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Dynamics on a Graph as the Limit of the Dynamics on a "Fat Graph"

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Abstract We discuss how the vertex boundary conditions for the dynamics of a quantum particle constrained on a graph emerge in the limit of the dynamics of a particle in a tubular region around the graph ("fat graph") when the transversal section of this region shrinks to zero. We give evidence of the fact that if the limit dynamics exists and is induced by the Laplacian on the graph with certain self-adjoint boundary conditions, such conditions are determined by the possible presence of a zero energy resonance on the fat graph. Pictorially, one may say that in the shrinking limit the resonance acts as a bridge connecting the boundary values at the vertex along the different rays.

1 Introduction and Motivation

The study of quantum graphs has flourished in recent years both on the purely mathematical side and with reference to applications. A typical example is seen in Chemical Physics [4] and in Mathematical Physics, where organic molecules such as graphene are *modeled by metric graphs* and conductivity and other physical properties are derived from the properties of the solutions to the Schrödinger equation *on the metric graph*.

In order to define the Schrödinger dynamics on a metric graph it is necessary to impose suitable (self-adjoint) boundary conditions at the vertices [13, 14]. While

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in mathematics one is free to choose the boundary conditions that suit best the analytical tools used, in applications it is convenient to use the boundary conditions that are suggested by the problem under study. It is customary both in Chemical Physics and in Mathematical Physics to choose vertex boundary conditions of Kirchhoff type, or sometimes also boundary conditions in which at each vertex the wave function is continuous and the sum of the directional derivatives is proportional to the value that the function attains at the vertex itself. These choices are seldom motivated theoretically, and are usually made to fit experimental data [4].

Quantum graphs are an idealisation of a physical system constrained (e.g., by constraining forces) to a very small neighbourhood of a graph-like structure. For the physical system the Schrödinger operator is well-defined as a self-adjoint operator; it is therefore of interest to see what is the origin of the plurality of choices on the graph.

For example the density of conducting electrons in graphene has the form of a "fat graph" with a hole at the vertices. One justifies this shape as due to the strong attractive forces of the nuclei and to the valence electrons which forbid the presence of conducting electrons near the vertices. We would like to know whether this shape justifies the choice of the boundary condition that is actually made, and whether the addition of an impurity (e.g., by changing the shape) forces a change of the boundary conditions for the model.

In this report we study the case of a graph with only one vertex ("*star graph*") and we restrict our attention to the case in which the operator on the edges is the negative Laplacian; all conclusions remain essentially unchanged if one adds to it a potential that is sufficiently regular. We content ourselves to provide only the sketch of the main proofs, full details are deferred to a future publication [7]. The techniques we use can be adapted to study the case of a Schrödinger particle constrained on a generic metric graph (i.e., a graph with many vertices and hence finite internal edges next to the infinite external ones), as well as to geometries consisting of a metric graph intersecting a surface in some points, for instance a plane and a line perpendicular to it, or more generally a so-called "hedgehog manifold".

We consider in $\mathbb{R}^3$ a star graph Γ with vertex in the origin and N "*rays*" (half-lines) $K^{(n)}$, $n = 1 \dots N$. We also consider a suitable neighbourhood 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" Ω_ε at the centre of the fat graph, attached to which there are N "tubes" $K_\varepsilon^{(n)}$, $n = 1, \dots, N$, namely N

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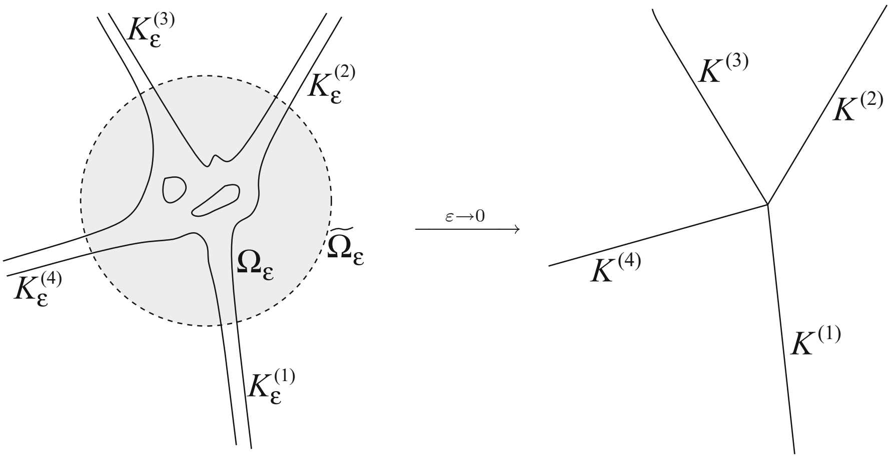
non-intersecting infinite half-cylinders with transversal radius ε, whose axes are the rays $K^{(n)}$. The domain Ω_ε need not be connected or simply connected (for example, it can be a spherical shell): we shall just assume it to be bounded and closed, and such that the bases of the cylinders are part of the boundary $\partial\Omega_\varepsilon$. Later it will be convenient to introduce an "effective central region" $\tilde{\Omega}_\varepsilon$, with the purpose of ignoring the geometric details of Ω_ε while retaining only the necessary information for our spectral analysis. $\tilde{\Omega}_\varepsilon$ is meant to be a smooth and simply connected domain centred at the vertex of the star graph Γ, which includes Ω_ε and has, in common with Ω_ε, the bases of the cylinders $K_\varepsilon^{(n)}$.



The limit $\varepsilon \to 0$ that we have in mind is a homotetic shrinking of Γ_ε to its skeleton Γ: thus each cylinder shrinks to its axis, and the vertex region Ω_ε shrinks homotetically to the vertex of Γ. In symbols, $\Gamma_\varepsilon = \varepsilon\Gamma_1$, $\Omega_\varepsilon = \varepsilon\Omega_1$, and $\varepsilon \to 0$.

Let $\Delta_{\Gamma_\varepsilon}$ be the Laplacian on Γ_ε with Dirichlet boundary conditions at $\partial\Gamma_\varepsilon$. It is well defined as a positive self-adjoint operator for all $\varepsilon > 0$ and therefore it determines a dynamics (free particle dynamics) on Γ_ε. On the other hand, the Laplacian on the graph Γ is defined as a self-adjoint operator only if one specifies self-adjoint boundary conditions at the vertex [13, 14]. We are interested in the connection between the properties of Ω_ε (e.g., its *shape*) and the boundary conditions at the vertex of Γ for the limit dynamics.

We observe that an obvious renormalisation of $-\Delta_{\Gamma_\varepsilon}$ is in order, for one immediately sees that the bottom of its spectrum diverges to $+\infty$ as $\varepsilon \to 0$. To this aim, let us consider the transversal section of each tube, that we take to be a two-dimensional disk of radius ε. The two-dimensional negative Laplacian on such a disk with Dirichlet boundary conditions is a positive self-adjoint operator with discrete spectrum. We denote by $\lambda_\varepsilon > 0$ and $\xi_\varepsilon^{(1)}$, respectively, its lowest eigenvalue and the corresponding normalised eigenfunction. It is clear by scaling that $\lambda_\varepsilon \sim \varepsilon^{-2}$. Then we define $H_\varepsilon := -\Delta_{\Gamma_\varepsilon} - \lambda_\varepsilon \mathbb{1}$. We have thus obtained a self-adjoint operator on the fat graph Γ_ε such that, for all values of $\varepsilon > 0$, H_ε has possibly negative point spectrum and an absolutely continuous spectrum coinciding with $\mathbb{R}^+$.

The relation between the dynamics induced by H_ε on Γ_ε and a limit dynamics on Γ when $\varepsilon \to 0$ is far from trivial and very few results are available. We shall investigate the limit in the sense of convergence of the resolvent of H_ε, more precisely of a suitable reduction of the resolvent of H_ε to a natural space $\mathcal{K}$. For all $\varepsilon > 0$ the space $\mathcal{K}$ can be identified with $L^2(\Gamma)$ [note that $L^2(\Gamma)$ is *not* a subspace of $L^2(\Gamma_\varepsilon)$].

It turns out that a deep understanding 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 $\frac{1}{|k|}$. It corresponds in our case, due to the special form of the domain Γ_ε, to a generalised (i.e., distributional) solution Φ_ε to $H_\varepsilon\Phi_\varepsilon = 0$ which is square-integrable only locally.

Remark 1.1. An analogous situation occurs for the Laplacian on the star graph initially restricted to smooth functions compactly supported away from the graph's vertex: all its self-adjoint extensions, other than the Dirichlet one, are characterised by their (singular) behaviour at the origin in momentum space [3, 13, 14].

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, see also (2) below); the latter have the very same behaviour on the corresponding rays of the star graph.

We take this as a *strong indication* that the limit dynamics on the star graph is determined by the possible occurrence of a zero energy resonance for H_ε on the fat graph. In particular, if H_ε is not resonant, we expect that the limit dynamics is given by the negative Laplacian with Dirichlet boundary conditions at the vertex.

For the fat graph the occurrence of resonances is intimately linked to the *shape* of the central region Ω_ε and it is very sensitive to this shape: if the shape changes slightly the resonance in general immediately disappears. The fragility of resonances makes the analytic proof of convergence extremely difficult.

In this report we will give evidence of the following two facts:

1. *If* the operator H_ε has a zero energy resonance and *if* the limit of a suitable reduction of the resolvent $(H_\varepsilon - \lambda)^{-1}$ to $\mathcal{K} \cong L^2(\Gamma)$ is the resolvent $(H - \lambda)^{-1}$ of a self-adjoint operator H on the star graph, such H must be that self-adjoint negative Laplacian on the star graph identified by the fact that $(H - \lambda)^{-1}$ and $(H_\varepsilon - \lambda)^{-1}$ have *the same singularity* in momentum space at $\lambda = 0$.

2. In addition, the self-adjointness boundary conditions of H at the graph's vertex turn out to be determined by the spatial asymptotic behaviour of the resonance of H_ε.

Remark 1.2. Let us conclude this Introduction by remarking that the problem of describing the limit of the Laplacian in shrinking tubular domains has been attacked previously [5, 8–10, 16–18], but the role of a resonance at the bottom of the continuous spectrum was not fully appreciated.

2 Setting Up the Problem

We have already emphasized that the occurrence of a zero energy resonance for H_ε on the fat graph, which in turn is crucial for the limit dynamics, is related in a very subtle and delicate way to the shape of the internal region Ω_ε. Recall that in our model Ω_ε is a compact, not-necessarily connected region in $\mathbb{R}^3$, which the tubes of the fat graph are attached to; part of its boundary $\partial\Omega_\varepsilon$ coincides therefore with the bases of the cylinders. (We also tacitly assume that Ω_ε has a sufficiently smooth boundary.)

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 Dirichlet type on the rest of $\partial\Omega_\varepsilon$. More precisely, the boundary condition α is a linear constraint between the value of the function and the value of its normal derivative at each point of $\partial\Omega_\varepsilon$ that belongs to the basis of a cylinder (see the figure displayed in the Introduction). Ω_ε being compact, this problem has a discrete spectrum. With this choice, we denote by $\mu_+(\Omega_\varepsilon)$ and $\mu_-(\Omega_\varepsilon)$, respectively, the lowest eigenvalue of the internal region problem when α = Dirichlet or α = 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.

Next to this, we recall that on the whole fat graph Γ_ε we have defined the Hamiltonian H_ε to be the Schrödinger operator $-\Delta_{\Gamma_\varepsilon} - \lambda_\varepsilon \mathbb{1}$ with *Dirichlet boundary conditions* at the boundary $\partial\Gamma_\varepsilon$. Here $\lambda_\varepsilon = \lambda_1 \varepsilon^{-2}$ is the lowest eigenvalue of the Laplacian on a two-dimensional disk of radius ε (the transversal section of each cylinder) with Dirichlet boundary conditions. The choice of the subtraction constant is such that the continuous spectrum of H_ε coincides with the positive real axis for all ε.

Our *key remark* in the comprehension of the problem is the following. Suppose that the internal region problem with a given boundary condition α (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 $\partial\Omega_\varepsilon$) 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, prolong ϕ_ε, by continuity of the function and its derivatives, to a function Φ_ε 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

$$\Phi_\varepsilon(x_1, y_1, z_1, \dots, x_N, y_N, z_N) \;=\; \prod_{n=1}^{N} \tilde{\phi}_\varepsilon^{(n)}(x_n, y_n)(a_n + b_n z_n)\,, \qquad z_n \geqslant 0\,, \tag{1}$$

where the constants a_n and b_n are those determined by the boundary condition α on ϕ_ε, and $\tilde{\phi}_\varepsilon^{(n)}(x_n, y_n)$ is the value that ϕ_ε attains at the basis of the n-th cylinder. In fact, if as in the figure of the Introduction the bases of the cylinders are taken "along the actual cylinders", but sufficiently far from the junction, and if $\mu_\alpha(\Omega_\varepsilon)$ is a sufficiently "low energy", then (1) reads

$$\Phi_\varepsilon(x_1, y_1, z_1, \dots, x_N, y_N, z_N) \;=\; \prod_{n=1}^{N} \xi_\varepsilon^{(1)}(x_n, y_n)(a_n + b_n z_n)\,, \qquad z_n \geqslant 0\,, \tag{2}$$

It is immediate to see by construction that $H_\varepsilon \Phi_\varepsilon = (\mu_\alpha(\Omega_\varepsilon) - \lambda_\varepsilon)\phi_\varepsilon$. (Of course Φ_ε is *not* square integrable, unless $a_n = b_n = 0\ \forall n \in \{1, \dots, N\}$, so by $H_\varepsilon \Phi_\varepsilon$ we mean here the result of the formal action of the differential operator H_ε on Φ_ε in the distributional sense.) The function $H_\varepsilon \Phi_\varepsilon$ is therefore only supported inside Ω_ε, and if the shape of Ω_ε is such that $\mu_\alpha(\Omega_\varepsilon) = \lambda_\varepsilon$, and if we exclude the exceptional case $a_n = b_n = 0\ \forall n \in \{1, \dots, N\}$, then Φ_ε is a *zero energy resonance* for H_ε, in the sense of a non square-integrable distributional solution to $H_\varepsilon \Phi_\varepsilon = 0$.

We have therefore come to the fundamental observation that 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 $\mu_\alpha(\Omega_\varepsilon)$ coincides with the lowest eigenvalue λ_ε of the negative Laplacian on the cylinders transversal section.

Let us tacitly assume, without loss of physical generality, that the geometry of Ω_ε is such that *any* intermediate value in $[\mu_-(\Omega_\varepsilon), \mu_+(\Omega_\varepsilon)]$ can be obtained as the lowest eigenvalue $\mu_\alpha(\Omega_\varepsilon)$ of the internal region problem for a suitable boundary condition α at the bases of the cylinders. Under this restriction our conclusion is therefore that a zero energy resonance for H_ε on Γ_ε occurs if and only if

$$\mu_-(\Omega_\varepsilon) \leqslant \lambda_\varepsilon \leqslant \mu_+(\Omega_\varepsilon)\,. \tag{3}$$

As remarked above, for every fixed $\varepsilon > 0$ we can decrease $\mu_-(\Omega_\varepsilon)$ and $\mu_+(\Omega_\varepsilon)$ by increasing the size of Ω_ε, which indicates that (3) can be matched (by a suitable geometry and) by a suitable change of the size of the internal region.

With such a discussion in mind, let us go back to the analysis of the limit dynamics as $\varepsilon \to 0$. It is clear that the Hilbert space $L^2(\Gamma_\varepsilon)$ changes with ε. We shall now describe in which sense the dynamics induced by the Hamiltonian H_ε may have a limit when $\varepsilon \to 0$. Such a limit, if it exists, describes the dynamics on the metric star graph Γ.

Remark 2.1. The analogous problem where Neumann (instead of Dirichlet) boundary conditions are taken at $\partial\Gamma_\varepsilon$ is easier, because of the fact that one has a natural restriction on the graph of the Sobolev space $H^2(\Gamma_\varepsilon)$, see [11, 17, 18]. One can use this restriction to define the topology of convergence. In this case it is known that the limit operator is the Schrödinger operator on Γ with boundary conditions of Kirchhoff type at the vertices. In the case we are studying, namely with Dirichlet boundary conditions at $\partial\Gamma_\varepsilon$, the limit is singular and part of the problem is to find a proper setting.

Remark 2.2. One expects to obtain the same results in the limit $\varepsilon \to 0$ if instead of assuming Dirichlet boundary conditions at $\partial\Gamma_\varepsilon$ one introduces a constraining potential $V_\varepsilon(x) = \frac{1}{\varepsilon^2} d(x,\Gamma)^2$, where $d(x,\Gamma)$ is the Euclidean distance between a point $x \in \mathbb{R}^3$ and the star graph Γ. A first step in this direction has been taken in [8]. The method presented here can be adapted to that case.

We want to take a convenient restriction ("reduction") of the resolvent of H_ε to a subspace of $L^2(\Gamma_\varepsilon)$ which can be *identified* for all values of ε with $L^2(\Gamma)$. To this aim, we introduce the following decomposition of the Hilbert space $L^2(\Gamma_\varepsilon)$ (with Lebesgue measure)

$$L^2(\Gamma_\varepsilon) \;\cong\; L^2(\Omega_\varepsilon) \,\oplus \big(\oplus_{n=1}^N L^2(K_\varepsilon^{(n)})\big) \tag{4}$$

where Ω_ε is the central region and the $K_\varepsilon^{(n)}$'s are the cylinders. In turn, the Hilbert space of the n-th cylinder can be decomposed as

$$\begin{aligned} L^2(K_\varepsilon^{(n)}) \;&\cong\; L^2(K^{(n)}) \otimes L^2(D_\varepsilon) \\ &\cong\; \Big(L^2(\mathbb{R}^+) \otimes \mathrm{Span}\{\xi_\varepsilon^{(1)}\}\Big) \oplus \Big(L^2(\mathbb{R}^+) \otimes \big(\oplus_{k=2}^\infty \mathrm{Span}\{\xi_\varepsilon^{(k)}\}\big)\Big)\,; \end{aligned} \tag{5}$$

here $K^{(n)}$ is the corresponding ray of the star graph Γ around which the tube $K_\varepsilon^{(n)}$ is taken (hence $L^2(K^{(n)}) \cong L^2(\mathbb{R}^+)$), D_ε is the disk in $\mathbb{R}^2$ centred at the origin and with radius ε, and $\{\xi_\varepsilon^{(k)} | k \in \mathbb{N}\}$ is the orthonormal basis of $L^2(D_\varepsilon)$ consisting of all (normalised) eigenfunctions of the negative Laplacian on D_ε with Dirichlet boundary conditions, labelled in such a way that $\xi_\varepsilon^{(1)}$ is the ground state, corresponding to the ground state energy λ_ε considered in the Introduction.

Notice that the decomposition (4) and (5) *is not left invariant* by the flow of H_ε [namely the evolution unitary group $e^{-\mathrm{i}tH_\varepsilon}$ acting on $L^2(\Gamma_\varepsilon)$] and therefore one cannot use it to define a reduced Hamiltonian. Instead, in view of (4) and (5) we shall exploit a 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 living 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 $\xi_\varepsilon^{(1)}$. Explicitly, if $\Psi \in L^2(\Gamma_\varepsilon)$ and, according to (4), $\Psi = \Psi^{(0)} \oplus (\oplus_{n=1}^N \Psi^{(n)})$, then

$$\begin{aligned} \Psi = \Psi^{(0)} \oplus (\oplus_{n=1}^N \Psi^{(n)}) \;\stackrel{\Pi_\varepsilon}{\longmapsto}\; \psi \;=\; \oplus_{n=1}^N \psi^{(n)} \;\in\; \bigoplus_{n=1}^N L^2(K^{(n)}) \;\cong\; L^2(\Gamma) \\ \psi^{(n)}(z_n) = \iint \mathrm{d}x_n \mathrm{d}y_n \, \xi_\varepsilon^{(1)}(x_n, y_n) \Phi(x_n, y_n, z_n)\,. \end{aligned} \tag{6}$$

It is easy to see that Π_ε is a bounded linear map with operator norm 1. This map allows us to control, for each $\varepsilon > 0$, the "squeezed" Hamiltonian

$$\Pi_\varepsilon H_\varepsilon \Pi_\varepsilon^*$$

as a well-defined operator on $L^2(\Gamma)$, and to study its limit as $\varepsilon \to 0$. Physically this procedure is inspired by the idea that we want to study only the *low-energy* behaviour of a free particle on the fat graph, and hence it is enough to consider in practice only those wave-functions on $L^2(\Gamma_\varepsilon)$ that transversally on each tube are in the span of the lowest energy eigenmode $\xi_\varepsilon^{(1)}$.

We consider now the resolvent $(H_\varepsilon - k^2)^{-1}$, where k^2 belongs to the resolvent set of H_ε and $\mathrm{Im}\, k > 0$, and its "squeezed" (reduced) version on $L^2(\Gamma)$, i.e.,

$$\Pi_\varepsilon (H_\varepsilon - k^2)^{-1} \Pi_\varepsilon^*\,.$$

It is the convergence of this effective (reduced) resolvent on the star graph as $\varepsilon \to 0$ that we can study.

In doing so, since the decomposition (4) and (5) is not left invariant by the flow of H_ε, the restriction of each element in $L^2(\Gamma_\varepsilon)$ to the central region Ω_ε will play a crucial role, and so will the behaviour in the central region of possible zero energy resonant functions. Pictorially, we will see that the resonance *in the limit* $\varepsilon \to 0$ acts as a bridge connecting the boundary values at the vertex along the different rays.

3 Limit to the Star Graph: The Resonant Case (The Case in Which (3) is Satisfied)

We begin with the case when (3) is satisfied. In this case, there is a choice of a boundary conditions α at the bases of the cylinders such that the lowest eigenvalue $\mu_\alpha(\Omega_\varepsilon)$ of the internal region problem satisfies $\mu_\alpha(\Omega_\varepsilon) = \lambda_\varepsilon$. This also means, as discussed in the previous Section, that there exists a zero energy resonance Φ_ε for H_ε:

$$\begin{aligned} \Phi_\varepsilon &\in L^2_{\mathrm{loc}}(\Gamma_\varepsilon)\setminus L^2(\Gamma_\varepsilon) \\ H_\varepsilon \Phi_\varepsilon &= 0 \quad \text{distributionally}\,. \end{aligned} \tag{7}$$

Whereas the problem of what limit, if any, the reduced resolvent $\Pi_\varepsilon(H_\varepsilon - k^2)^{-1}\Pi_\varepsilon^*$ attains as $\varepsilon \to 0$ is, to our understanding, a real hard one, at least at this level of generality, nevertheless there are important conclusions that one can deduce if the limit exists, which have a natural formulation in terms of resonances.

To this aim, we recall on the one hand that Φ_ε has a non-square integrable profile on (some) cylinders: on the n-th cylinder $K_\varepsilon^{(n)}$ it has the form

$$\Big(\Phi_\varepsilon\Big|_{K_\varepsilon^{(n)}}\Big)(x_n, y_n, z_n) \;=\; \xi_\varepsilon^{(1)}(x_n, y_n)(a_n + b_n z_n)\,. \tag{8}$$

On the other hand, we recall from the literature (e.g., [13, 14]) that each self-adjoint Laplacian on the star graph Γ, denoted here as $\Delta_{A,B}$, is identified by a vertex boundary condition on each $f \equiv (f^{(1)}, \dots, f^{(N)})$ of the domain of $\Delta_{A,B}$ which has the form a linear relation between the values of f and f' at the origin of each ray, say,

$$A\begin{pmatrix} f^{(1)}(0) \\ \vdots \\ f^{(N)}(0)\end{pmatrix} + B\begin{pmatrix} f^{(1)\prime}(0) \\ \vdots \\ f^{(N)\prime}(0)\end{pmatrix} \;=\; 0 \tag{9}$$

where A and B are $N \times N$ matrices satisfying certain self-adjointness conditions. It is not difficult to argue that each $\Delta_{A.B}$ admits a zero-energy resonance, in the sense of our definition, namely an element in $L^2_{\mathrm{loc}}(\Gamma)\setminus L^2(\Gamma)$, that on each ray $K^{(n)}$, $n = 1, \dots, N$, behaves as $\alpha_n + \beta_n z_n$ for certain couples of coefficients (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 intend now to develop further.

Our main point in this case is the following: *if* $\Pi_\varepsilon(H_\varepsilon - k^2)^{-1}\Pi_\varepsilon^*$ converges as $\varepsilon \to 0$ to the resolvent $(-\Delta_{A,B} - k^2)^{-1}$ of a self-adjoint realisation $-\Delta_{A,B}$ of the negative Laplacian on the star graph Γ, and if this convergence has suitable distributional properties (in the sense that we will comment in a moment), then $-\Delta_{A,B}$ must be that Laplacian whose resonance's behaviour is given by $\alpha_n = a_n$, $\beta_n = b_n$. In this sense we say that the limit, if it exists and corresponds to *a* Laplacian $-\Delta_{A,B}$, is "selected by the resonance of H_ε" and must be *the* Laplacian with resonance $\alpha_n = a_n$, $\beta_n = b_n$. Note that this claim is well-posed, for the resonance function of H_ε is scale invariant, i.e., a_n and b_n do not depend on ε and thus make sense also in the limit $\varepsilon \to 0$.

The precise sense of the convergence

$$\Pi_\varepsilon (H_\varepsilon - k^2)^{-1} \Pi_\varepsilon^* \xrightarrow{\varepsilon \to 0} (-\Delta_{A,B} - k^2)^{-1} \tag{10}$$

is indicated by the following heuristic remarks. Although Φ_ε is not square-integrable, still $\Pi_\varepsilon \Phi_\varepsilon$ makes sense pointwise and on the n-th ray is the function $z_n \mapsto a_n + b_n z_n$. As long as the l.h.s. below is well-defined (e.g., distributionally or pointwise), one deduces from (7) that

$$\begin{aligned} \Pi_\varepsilon (H_\varepsilon - k^2)^{-1} \Pi_\varepsilon^* \big(\oplus_n (a_n + b_n z_n) \big) \; &= \; \Pi_\varepsilon (H_\varepsilon - k^2)^{-1} \Phi_\varepsilon \\ &= \; -k^{-2} \big(\oplus_n (a_n + b_n z_n) \big) \,, \end{aligned} \tag{11}$$

the identity above being meant distributionally or pointwise. (Incidentally, we observe that the function Φ_ε in any bounded region of Γ_ε approximates in the L^2-norm a function in the domain of H_ε, so we also expect to give meaning to (11) above in the L^2-sense, if a suitable localisation is introduced.) Most importantly, the r.h.s. of (11) does *not* depend on ε, and combining it with (10) yields

$$(-\Delta_{A,B} - k^2)^{-1} \big(\oplus_n (a_n + b_n z_n) \big) \; = \; -k^{-2} \big(\oplus_n (a_n + b_n z_n) \big) \,, \tag{12}$$

at least if the convergence is robust enough to hold true pointwise. In turn, (12) indicates that $-\Delta_{A,B} \big(\oplus_n (a_n + b_n z_n) \big) \equiv 0$, thus $\Delta_{A,B}$ must be the self-adjoint Laplacian on the star graph whose resonance is such that $\alpha_n = a_n$, $\beta_n = b_n$.

Clearly, in the exceptional case $a_n = b_n = 0$ for some n the limit operator on the star graph, *if* it exists, has Dirichlet boundary conditions at the origin in the n-th ray.

4 Limit to the Star Graph: The Non-resonant Case (The Case in Which (3) is Violated)

In this case H_ε has no resonance any longer which may act as a bridge connecting the boundary values at the vertex along different rays: what one expects is that the limit dynamics, if it exists, has Dirichlet boundary conditions at the vertex. This was already indicated in an alternative setting by the analysis performed in [6] (a *dynamical* analysis, unlike the *static* one carried on here, see Remark 4.4. below).

We distinguish two sub-cases.

$$\underline{\text{First case}}: \qquad \lambda_\varepsilon < \mu_-(\Omega_\varepsilon)\,. \tag{13}$$

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.

We can also argue as follows: when (13) holds, the bottom of the spectrum of H_α is zero and the spectral measure is regular around zero, the closest singularity being located at the positive spectral point $\mu_-(\Omega_\varepsilon) - \lambda_\varepsilon$. This holds true uniformly in ε, because of the scaling invariance, and hence *if* $\Pi_\varepsilon(H_\varepsilon - k^2)^{-1}\Pi_\varepsilon^*$ converges as $\varepsilon \to 0$ to the resolvent of a self-adjoint negative Laplacian on the star graph Γ, the limit is precisely that self-adjoint negative Laplacian on Γ with regular spectral measure at the spectral point zero, and this can only be the negative Laplacian with Dirichlet boundary conditions.

$$\underline{\text{Second case}}: \qquad \lambda_\varepsilon > \mu_+(\Omega_\varepsilon)\,. \tag{14}$$

Now the energy threshold for the internal region is low (compared to λ_ε) and the argument above does not apply. This second sub-case is more problematic: in fact, as we shall see in a moment, it even remains unclear to us whether it is too strong to monitor the convergence of H_ε in the resolvent sense (namely, the (weak) limit $\varepsilon \to 0$ of the "squeezed" resolvent $\Pi_\varepsilon(H_\varepsilon - k^2)^{-1}\Pi_\varepsilon^*$): a reasonable limit might only be meaningful in some kind of ultra-weak sense on which we give some indications in the discussion that follows.

In this case too we expect the limit dynamics on the star graph be the Dirichlet one. Correspondingly, we expect that the resolvent $\Pi_\varepsilon(H_\varepsilon - k^2)^{-1}\Pi_\varepsilon^*$ becomes *regular* at $k^2 \to 0$ in the limit $\varepsilon \to 0$, because on the star graph the Dirichlet Laplacian is the only self-adjoint Laplacian whose spectral measure is regular at zero [13, 14]. 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 (13), instead, the resolvent of H_ε is regular at zero 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 resolvent of a second operator $H_\varepsilon + V_\varepsilon$ constructed as follows. We introduce an additional constant potential

$$V_\varepsilon := C\varepsilon^{-2}\mathbb{1}_{\Omega_\varepsilon} \tag{15}$$

supported on Ω_ε ($\mathbb{1}_{\Omega_\varepsilon}$ is the indicator function of Ω_ε). We choose the constant $C > 0$, which is always possible, in such a way 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 coincides precisely 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 quota λ_ε).

The spectrum of the resulting operator $H_\varepsilon + V_\varepsilon$ on $L^2(\Gamma_\varepsilon)$ is the whole $[0, +\infty)$ and by means of a completely analogous discussion to that developed in Sect. 2 we argue that $H_\varepsilon + V_\varepsilon$ 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 to re-write the difference of the resolvents of such two operators in a way that is well suited for taking the limit $\varepsilon \to 0$ and for implementing the existence of a zero-energy resonance. We quickly revise this approach in the remaining part of this section, after the following two remarks.

Remark 4.1. We observe that for explicit computations and estimates it is convenient to replace the actual internal region problem on Ω_ε with an effective internal region problem on the smoother and geometrically simple (e.g., a sphere) enlarged region $\widetilde{\Omega}_\varepsilon$, where the *same* boundary condition α is taken at the bases of the cylinder, and Dirichlet boundary conditions are taken on the remaining part of $\partial\Omega_\varepsilon$. This way H_ε and $H_\varepsilon + V_\varepsilon$ now act on a modified $L^2(\Gamma_\varepsilon)$ where the shape of Γ_ε has been modified around the vertex, still retaining the spectral properties of the original problem.

Remark 4.2. We also remark that the potential is added in the internal region Ω_ε, that is, it makes sense to add it only in the fat graph Γ_ε and this has no counterpart on the graph Γ. In fact, one can prove [7] that adding to a self-adjoint Laplacian in a star graph a potential supported in a ε-neighbourhood of the vertex, and with magnitude blowing up as some inverse power of ε, in general does *not* produce boundary conditions in the limit, in the sense that either the scaling of the potential is too weak, and therefore the potential is ineffective in the limit $\varepsilon \to 0$, or the limit of the resolvent is not the resolvent of a self-adjoint Laplacian with the original or with new boundary conditions at the vertex. 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 $\varepsilon^{-1}\mathbb{1}_{\{|x|\leqslant\varepsilon\}}$ 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 [1].

Let us now complete the argument above for the study of the difference of the resolvents of H_ε and $H_\varepsilon + V_\varepsilon$. As said, we make use of the theory of Birman–Schwinger as developed among others by Krein, Kato, and Kuroda in [11, 12, 15] (for concreteness, we refer to the explicit formulation given in [1], Theorem B.1). This theory describes the difference of the resolvents of two self-adjoint operators $H^{(1)}$ and $H^{(2)}$ acting on a common Hilbert space $\mathcal{H}$ in terms of an operator Ξ_λ as

$$\frac{1}{H^{(2)} - \lambda} - \frac{1}{H^{(1)} - \lambda} = \frac{1}{H^{(1)} - \lambda}\,\Xi_\lambda\,\frac{1}{H^{(1)} - \lambda}\,, \tag{16}$$

where $\lambda \in \mathbb{C}$ is chosen away from the spectrum of both $H^{(2)}$ and $H^{(1)}$. Here it is assumed that $H^{(2)} - H^{(1)} = D_1 D_2$ for some two closed operators D_1 and D_2 that are infinitesimally bounded with respect to $|H^{(1)}|^{1/2}$ and such that $D_1(H^{(1)} - \lambda)^{-1} D_2$ is compact (compactness is actually needed to guarantee that $D_1(H^{(1)} - \lambda)^{-1} D_2$ has discrete spectrum). Also, we make use of the notation $\frac{1}{H-\lambda} \equiv (H - \lambda)^{-1}$ to make the forthcoming formulas more readable.

Remark 4.3. The properties of the operator Ξ_λ were used in [2] in the case

$$H^{(1)} = -\Delta, \qquad H_\varepsilon^{(2)} = H^{(1)} + V_\varepsilon(x), \qquad V_\varepsilon(x) = \varepsilon^{-2} V(x/\varepsilon), \tag{17}$$

where the potential V belongs to the Rollnik class (this is assumed to have the needed compactness, any other condition that implies such a compactness can be assumed as well). There it is proved that $H_\varepsilon^{(2)}$ is convergent in norm resolvent sense as $\varepsilon \to 0$, and the limit is $H^{(1)}$ itself, if $H_\varepsilon^{(2)}$ is non-resonant at energy zero, whereas the resolvent is a rank-one perturbation of the resolvent of $H^{(1)}$, if $H_\varepsilon^{(2)}$ has a zero energy resonance.

We plan to use the same strategy in the present setting, with respect to the operators

$$H_\varepsilon + V_\varepsilon, \qquad V_\varepsilon = \frac{C}{\varepsilon^2} \mathbb{1}_{\Omega_\varepsilon}.$$

Our choice of the potential makes the resolvent formula (16) applicable and the operator Ξ_λ well defined. We set

$$v_\varepsilon := \sqrt{V_\varepsilon} \tag{18}$$

and also

$$G_\varepsilon^{(V_\varepsilon)}(k) := \frac{1}{H_\varepsilon + V_\varepsilon - k^2}. \tag{19}$$

Then (Konno–Kuroda resolvent identity)

$$\frac{1}{H_\varepsilon - k^2} = \frac{1}{H_\varepsilon + V_\varepsilon - k^2} + G_\varepsilon^{(V_\varepsilon)}(k) v_\varepsilon \frac{1}{1 + v_\varepsilon G_\varepsilon^{(V_\varepsilon)}(k) v_\varepsilon} v_\varepsilon G_\varepsilon^{(V_\varepsilon)}(k). \tag{20}$$

Through the reduction map $\Pi_\varepsilon : L^2(\Gamma_\varepsilon) \to L^2(\Gamma)$ the identity above takes the form

$$\begin{aligned} \Pi_\varepsilon \frac{1}{H_\varepsilon - k^2} \Pi_\varepsilon^* = \Pi_\varepsilon \frac{1}{H_\varepsilon + V_\varepsilon - k^2} \Pi_\varepsilon^* + \\ + \Pi_\varepsilon G_\varepsilon^{(V_\varepsilon)}(k) v_\varepsilon \frac{1}{1 + v_\varepsilon G_\varepsilon^{(V_\varepsilon)}(k) v_\varepsilon} v_\varepsilon G_\varepsilon^{(V_\varepsilon)}(k) \Pi_\varepsilon^*. \end{aligned} \tag{21}$$

The R.H.S. of (21), an identity between bounded operators on $L^2(\Gamma)$, shows how the mechanism of "removal of singularity" may occur. The first summand, if it has a limit, is expected to be asymptotically close to $(-\Delta_\alpha - k^2)^{-1}$, the resolvent of the negative self-adjoint Laplacian on the star graph with the vertex boundary condition α induced by the boundary condition α that was taken above at the bases of the cylinders for the internal region problem. The second summand is the one that is sensitive to the presence of a resonance: exploiting the scaling $x \mapsto \varepsilon^{-1}x$, $k^2 \mapsto \varepsilon^2 k^2$, one sees, following the analysis of [2] (see also [1], Lemma 1.2.4, for details), that *because of the fact that* $H_\varepsilon + V_\varepsilon$ *is zero-resonant* this second summand can only have a non-trivial (i.e., non-zero) limit, and this limit has the form of a rank-one operator $C(k)|\eta_k\rangle\langle\overline{\eta_k}|$. The removal of singularity that is expected to occur in the limit is precisely a compensation between these two terms. This is consistent with the analysis of [14], where it is shown that the resolvents of the self-adjoint Laplacians on a star graph are rank-one perturbation of each other.

For example we could make the special choice $\alpha =$ Neumann: that is, we could lift, by addition of a suitable V_ε, the lowest eigenvalue of the modified central region problem with Neumann boundary conditions at the basis of the cylinders (and Dirichlet boundary conditions elsewhere) up to the threshold λ_ε. In the resulting identity (21) the R.H.S. gives rise to the following compensation. The first term converges to the resolvent $(-\Delta_N - k^2)^{-1}$ of the negative Laplacian on the star graph with Neumann vertex condition; the second term converges to an operator of the form

$$C(k)\,\big|G_k^{(\alpha)}(\cdot,0)\big\rangle\big\langle\overline{G_k^{(\alpha)}(0,\cdot)}\big|$$

where $G_k^{(\alpha)}(x_1,\dots,x_n;y_1,\dots,y_N)$ is the integral kernel of $(-\Delta_N - k^2)^{-1}$. Using the explicit form of $C(k)$, it can be deduced from the classification [14] of the resolvents of the self-adjoint Laplacians on the star graph that the latter rank-one operator is precisely the resolvent difference

$$\frac{1}{-\Delta_D - k^2} - \frac{1}{-\Delta_N - k^2}\,,$$

where $-\Delta_D$ is the self-adjoint Laplacian with Dirichlet boundary conditions at the vertex. This way, in the limit $\varepsilon \to 0$ the second summand of (21) produces a term that regularizes the singularity of the resolvent $(-\Delta_N - k^2)^{-1}$ and gives the regular (at the origin) resolvent $(-\Delta_D - k^2)^{-1}$.

Under the conditions for which such limits exist our conclusion is therefore

$$\Pi_\varepsilon \frac{1}{H_\varepsilon - k^2}\Pi_\varepsilon^* \xrightarrow{\ \varepsilon\to 0\ } \frac{1}{-\Delta_D - k^2} \qquad (\mathrm{Im}\,k > 0)\,. \tag{22}$$

The precise sense in which (22) holds true depend on the class of states on which it is meant to be applied to: they have to be states that guarantee that all the above-mentioned approximations are correct in the limit. In fact, we doubt that the convergence (22) can take place in the standard resolvent sense (that is, weakly in the resolvent sense, and hence also strongly, for the limit is the resolvent of a self-adjoint operator). We rather believe that the convergence sense has to be further weakened and we plan to make it precise in a future work.

In this perspective, let us stress that the addition of the central region potential V_ε is only a convenient artifice to produce a zero-energy resonance and to apply the Konno–Kuroda scheme. This scheme has the virtue of producing, in the limit $\varepsilon \to 0$, a removal of singularity in the resolvent $\Pi_\varepsilon(H_\varepsilon - k^2)^{-1}\Pi_\varepsilon^*$ that asymptotically takes the form (in the example above, where α = Neumann)

$$\frac{1}{-\Delta_N - k^2} + \left(\frac{1}{-\Delta_D - k^2} - \frac{1}{-\Delta_N - k^2}\right) = \frac{1}{-\Delta_D - k^2}$$

A convenient choice of the boundary condition α at the bases of the cylinder, as well as a convenient choice of the geometry for the effective central region $\tilde{\Omega}_\varepsilon$ so to carry on explicit computations, are expected to lead to a complete derivation of (22) in some "ultra-weak" sense.

In either case (13) and (14) our conclusion is that, opposed to the resonant case, if in the non-resonant case the limit dynamics exist, then it has to be the free particle dynamics on the star graph with Dirichlet conditions at the vertex.

Remark 4.4. In [6] the problem of finding the limit dynamics of a fat graph was attacked by studying the limit when $\varepsilon \to 0$ of the solutions to the free Schrödinger equation on the fat graph in the subspace corresponding to initial data of uniformly finite energy *supported away from the region* Ω_ε. It was therefore a *dynamical* analysis. It was proved there that these solutions converge when $\varepsilon \to 0$ to solutions to the Schrödinger equation on the graph satisfying Dirichlet boundary conditions at the vertex *if there are no resonances at the bottom of the continuous spectrum.* If there are zero energy resonances, then the convergence is instead to solutions to the Schrödinger equation on the graph satisfying vertex boundary conditions that depend on the resonances. The connection between these boundary conditions and the resonance function was obtained through a suitable use of Green's theorem. In this report we studied the limit by considering instead the resolvents.

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