U_{jn} f = k^2 f$ satisfying $u_{jn}(\ell_{jn}) = 1 - (u_{jn})'(\ell_{jn}) = 0$ and $v_{jn}(0) = 1 - (v_{jn})'(0) = 0$ (Dirichlet b.c. at $\mathcal{B}$); one has $W_{jn} = -v_{jn}(\ell_{jn}) = u_{jn}(0)$

A preliminary: graph duality

Let H_α^D be obtained Dirichlet decoupling of H_α and denote $\mathcal{K} := \{k :\ k^2 \in \sigma(H_\alpha^D)\}$. Moreover, assume that

(i) there is $C > 0$ s.t. $\|U_{jn}\|_\infty \le C$ for all $(j,n) \in I_\mathcal{L}$

(ii) $\ell_0 := \inf\{\,\ell_{jn} :\ (j,n) \in I_\mathcal{L}\} > 0$

(iii) $L_0 := \sup\{\,\ell_{jn} :\ (j,n) \in I_\mathcal{L}\} < \infty$

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Theorem [E.'97]: (a) Suppose that *(i)-(iv)* are satisfied and $\psi \in D_{loc}(H_\alpha)$ solves $-f'' + U_{jn}f = k^2 f$ for some $k \notin \mathcal{K}$ with $k^2 \in \mathbb{R}$, $\mathrm{Im}\, k \ge 0$. Then the boundary values satisfy

$$\sum_{n\in\nu(j)\cap I_\mathcal{I}} \frac{\psi_n}{W_{jn}} - \left(\sum_{n\in\nu(j)} \frac{(v_{jn})'(\ell_{jn})}{W_{jn}} - \alpha_j \right) \psi_j = 0$$

Graph duality, continued

Conversely, any solution $\{\psi_j : j \in I_{\mathcal{I}}\}$ to the above system determines a solution of $-f'' + U_{jn}f = k^2 f$ by

$$\psi_{jn}(x) = \frac{\psi_n}{W_{jn}}\, u_{jn}(x) - \frac{\psi_j}{W_{jn}}\, v_{jn}(x) \qquad \text{if} \quad n \in \nu(j) \cap I_{\mathcal{I}}\,,$$

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(b) Under *(i)*, *(ii)*, $\psi \in L^2(\Gamma)$ implies that the solution $\{\psi_j\}$ of the “discrete” system belongs to $\ell^2(I_{\mathcal{I}})$

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Remark: There is a natural relation between the dual system specified above and the *spectral determinant* of Γ

Approximation by lattice graphs

Let us specify the above result to the situation when
(a) all the graph edges have *the same length* $\ell > 0$, and
(b) all the *potentials* U_{jn} *vanish*. Then we have

$$u_{jn}(x) = \frac{1}{k} \sin k(x-\ell)\,, \quad v_{jn}(x) = \frac{1}{k} \sin kx\,,$$

with $W_{jn} = -\frac{1}{k} \sin k\ell$ and the dual system becomes

$$-\sum_{n\in\nu(j)} \frac{\psi_n - \psi_j \cos k\ell}{k^{-1} \sin k\ell} + \alpha_j \psi_j = 0\,, \quad j \in I\,;$$

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Let now local metric on Γ come from *embedding*, the graph being a *subset in* $\mathbb{R}^\nu$. In particular, consider a *cubic lattice graph* $\mathcal{C}^\nu \equiv \mathcal{C}^\nu(\ell) \subset \mathbb{R}^\nu$ whose vertices are lattice points $\{x_j(\ell) = (j_1\ell,\dots,j_\nu\ell):\ j_i\in\mathbb{Z}\}$, as well as subgraphs of $\mathcal{C}^\nu$

Approximation by lattice graphs

Theorem [E.-Hejčík-Šeba'05]: (a) Let $V:\mathbb{R}^\nu \to \mathbb{R}$ be C^1 with ∇V bounded and put $\alpha_j(\ell) := V(x_j)\ell$. Let for any $\ell > 0$ and k with $k^2 \in \mathbb{R},\ \mathrm{Im}\, k \ge 0$, the family $\{\psi_j^\ell\}$ solve the dual system, and define a step function $\psi_\ell : \mathbb{R}^\nu \to \mathbb{C}$ by

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(b) The analogous result holds for Schrödinger equation in a region $\Omega \subset \mathbb{R}^\nu$ with Dirichlet b.c. if $\partial\Omega$ is piecewise smooth

Approximation by lattice graphs

Proof: For $f \in C^2$ we use Taylor expansion,

$$\frac{f(x+\ell)-f(x-\ell)-2f(x)\cos k\ell}{\ell k^{-1}\sin k\ell} = \frac{2k}{\ell} f(x)\tan\frac{k\ell}{2} + f''(x)\frac{k\ell}{\sin k\ell} + o(\ell)\,,$$

so the right-hand side tends to $f''(x)+k^2 f(x)$ as $\ell \to 0$. Applying this to ψ w.r.t. *each of the ν variables* we find

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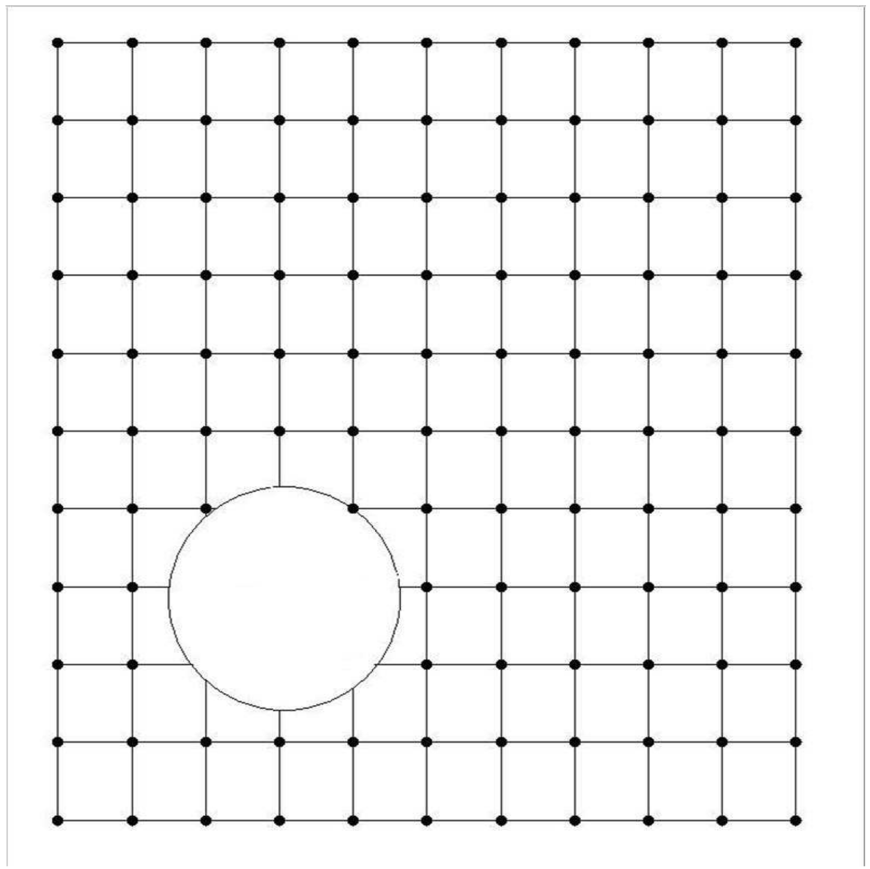
Remarks: (a) We do not discuss here *existence of ψ*
(b) The restriction $k \notin \mathcal{K}$ is satisfied for ℓ is small enough
(c) The limiting energy is νk^2, because all the "local" momentum components are equal (and the particle moves naturally over the graph in a zig-zag way)

Example

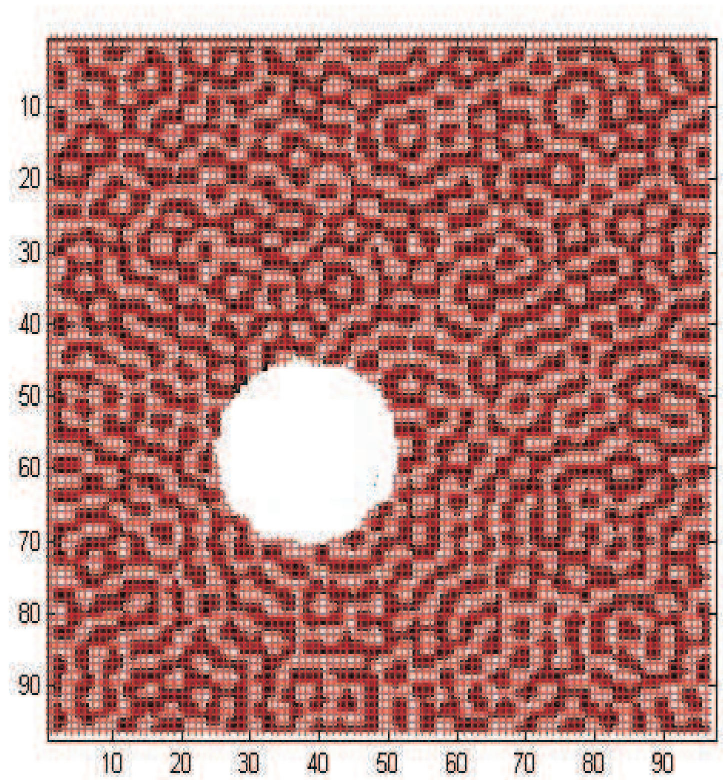
Take a *"Sinai-billiard" graph* made of a $N \times N$ rectangular lattice with *Dirichlet b.c.* at the boundary of Γ



The computation will be made with $N = 97$ and $\alpha = 0$, $U = 0$

Nodal domains

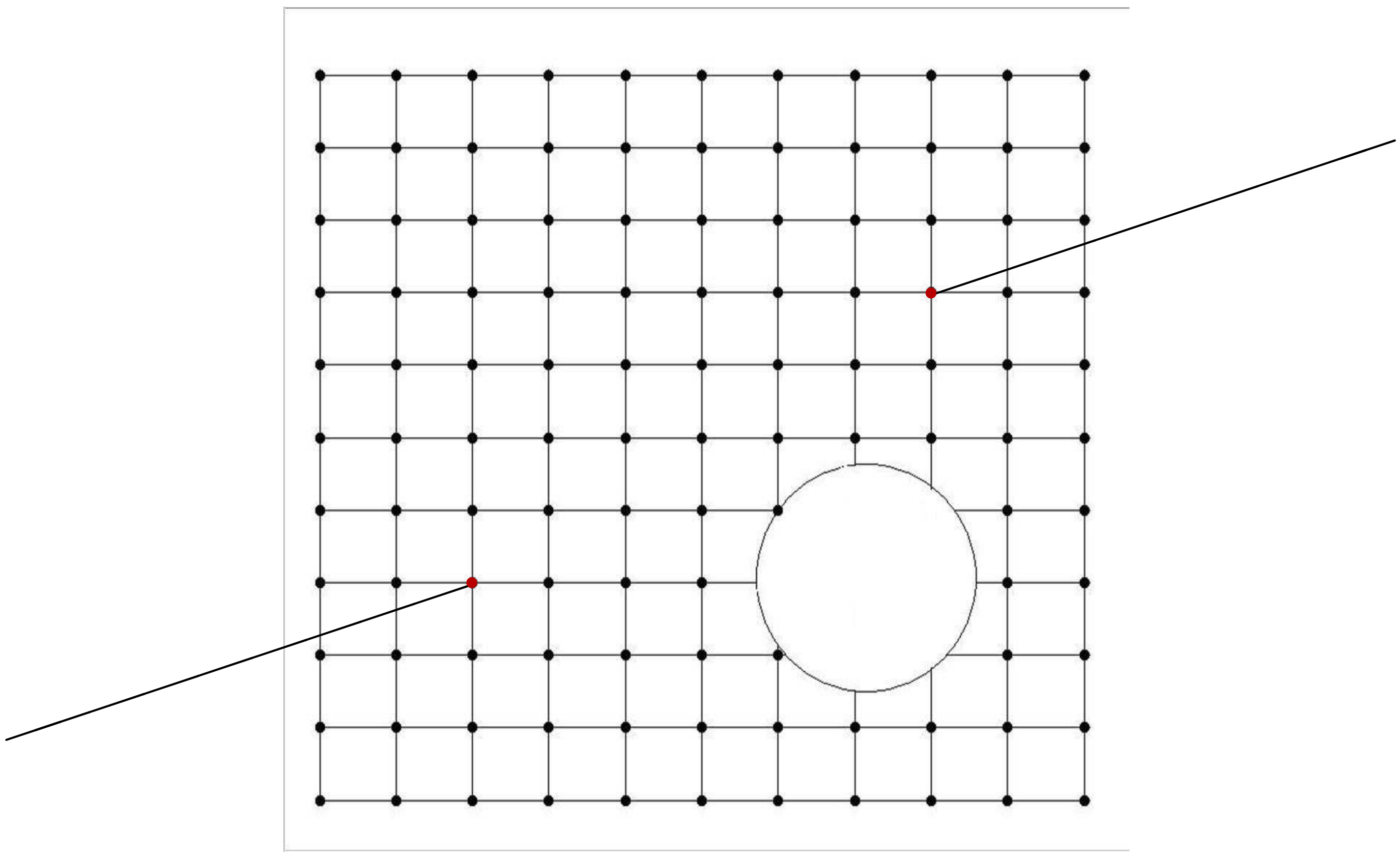
Take first an *eigenfunction* of the graph Hamiltonian corresponding to high enough eigenvalue



The nodal domains *on the graph* look similar to those of the "usual" Sinai billiard

Sinai graph transport

We attach to the above graph *two external leads* at points $(14, 40)$ and $(59, 80)$ of the 97×97 lattice



The b.c. are again supposed to be *free*

Billiards with leads

To have something to compare with, recall how one can describe transport through a billiard Ω with a *pair of leads* attached at internal points of Ω

The billiard Hamiltonian is, of course, the Dirichlet Laplacian $-\Delta_D^\Omega$ on $L^2(\Omega)$ and 1D Laplacians describe the leads

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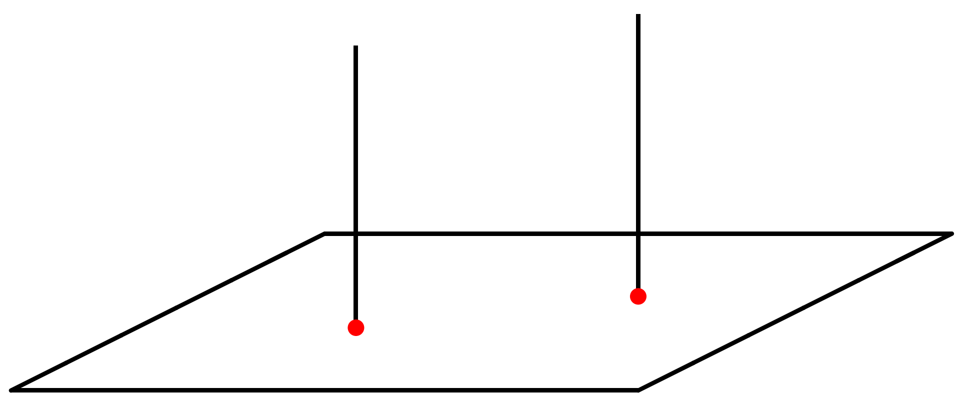
The direct sum $\mathcal{H} = L^2(\mathbb{R}_-) \oplus L^2(\Omega) \oplus L^2(\mathbb{R}_+)$ is naturally associated with the full system, so the wavefunctions are triples $\Phi = (\phi_-, \phi, \phi_+)$ of square integrable functions



Coupling of the leads

It describes by b.c. which involve *generalized boundary values*

$$L_0(\Phi) := \lim_{r\to 0} \frac{\Phi(\vec{x})}{\ln r}\,, \;\; L_1(\Phi) := \lim_{r\to 0} \left[\, \Phi(\vec{x}) - L_0(\Phi)\ln r \,\right]$$

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Typical b.c. determining a s-a extension

$$\begin{aligned} \pm\phi'_{\mp}(0\mp) &= A\phi_{\mp}(0\mp) + BL_0(\phi)\,, \\ L_1(\phi) &= C\phi_{\mp}(0\mp) + DL_0(\phi)\,, \end{aligned}$$

where

$$A,\, D \in \mathbb{R} \quad \text{and} \quad B = 2\pi\bar{C}$$

N.B.: If we use such a coupling between *plane and halfline* one can derive the S-matrix as a function of A, B, C, D

Billiard transport

Let the leads be attached at points $x_1, x_2 \in \Omega$. Construction of generalized eigenfunctions means *to couple plane-wave solution at leads* with

$$\phi(x) = a_1 G(x, x_1; k) + a_2 G(x, x_2; k)\,,$$

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The latter has a logarithmic singularity so $L_j(\phi)$ express in terms of $g := G(x_1, x_2; k)$ and

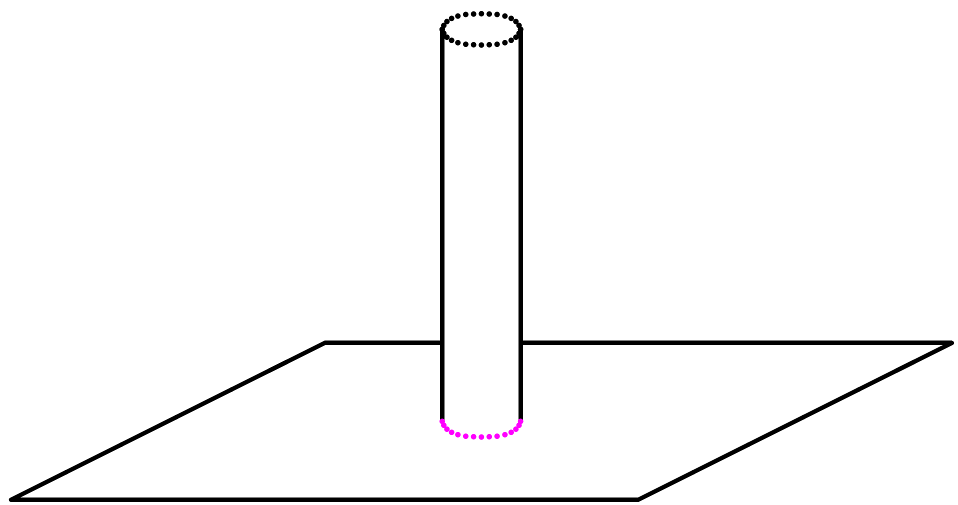
$$\xi_j \equiv \xi(x_j; k) := \lim_{x \to x_j} \left[G(x, x_j; k) + \frac{\ln|x - x_j|}{2\pi} \right]\,;$$

the b.c. then determine *scattering*, i.e. transmission and reflection amplitudes, as well as the *coefficients* a_1, a_2

How to choose coupling parameters

A heuristic way to do that is to *compare low-energy scattering* in the *plane+halfline* model mentioned above

with the situation when the halfline is replaced by tube of radius a (for simplicity we disregard effect of the sharp edge at interface of the two parts)



Plane plus tube scattering

Rotational symmetry allows us to treat each partial wave separately. Given orbital quantum number ℓ one has to match smoothly the corresponding solutions

$$\psi(x) := \begin{cases} e^{ikx} + r_a^{(\ell)}(t)e^{-ikx} & \dots \qquad x \le 0 \\ \sqrt{\frac{\pi kr}{2}}\, t_a^{(\ell)}(k) H_\ell^{(1)}(kr) & \dots \qquad r \ge a \end{cases}$$

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This yields

$$r_a^{(\ell)}(k) = -\frac{\mathcal{D}_-^a}{\mathcal{D}_+^a}, \quad t_a^{(\ell)}(k) = 4i\sqrt{\frac{2ka}{\pi}}\,\left(\mathcal{D}_+^a\right)^{-1}$$

with

$$\mathcal{D}_\pm^a := (1 \pm 2ika) H_\ell^{(1)}(ka) + 2ka \left(H_\ell^{(1)}\right)'(ka)$$

Choice of the parameters

This has to be compared with the plane-and-halfline result. Only the *s-wave* is important: for the halfline there is no scattering if $\ell \neq 0$ while for the tube transmission probability vanishes as $a^{2\ell-1}$ for $a \to 0$

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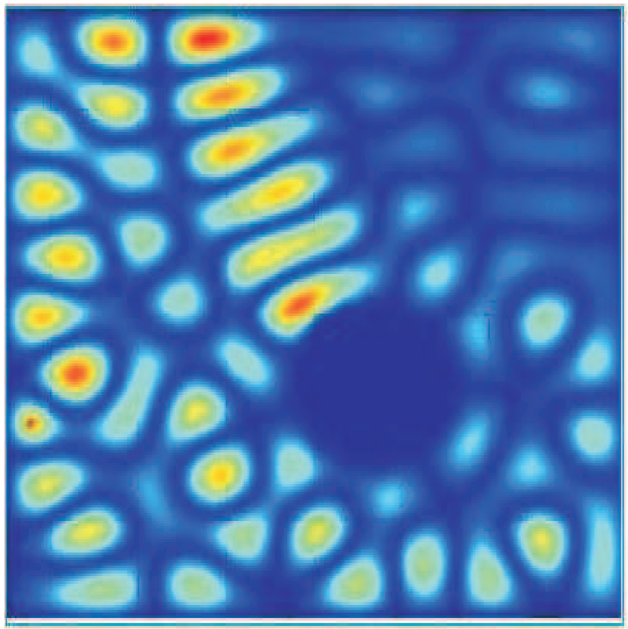
Comparison shows that the two amplitudes coincide, in the leading order as $k \to 0$, with *plane+halfline* expression if

$$A := \frac{1}{2a}\,, \quad D := -\ln a\,, \quad B = 2\pi C = \sqrt{\frac{2\pi}{a}}$$

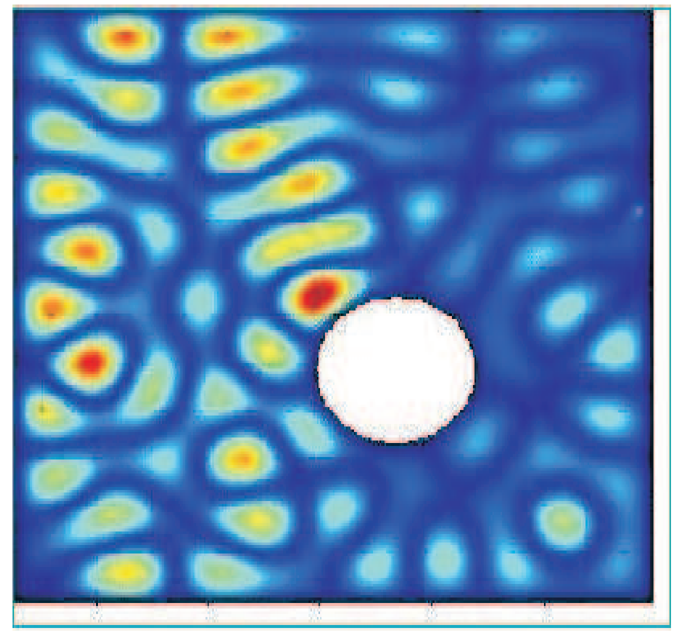
Notice that the "natural" coupling depend on a *single parameter*, namely radius of the "thin" component

In the example below we choose the tube radius a to be *one tenth* of the distance between the lattice graph nodes

Eigenfunctions comparison



graph with energy E



Schrödinger with energy $2E$

Energy E refers to incident momentum $k = \sqrt{E} = 1.65$

Probability currents

Apart of being less numerically demanding, study of transport with complex-valued generalized eigenfunctions allows us to analyze also *phase-related effects* and to compare them to their analogues in “true” billiards

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A primary quantity of interest is the *probability current* which in (an open) billiard is given conventionally by

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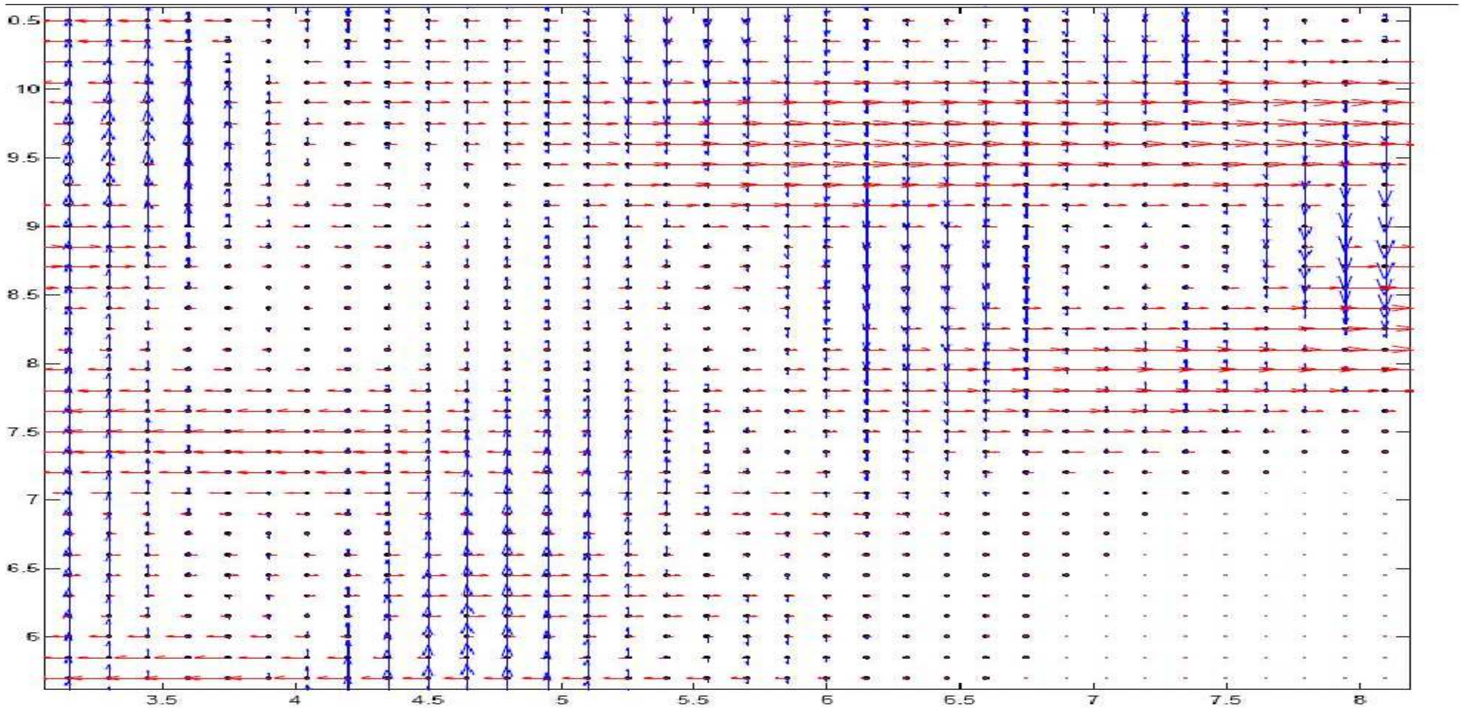
$$\vec{\jmath}(\vec{x}) = \mathrm{Im}\,\left(\bar{\psi}\nabla\psi\right)(\vec{x})$$

What is a quantity to compare on Γ? One possibility is to take *vertex values* as *discretization* of a smooth complex function and to compute the current in analogy with the above formula, by discrete approximation of differentiation

There is also an *alternative way*, more or less equivalent

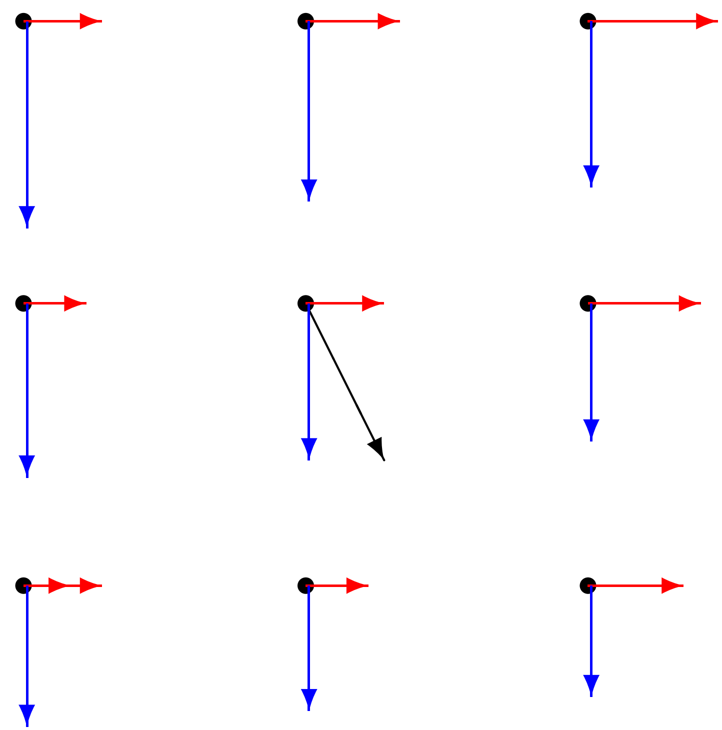
Graph probability flows



“Microscopically”, of course, they follow graph edges

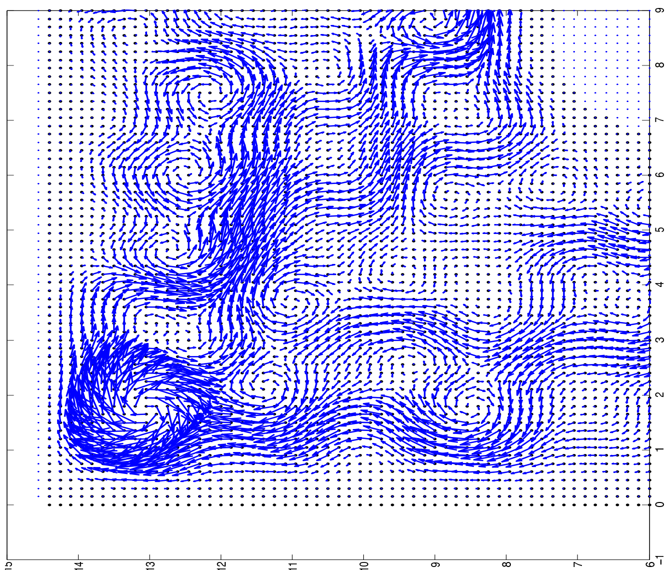
Graph probability flows, continued

Construct now the “overall” flow on the graph as a *vector sum* of the “red” and “blue” components:

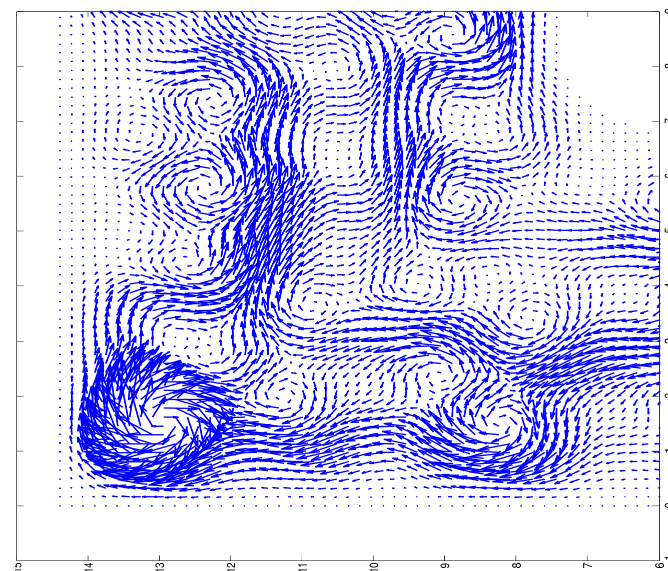


In this way, we find the vector field on Γ, to be compared with that of the billiard with leads

Comparison with Sinai billiard



vector addition, energy E



$\mathrm{Im}\,\left(\bar{\psi}\nabla\psi\right)(\vec{x})$, energy $2E$

For simplicity, we show here just the lower left corner of the two pictures

Summary and outlook

- *Fat graph approximations:* progress in the Neumann-like case, free boundary conditions arise generically. The Dirichlet case is open (and frustrating)

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- *Interesting applications:* the obtained phase portraits of our large graphs are strikingly similar to structures observed in neural networks such a visual cortex

The talk was based on

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

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

[E96] P.E.: Weakly coupled states on branching graphs, *Lett. Math. Phys.* **38** (1996), 313-320

[E97] P.E.: A duality between Schrödinger operators on graphs and certain Jacobi matrices, *Ann. Inst. H. Poincaré: Phys. Théor.* **66** (1997), 359-371

[EHŠ05] P.E., P. Hejčík, P. Šeba: Emergence of global structures in large quantum graphs, *in preparation*

[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

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