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From "fat" graphs to metric graphs: the problem of boundary conditions

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We discuss how the vertex boundary conditions for the dynamics of a quantum particle on a metric graph emerge when the dynamics is regarded as a limit of the dynamics in a tubular region around the graph. We give evidence for the fact that the boundary conditions are determined by the possible presence of a zero-energy resonance. Therefore, the boundary conditions depend on the shape of the fat graph near the vertex. We also give evidence, by studying the case of the half-line, for the fact that on the contrary, in general, adding on a graph a shrinking support potentials at the vertex either does not alter the boundary condition or does not produce a self-adjoint dynamics. Convergence, throughout, is meant in the sense of strongly resolvent convergence.

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1. Introduction

We consider in $\mathbb{R}^3$ a star graph Γ with vertex at the origin and N "*rays*" (half-lines) $K^{(n)}$, $n = 1 \dots N$. We consider also a suitable vicinity of Γ ("*fat graph* "), denoted by Γ_ε, whose "width" is proportional to $\varepsilon > 0$. More concretely, we consider Γ_ε as consisting of a junction region contained in a ball B_ε of radius $C \cdot \varepsilon$ $(C > 1)$, attached to which there are N tubes" $K_\varepsilon^{(n)}$, $n = 1, \dots, N$, namely N non-intersecting infinite half-cylinders with transversal radius ε, whose axes are the rays $K^{(n)}$.

The limit $\varepsilon \to 0$ that we have in mind is a homotetic shrinking of Γ_ε to its skeleton Γ.

The internal region may be arbitrary and need not be connected; it may also be fragmented. In the case of graphene, the image in an electronic microscope shows that the density of conducting electrons is essentially localized in a spherical corona of width approximately equal to the diameter of the cylinders.

This may be considered as a result of the combined action of the attraction to the nucleus and of the presence near the nucleus of the valence electrons.

Let $\Delta_{\Gamma_\varepsilon}$ be the Laplacian on Γ_ε with Dirichlet boundary conditions at $\partial\Gamma_\varepsilon$.

We denote by $\lambda_\varepsilon > 0$ and $\xi_\varepsilon^{(1)}$, respectively, the lowest eigenvalue and the corresponding normalized eigenfunction of the two-dimensional negative Laplacian on a disk with Dirichlet boundary conditions. By scaling $\lambda_\varepsilon \sim \varepsilon^{-2}\lambda$.

We define the following:

$$H_\varepsilon := -\Delta_{\Gamma_\varepsilon} - \lambda_\varepsilon \mathbf{1}.$$

We have thus obtained a self-adjoint operator on the fat graph Γ_ε. Dependng on the shape of Ω_ε for all values of $\varepsilon > 0$, H_ε may possibly have a negative point spectrum and an absolutely continuous spectrum coinciding with $\mathbb{R}^+$.

It turns out that a deep understanding of the structure of the limit $\varepsilon \to 0$ is achieved by means of the notion of *zero energy resonance*. For the present purposes, we define a zero energy resonance of H_ε as a singularity of the spectral measure of H_ε at the bottom of the continuous spectrum, equivalently, as a singularity in k^2 at $k = 0$ of the resolvent $(H_\varepsilon - k^2)^{-1}$.

If the boundary $\partial\Gamma_\varepsilon$ is smooth, the singularity at the bottom of the continuous spectrum is of the type $\frac{1}{|k|}$. This corresponds, in our case, due to the special form of the domain Γ_ε, to a generalized (i.e., distributional) solution Φ_ε to $H_\varepsilon\Phi_\varepsilon = 0$ which is only square-integrable locally.

There is in fact a **one-to-one correspondence** between the possible singularities at zero of the resolvent of H_ε, due to **resonances**, and the singularities at zero of the resolvents of each self-adjoint Laplacian on the star graph. The former are non square-integrable functions that on each cylinder behave, axially, as a constant plus linear function $a_n + b_n z_n$ (z_n is the axial coordinate on the n-th cylinder); the latter have the very same behavior on the corresponding rays of the star graph.

2. Setting the problem up

We want to study the effect of Ω_ε on the limit $\varepsilon \to 0$ by means of the associated problem – we shall call it "the internal region problem" – consisting of the negative Laplacian in the internal region Ω_ε with boundary conditions that are of some assigned type, denoted by α, on the bases of the cylinders, and are of the Dirichlet type on the rest of $\partial\Omega_\varepsilon$.

With this choice, we denote by $\mu_+(\Omega_\varepsilon)$ and $\mu_-(\Omega_\varepsilon)$, respectively, the lowest eigenvalue of the internal region problem when $\alpha =$ Dirichlet or $\alpha =$ Neumann, and by $\mu_\alpha(\Omega_\varepsilon)$ the lowest eigenvalue with generic boundary condition α (recall that on the rest of $\partial\Omega_\varepsilon$ we always take Dirichlet boundary conditions). Clearly:

$$\mu_-(\Omega_\varepsilon) \leqslant \mu_\alpha(\Omega_\varepsilon) \leqslant \mu_+(\Omega_\varepsilon),$$

and each $\mu_\alpha(\Omega_\varepsilon)$ scales as ε^{-2}. We also note that by min-max, when one increases Ω_ε, both $\mu_-(\Omega_\varepsilon)$ and $\mu_+(\Omega_\varepsilon)$ decrease.

Suppose that the internal region problem with a given boundary condition $\boldsymbol{\alpha}$ has a lowest-energy solution given by the eigenfunction $\phi_\varepsilon(\mathbf{x})$ and the eigenvalue $\mu_\alpha(\Omega_\varepsilon)$, where $\mathbf{x}$ is the three-dimensional coordinate in Ω_ε.

Correspondingly, prolonging ϕ_ε by continuity of the function and its derivatives, to a function Φ_ε, also defined also on the external cylinders in such a way that, if (x_n, y_n) are the transversal coordinates and z_n is the axial coordinate in $K_\varepsilon^{(n)}$, then:

$$\Phi_\varepsilon(x_1, y_1, z_1, \ldots, x_N, y_N, z_N) = \prod_{n=1}^{N} \xi_\varepsilon^{(1)}(x_n, y_n)(a_n + b_n z_n)\,, \qquad z_n \geqslant 0\,,$$

Fundamental observation: a zero energy resonance for H_ε on Γ_ε *can occur* only if for the associated internal region problem there exists a boundary condition α at the bases of the cylinders such that the first eigenvalue $\mu_\alpha(\Omega_\varepsilon)$ of the internal region problem (namely the negative Laplacian inside Ω_ε with boundary condition α at the bases of the cylinders and Dirichlet boundary conditions on the remaining part of $\partial\Omega_\varepsilon$) **coincides** with the lowest eigenvalue λ_ε of the negative Laplacian on the cylinders transversal section, namely if

$$\mu_-(\Omega_\varepsilon) \leqslant \lambda_\varepsilon \leqslant \mu_+(\Omega_\varepsilon)\,.$$

Decomposition:

$$L^2(\Gamma_\varepsilon) \;\cong\; L^2(\Omega_\varepsilon) \,\oplus \big(\oplus_{n=1}^N L^2(K_\varepsilon^{(n)})\big)$$

(Ω_ε = the central region, $K_\varepsilon^{(n)}$ = the cylinders). In turn,

$$\begin{aligned} L^2(K_\varepsilon^{(n)}) \;&\cong\; L^2(K^{(n)}) \otimes L^2(D_\varepsilon) \\ &\cong\; \Big(L^2(\mathbb{R}^+) \otimes \mathrm{Span}\{\xi_\varepsilon^{(1)}\}\Big) \oplus \Big(L^2(\mathbb{R}^+) \otimes \big(\oplus_{k=2}^\infty \mathrm{Span}\{\xi_\varepsilon^{(k)}\}\big)\Big)\,; \end{aligned}$$

($K^{(n)}$ = corresponding ray of the star graph Γ) (hence $L^2(K^{(n)}) \cong L^2(\mathbb{R}^+)$), D_ε is the disk in $\mathbb{R}^2$ centered at the origin and with radius ε, and $\{\xi_\varepsilon^{(k)} \,|\, k \in \mathbb{N}\}$ is the o.n.b. of $L^2(D_\varepsilon)$ consisting of all Dirichlet Laplacian eigenfunctions.

We note that this decomposition *is not left invariant* by the flow of H_ε.

Consider the natural map:

$$\Pi_\varepsilon : L^2(\Gamma_\varepsilon) \to L^2(\Gamma)$$

which "crushes" the square integrable functions on the fat graph to square integrable functions on the star graph by first taking only the part of the function existing on the cylinders $K_\varepsilon^{(n)}$'s and neglecting the part supported on the vertex region Ω_ε, and then on each cylinder projecting the transversal part of the wave-function onto $\xi_\varepsilon^{(1)}$.

We want to investigate the limit of the **"squeezed resolvent"**:

$$\Pi_\varepsilon (H_\varepsilon - k^2)^{-1} \Pi_\varepsilon^* \xrightarrow{\varepsilon \to 0} ?$$

2.1. Resonant case

Resonant case: $\exists$ a zero energy resonance Φ_ε for H_ε:

$$\begin{aligned} \Phi_\varepsilon \;&\in\; L^2_{\mathrm{loc}}(\Gamma_\varepsilon) \backslash L^2(\Gamma_\varepsilon) \\ H_\varepsilon \Phi_\varepsilon \;&=\; 0 \quad \text{distributionally}\,. \end{aligned}$$

on the n-th cylinder, $K_\varepsilon^{(n)}$ it has the form

$$\Big(\Phi_\varepsilon\Big|_{K_\varepsilon^{(n)}}\Big)(x_n, y_n, z_n) \;=\; \xi_\varepsilon^{(1)}(x_n, y_n)(a_n + b_n z_n)\,.$$

Each self-adjoint Laplacian $\Delta_{A,B}$ on the star graph Γ is identified by a vertex boundary condition on each $f \equiv (f^{(1)}, \ldots, f^{(N)})$

$$A \begin{pmatrix} f^{(1)}(0) \\ \vdots \\ f^{(N)}(0) \end{pmatrix} + B \begin{pmatrix} f^{(1)\prime}(0) \\ \vdots \\ f^{(N)\prime}(0) \end{pmatrix} \;=\; 0$$

for suitable $N \times N$ matrices A and B [Kostrykin-Schrader]. Each $\Delta_{A.B}$ admits a zero-energy resonance in $L^2_{\mathrm{loc}}(\Gamma) \backslash L^2(\Gamma)$, that on each ray $K^{(n)}$, $n = 1, \ldots, N$, behaves as $\alpha_n + \beta_n z_n$ for certain coefficient pairs (α_n, β_n) determined by A and B.

There is an evident **one-to-one correspondence** between the set of parameters qualifying a **resonance on the fat graph** and the set of parameters qualifying a **resonance on a star graph**, an observation that we now intend to develop further.

Let $-\Delta_{A,B}$ be that Laplacian whose resonance's behavior is given by $\alpha_n = a_n$,$\beta_n = b_n$.

It can be argued that if $\Pi_\varepsilon H_\varepsilon \Pi_\varepsilon - (-\Delta_{A,B})$ has no further resonance, and if the resolvent convergence has suitable distributional properties then the limit exists and corresponds to *a* Laplacian $-\Delta_{A,B}$ i.e. $\Pi_\varepsilon H_\varepsilon - k^2)\Pi_\varepsilon^* \xrightarrow{\varepsilon\to 0} (-\Delta_{A,B} - k^2)^{-1}$

"the limit is selected by the resonance of H_ε".
Note that this claim is well-posed, for the resonance function of H_ε is scale invariant.

The claim is proved by the following argument. Let $H_0 \equiv \Pi_\varepsilon H_\varepsilon \Pi_\varepsilon$ and let $V_\varepsilon W_\varepsilon^* = H_0 + \Delta_{A,B}$. One has:

$$\frac{1}{H_0 + V_\varepsilon W_\varepsilon^* - z} - \frac{1}{H_0 + z} = \frac{1}{H_0 - z} V_\varepsilon C_\varepsilon W_\varepsilon^* \frac{1}{H_0 - z}$$

$$C_\varepsilon \equiv \frac{1}{1 - W_\varepsilon^* \frac{1}{H_0 - z} V_\varepsilon}$$

If V_ε and W_ε are H_0-compact and converge weakly to zero when $\varepsilon \to 0$ and if H_0 and $\Delta_{A,B}$ have the same zero-energy resonances, then C_ε vanishes in the limit $\epsilon \to 0$.

2.2. Non-resonant case

Non-resonant case: no zero-resonance for H_ε.
Two subcases:

<u>First case</u>: $\lambda_\varepsilon < \mu_-(\Omega_\varepsilon)$.

In this case, the energy threshold for the internal region is high (compared to λ_ε), which means that the domain Ω_ε has to be "very small" (in order for the spectrum of the internal region problem to have such a high bottom). Functions that belong to the continuous spectrum of H_ε have a component in Ω_ε vanishing in the sup-norm as $\varepsilon \to 0$, in order for their H^2-norm to stay finite. Therefore, the functions in the domain of any limit operator on the graph must be zero at the vertex.
$\Rightarrow$ The limit is the Dirichlet Laplacian.

<u>Second case</u>: $\lambda_\varepsilon > \mu_+(\Omega_\varepsilon)$.

Now the energy threshold for the internal region is low (compared to λ_ε) and the argument above does not apply. We expect that the projection Π_ε "kills" in the limit the wave function (the fast transversal oscillations average to zero).

Therefore, in this case too, we expect that if the limit dynamics on the star graph exists they are Dirichlet-based.

But consider that strong convergence of the resolvents as bounded operators in the Hilbert space does not imply that the limit be the resolvent of a self-adjoint operator even if the convergence is strong and the resolvent identities are satisfied. The limit must be analytic away from the real axis and strong convergence need not preserve analyticity. We shall later give a simple example.

We expect that in the limit $\Pi_\varepsilon(H_\varepsilon - k^2)^{-1}\Pi_\varepsilon^*$ becomes analytic for $Imk^2 > 0$ and *regular* at $k^2 \to 0$ as $\varepsilon \to 0$, because on the star graph, the Dirichlet Laplacian is the *only* self-adjoint Laplacian whose spectral measure is regular at zero [Kostrykin-Schrader].

A *removal of singularity* of the resolvent must therefore take place in the limit $\varepsilon \to 0$. This is typical of this second sub-case: in the first sub-case $\lambda_\varepsilon < \mu_-(\Omega_\varepsilon)$, instead, the resolvent of H_ε is regular at $k^2 = 0$ uniformly in $\varepsilon > 0$ and hence also in the limit.

A way to monitor this *removal of singularity* for the limiting resolvent is to compare (the resolvent of) H_ε with the second operator:

$$H_\varepsilon + V_\varepsilon \qquad V_\varepsilon := C\varepsilon^{-2}\mathbf{1}_{\Omega_\varepsilon}$$

We choose $C > 0$, which is always possible, so that the "modified internal region problem" $-\Delta + V_\varepsilon$ on Ω_ε, with a given boundary condition α at the bases of the cylinders and, as usual, Dirichlet boundary conditions on the remaining part of $\partial\Omega_\varepsilon$, has the lowest eigenvalue that precisely coincides with λ_ε (the role of V_ε is therefore merely to lift the bottom of the spectrum of the internal region problem up to the desired level λ_ε). For convenience, we denote by φ_ε the corresponding lowest energy eigenfunction, that is, $(-\Delta + V_\varepsilon)\varphi_\varepsilon = \lambda_\varepsilon\varphi_\varepsilon$ in Ω_ε with Dirichlet boundary conditions on the whole $\partial\Omega_\varepsilon$.

The internal region problem, consisting now of the negative Laplacian plus the potential V_ε with a given boundary condition α, has the lowest eigenvalue that can be lifted up by means of a suitable choice of the constant C so as to precisely match the value λ_ε. This does *not* alter, but for an overall phase factor, the solutions to the internal region problem and hence the matching conditions at the bases of the cylinders.

Notice:
$\sigma(H_\varepsilon + V_\varepsilon) = [0, +\infty)$
$H_\varepsilon + V_\varepsilon$ admits a zero energy resonance.

We thus have two operators on $L^2(\Gamma_\varepsilon)$, namely H_ε and $H_\varepsilon + V_\varepsilon$, where the latter is a perturbation of the former and it is zero-resonant.

This is the input for a well-established scheme developed by Kato, Konno, and Kuroda that allows one to re-write:

$$(H_\varepsilon + V_\varepsilon - \lambda)^{-1} - (H_\varepsilon - \lambda)^{-1},$$

in a way that is well suited for taking the limit $\varepsilon \to 0$ and for taking advantage of the existence of a zero-energy resonance.
For instance:

$$\Pi_\varepsilon\Big((H_\varepsilon^N + V_\varepsilon - \lambda)^{-1} - (H_\varepsilon^N - \lambda)^{-1}\Big)\Pi_\varepsilon^* \xrightarrow{\varepsilon\to 0}$$
$$\xrightarrow{\varepsilon\to 0} (-\Delta^N - \lambda)^{-1} + C(k)P_{N,k}$$

where $P_{N,k}$ is the projection onto the vector $|G_k^N(.,0) >$.

Using the explicit form of the resolvents on a graph given e.g. in [1], one verifies that the last term is:

$$\Big((-\Delta^D - \lambda)^{-1} - (-\Delta^N - \lambda)^{-1}\Big)$$

and therefore $\Rightarrow$ The limit is the resolvent of the Dirichlet Laplacian.

Notice: V_ε is added in the *internal region* Ω_ε and this can be done only in the case of a fat graph Γ_ε. This procedure has no counterpart on the graph Γ (because there is no internal region).

One may hope to obtain similar results by adding directly in the graph a potential V_ε supported around the vertex of the graph and taking the limit when the support shrinks to the vertex.

Prototype: a "star graph" with one edge only. The corresponding fat graph has the shape of a safety match.
By choosing suitably the shape of the head of the safety match, one can produce in the limit any boundary condition at the vertex.
We can now try to change boundary conditions at the vertex of the graph by adding a

potential shrinking around the origin
We introduce the Hamiltonian on $L^2(\mathbb{R}^+)$:

$$H_\varepsilon^{(\nu)} \;=\; -\Delta_\nu + V_\varepsilon\,, \qquad \mathcal{D}(H_\varepsilon^{(\nu)}) \;=\; \mathcal{D}(-\Delta_\nu)\,,$$
$$V_\varepsilon(x) \;:=\; \frac{1}{\varepsilon^{1+\gamma}}\,V\Big(\frac{x}{\varepsilon}\Big)\,,$$

where
→ V is real-valued, $V \in L^1(\mathbb{R}^+) \cap L^\infty(\mathbb{R}^+)$
→ self-adjoint boundary condition at the origin

$$f(0)\sin\nu \;=\; f'(0)\cos\nu \qquad \nu \in \Big(-\frac{\pi}{2},\frac{\pi}{2}\Big]$$

→ $\gamma < 0$ weak scaling, $\gamma = 0$ canonical, $\gamma > 0$ strong

The problem is simple enough to allow an explicit solution.

For $k^2 \in \mathbb{C}$ with im k¿0, we find that

$$(-\Delta_\nu + V_\varepsilon - k^2)^{-1} \;\xrightarrow{\varepsilon\to 0}\; (-\Delta_\nu - k^2)^{-1} \;+\; \Theta_{\nu,V,k}(\gamma)\,|\,\eta_{\nu,k}\,\rangle\langle\,\overline{\eta_{\nu,k}}\,|$$

in the norm operator sense, where

$$\eta_{\nu,k}(x) \;:=\; (\tan\nu - k)^{-1}\,e^{ikx}\,, \qquad x \in [0,+\infty)\,,$$

$$\Theta_{\nu,V,k}(\gamma) \;=\; \begin{cases} 0 & \text{if } \gamma < 0 \text{ (weak scaling)} \\ -\dfrac{(\int_{\mathbb{R}^+}V)}{1 + (\tan\nu - \mathrm{i}k)^{-1}(\int_{\mathbb{R}^+}V)} & \text{if } \gamma = 0 \text{ (canonical scaling)} \\ -(\tan\nu - \mathrm{i}k) & \text{if } 0 < \gamma < 1 \text{ (strong scaling).} \end{cases}$$

The convergence being in operator norm, the limit operator R_k satisfies the resolvent identity.

In the weak scaling regime the boundary conditions are not changed.

In the canonical or strong scaling, in general R_k is not the resolvent of a self-adjoint operator (in particular the limit does not produce new boundary conditions at $x = 0$), because R_k is not holomorphic in k^2:

in fact $R_k = (-\Delta_D - k^2)^{-1}$ for all $k^2 \in (-\infty, 0)$,
but $R_k \neq (-\Delta_D - k^2)^{-1}$ for some values $k^2 \in \mathbb{C} \setminus (-\infty, 0)$

Exceptions:
→ $\int_{\mathbb{R}^+}V = 0$ in the canonical scaling ($\gamma = 0$)
→ Dirichlet boundary conditions are preserved in any scaling

This phenomenon can be proved for a general metric graph as well.

Remarkably, the only exception is a "fake" star graph consisting of the real line $\mathbb{R}$ regarded as the union of the two rays $\mathbb{R}^+$ and $\mathbb{R}^-$.

In this case one can add to the self-adjoint Laplacian on $\mathbb{R}$ a potential $\varepsilon^{-1}\mathbf{1}_{\{|x|\leqslant\varepsilon\}}$ at the "vertex" of the graph so to obtain in the limit $\varepsilon \to 0$ a so-called "point interaction" at the origin, namely a self-adjoint operator with certain boundary conditions at the origin [2].

References

[1] K. Kostrykin, S. Schrader. Kirchhoff's rule for quantum wires. *J. Phys. A: Math. Gen.*, 1999, **32**, P. 595–630.

[2] S. Albeverio, R. Høegh-Krohn. Perturbation of resonances in quantum mechanics. *J. Math. Anal. Appl.*, 1984, **101**(2), P. 491-513.