Quantum Graphs and Quantum Waveguides with Dirichlet boundary conditions

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joint work with
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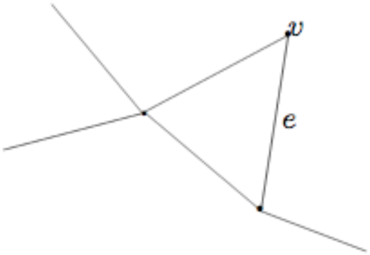
Introduction

A quantum graph is realized by a graph (i.e. a set of points, the vertices, connected by segments, the edges), together with a one dimensional, self-adjoint, differential (or pseudo-differential) operator on the graph



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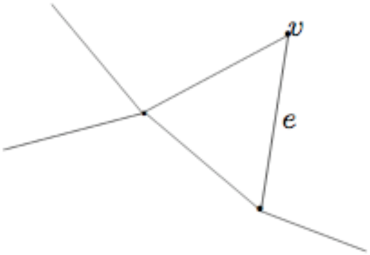

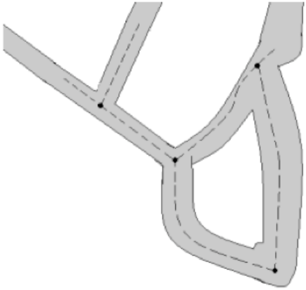

Quantum graphs can be used to describe the dynamics of a quantum particle constrained on a domain with transverse dimensions small with respect to the longitudinal ones

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Some old and recent examples of systems and problems for which quantum graphs are of interest

- Spectrum of valence electrons in organic molecules (Ruedenberg and Scherr '53)

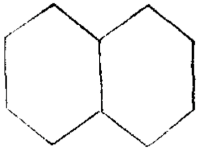

Figure: Molecular skeleton of the naphtalene molecule

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- Spectrum of valence electrons in organic molecules (Ruedenberg and Scherr '53)
- Nanotechnologies (circuits of quantum wires)

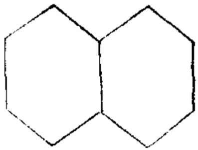

Figure: Molecular skeleton of the naphtalene molecule

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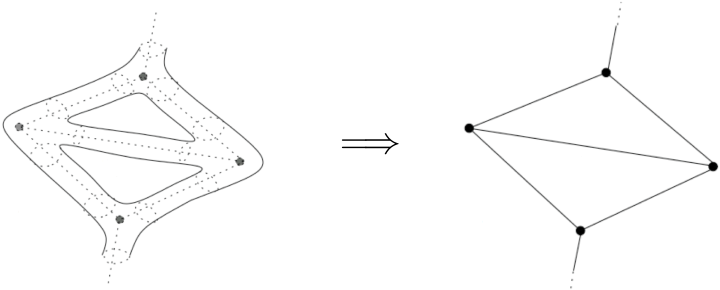
A natural approach to this problem consists in studying the one dimensional limit of the operator $-\Delta_\Omega$ when Ω "collapses" on a graph.



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Neumann Laplacian: (Kirchhoff's condition)

$$f_1(v) = f_2(v) = \cdots = f_n(v) \quad \text{and} \quad \sum_{j=1}^{n} f_j'(v) = 0$$

- Spectral convergence on compact graphs (Rubinstein and Schatzman '01, Kuchment and Zeng '01, Exner and Post '05)
- Weak convergence (Saitō '01)
- Spectral convergence on non-compact graphs (Post '06)

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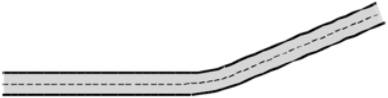
Dirichlet Laplacian: (Decoupling condition)

$$f_1(v) = f_2(v) = \cdots = f_n(v) = 0$$

- Spectral convergence on compact graphs (Post '05). The domain narrows around the vertices
- Convergence of the dynamics (Dell'Antonio and Tenuta '06). Simplified model with confining quadratic potentials
- Convergence of the scattering matrix in the generic case (Molchanov and Vainberg '06).

The Model

We are interested in studying the convergence of the Dirichlet Laplacian near the vertex. We shall consider a waveguide Ω of constant width $2d$ around a base curve Γ.



It is convenient to introduce global coordinates (s, u) on Ω: s is the arclenght coordinate along Γ and u is the transversal coordinate with respect to Γ. With these coordinates the domain Ω is given by $s \in \mathbb{R}$, $u \in [-d, d]$.

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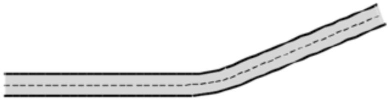

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$$\Gamma : \mathbb{R} \to \mathbb{R}^2 \quad \Gamma(t) := \{(\gamma_1(s), \gamma_2(s)) | \, s \in \mathbb{R}\} \, ; \quad \gamma_1'^2(s) + \gamma_2'^2(s) = 1$$

$$\gamma(s) := \gamma_2'(s)\gamma_1''(s) - \gamma_1'(s)\gamma_2''(t) \quad \text{(Signed Curvature)}$$

The Model

$$\text{Assumptions on } \Gamma : \quad \begin{cases} \Gamma \text{ has no self intersections} \\ supp[\gamma] \subseteq [a,b] \\ \gamma(s) \text{ is piecewise } C^2(\mathbb{R}) \\ \gamma'(s)\,,\ \gamma''(s) \text{ are bounded} \end{cases}$$

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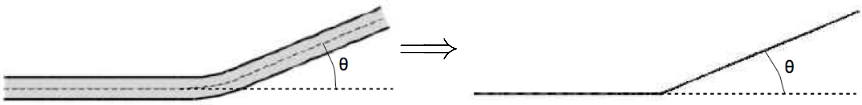
We rescale the domain Ω in the following way ($\Omega \longrightarrow \Omega_\varepsilon$)

$$\begin{cases} \gamma(s) & \longrightarrow \frac{1}{\varepsilon}\gamma\left(\frac{s}{\varepsilon}\right) \\ d & \longrightarrow \varepsilon^\alpha d \end{cases} \qquad \varepsilon > 0\,,\ \alpha \geqslant 1\,.$$



Preliminaries

- The angle
$$\theta = \int_{\mathbb{R}} \gamma(s) ds$$
between the straight parts of Γ is unchanged by the scaling
- The family of domains Ω_ε approximates, for $\varepsilon \to 0$, the broken line of angle θ

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The coordinates (s, u) allow to write the Hamiltonian as an operator on $L^2(\mathbb{R} \times [-d, d])$ defined by

$$H = -\frac{\partial}{\partial s} \frac{1}{(1 + u\gamma(s))^2} \frac{\partial}{\partial s} - \frac{\partial^2}{\partial s^2} + V(s, u)\,,$$

$$V(s, u) = -\frac{\gamma(s)^2}{4(1 + u\gamma(s))^2} + \frac{u\gamma''(s)}{2(1 + u\gamma(s))^3} - \frac{5}{4} \frac{u^2\gamma'(s)^2}{(1 + u\gamma(s))^4}$$

Preliminaries

Under our scaling we obtain

$$H_\varepsilon = -\frac{\partial}{\partial s}\frac{1}{(1+\varepsilon^{\alpha-1}u\gamma(s/\varepsilon))^2}\frac{\partial}{\partial s} - \frac{1}{\varepsilon^{2\alpha}}\frac{\partial^2}{\partial u^2} + \frac{1}{\varepsilon^2}V_\varepsilon(s,u)\,,$$

$$V_\varepsilon(s,u) = -\frac{\gamma(s/\varepsilon)^2}{4(1+\varepsilon^{\alpha-1}u\gamma(s/\varepsilon))^2} + \frac{\varepsilon^{\alpha-1}u\gamma''(s/\varepsilon)}{2(1+\varepsilon^{\alpha-1}u\gamma(s/\varepsilon))^3} - \frac{5}{4}\frac{\varepsilon^{2\alpha-2}u^2\gamma'(s/\varepsilon)^2}{(1+\varepsilon^{\alpha-1}u\gamma(s/\varepsilon))^4}$$

- We want to discuss the convergence of the operator H_ε to a suitable operator $\overline{H}$ defined on the graph
- A good notion of convergence for this problem is the uniform (strong) convergence of the resolvent operator since it gives information also on the convergence of the dynamics
- Notice that the initial Hamiltonian is defined on a strip while the limit operator is defined on a one dimensional (singular) manifold
- Notice also that the transversal kinetic energy is divergent in the limit $\varepsilon \to 0$ and therefore we shall have to subtract this divergent quantity to the spectral parameter of the resolvent

Main Result

We denote with $\{\phi_n(u)\}_{n\in\mathbb{N}}$ the solutions of

$$\begin{cases} -\dfrac{1}{\varepsilon^{2\alpha}}\dfrac{d^2}{du^2}\phi_n(u) = \lambda_{\varepsilon,n}\phi_{\varepsilon,n}(u) \\ \phi_n(-d) = \phi_n(d) = 0 \end{cases}$$

with

$$\lambda_{\varepsilon,n} = \left(\frac{n\pi}{2\varepsilon^\alpha d}\right)^2$$

We define the following operator $R^\varepsilon_{n,m}(k^2) : L^2(\mathbb{R}) \to L^2(\mathbb{R})$

$$R^\varepsilon_{n,m}(k^2) = (\phi_n, (H_\varepsilon - k^2 - \lambda_{m,\varepsilon})^{-1}\phi_m)$$

Main Result

Theorem

Assume that Γ *has no self intersections and that* γ *is piecewise* C^2*, has compact support and* γ', γ'' *are bounded. Moreover take* $\alpha > 5/2$ *and put* $\overline{V} = -\gamma^2/4$*. Then two cases can occur:*

Case 1. There does not exist a zero energy resonance for the Hamiltonian $\overline{H} = -\frac{d^2}{ds^2} + \overline{V}(s)$*. In such a case*

$$\mathrm{u} - \lim_{\varepsilon \to 0} R^{\varepsilon}_{n,m}(k^2) = \delta_{nm}(\overline{H}^D - k^2)^{-1} \qquad k^2 \in \mathbb{C}\backslash\mathbb{R},\ \mathrm{Im} k > 0$$

where

$$\mathscr{D}(\overline{H}^D) = \{f \in H^2(\mathbb{R}\backslash 0) \cap H^1(\mathbb{R})\ s.t.\ f(0) = 0\}$$

and

$$\overline{H}^D f = -\frac{d^2 f}{ds^2} \qquad s \neq 0$$

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Case 2. There exists a zero energy resonance for the Hamiltonian $\overline{H} = -\frac{d^2}{ds^2} + \overline{V}(s)$*. In such a case*

$$\mathrm{u}-\lim_{\varepsilon\to 0} R^{\varepsilon}_{n,m}(k^2) = \delta_{nm}(\overline{H}^r - k^2)^{-1} \qquad k^2 \in \mathbb{C}\backslash\mathbb{R},\ \mathrm{Im}k > 0$$

where

$$\mathscr{D}(\overline{H}^r) = \{f \in H^2(\mathbb{R}\backslash 0)\ s.t.\ (c_1 + c_2)f(0^+) = (c_1 - c_2)f(0^-)\,,\ (c_1 - c_2)f'(0^+) = (c_1 + c_2)f'(0^-)\}$$

and

$$\overline{H}^r f = -\frac{d^2 f}{ds^2} \qquad t \neq 0\,.$$

The constant c_1 *and* c_2 *depend on the resonance* $\psi_r \in L^\infty(\mathbb{R})$*.*

Main Result

Let us consider a one dimensional Hamiltonian $\overline{H}$ given by:

$$\overline{H} = -\frac{d^2}{ds^2} + \overline{V}(s)$$

We say that the Hamiltonian $\overline{H}$ has a zero energy resonance if there exist $\psi_r \in L^\infty(\mathbb{R})$, $\psi_r \notin L^2(\mathbb{R})$ such that $\overline{H}\psi_r = 0$ in distributional sense.

Proof

The proof is divided into two step: first we prove that, if $\alpha > 5/2$ we can approximate $R^{\varepsilon}_{n,m}(k^2)$ in norm with $\delta_{nm}(\overline{H}_{\varepsilon} - k^2)^{-1}$ where $\overline{H}_{\varepsilon}$ is the the following one dimensional Hamiltonian

$$\overline{H}_{\varepsilon} = -\frac{d^2}{ds^2} + \frac{1}{\varepsilon^2}\overline{V}(s/\varepsilon) \qquad \overline{V}(s) = -\frac{\gamma^2(s)}{4}$$

Now we have to study the convergence of this Hamiltonian under this singular scaling.

The resolvent of $\overline{H}$ can be written as

$$(\overline{H} - k^2)^{-1} = G_k - G_k v T(k) u G_k$$

where

$$G_k(s,s') = \frac{i}{2k} e^{ik|s-s'|} \qquad k^2 \in \mathbb{C}\backslash\mathbb{R}^+,\ \mathrm{Im}k > 0$$

and

$$T(k) = (1 + uG_k v)^{-1} \qquad \mathrm{Im}k \geqslant 0,\ k \neq 0,\ k^2 \notin \Sigma_p(\overline{H})$$

Proof

The following formula for $(\overline{H}_\varepsilon - k^2)^{-1}$ holds

$$(\overline{H}_\varepsilon - k^2)^{-1} = G_k - \frac{1}{\varepsilon} A_\varepsilon(k) T(\varepsilon k) C_\varepsilon(k)$$

where $A_\varepsilon(k)$ and $C_\varepsilon(k)$ have the following integral kernels:

$$A_\varepsilon(k; s, s') = G_k(s - \varepsilon s') v(s')$$
$$C_\varepsilon(k; s, s') = u(s) G_k(\varepsilon s - s') .$$

Using the low energy expansion of $T(k)$ given by Bollé, Gesztesy, and Wilk ('85), we end the proof in both cases

Final Remarks

- Non decoupling boundary conditions have been obtained for the first time in the Dirichlet case
- Our result cannot be trivially extended to the much more complicate case of a general graph
- The resonances provide a convergence mechanism which is too fragile to explain the physical applications
- The limit operator does simply not depend on the geometry of the graph, i.e. on the angle θ. It is possible to construct different curves with the same θ which give different limit operators and curves which has different θ but has the same limit operator.