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QUANTUM-GRAPH VERTEX COUPLINGS: SOME OLD AND NEW APPROXIMATIONS

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Abstract. In 1986 P. Šeba in the classic paper considered one-dimensional pseudo-Hamiltonians containing the first derivative of the Dirac delta function. Although the paper contained some inaccuracy, it was one of the starting points in approximating one-dimension self-adjoint couplings. In the present paper we develop the above results to the case of quantum systems with complex geometry.

Keywords: quantum graph; vertex coupling; singularly scaled potential

MSC 2010: 81Q35, 34L40

1. Introduction

Quantum graphs have attracted a lot of attention both in the physical and mathematical literature since their rediscovery in the end of the last century. One of the reasons for this is that quantum graphs represent natural models for complex systems prepared from semiconductor wires, carbon nanotubes, and photonic crystals. Applications also arise in dynamical systems and probability theory, spectral theory of differential operators on manifolds and in singular domains, in chemistry, for instance, in modeling electron spectra of aromatic molecules. Another reason is that such models provide a tool for studying properties of quantum dynamics in situations when the system has a nontrivial geometrical or topological structure. Among the systems that were successfully modeled by quantum graphs we mention, e.g., electron propagation in multiply connected media and quantum chaos. We refer the reader to the recent monograph [4] for a broad overview and an extensive bibliography.

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One of the fundamental questions in these models concerns the way in which the wave functions are coupled at the graph vertices. If n edges meet at a vertex, in the absence of external fields the requirement of self-adjointness or, in physical terms, probability current conservation leads to the condition $(U-I)\Psi(0)+\mathrm{i}(U+I)\Psi'(0)=0$ coupling the vectors of boundary values of the wave functions and their derivatives, in which U is an $n\times n$ unitary matrix. Different sets of parameters give rise to different dynamics on the graph and the choice of the parameters should be guided by the junctions to which the graph vertices should represent an idealized description. There are at least two natural approaches. On the one hand one may investigate the dynamics of a quantum particle confined to real-world mesoscopic waveguides of small width ε and compare it with the dynamics on the idealized one-dimensional "manifolds" obtained in the limit as ε vanishes. On the other hand we may start from the simplest coupling, often called Kirchhoff, and to investigate how the junction properties are influenced by a potential supported in the vicinity of the vertex, in particular if the support shrinks to a point and the potential is properly scaled. In this paper we will use the second approach due to which it is easy to obtain the so-called δ-coupling using the scaling which preserves the mean value of the potential. To obtain other couplings we need a different limiting procedure, for instance, using shrinking potentials with a more singular scaling of the type $Q(\cdot)\mapsto\varepsilon^{-2}Q(\cdot/\varepsilon)$.

The motivation for the present note was two-fold. First, we intended to review some recent achievements in this area. To be more exact the first aim of this paper is to discuss the asymptotic behaviour as $\varepsilon\to 0$ of the family of Schrödinger operators on the star graph given by

$$\mathscr{A}_\varepsilon := -\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\lambda(\varepsilon)}{\varepsilon^2}Q\Big(\frac{x}{\varepsilon}\Big). \tag{1.1}$$

In Section 2 we present this part without proofs referring for details to our recent papers [8], [14], [15]. We also discuss some historical aspects of the problem.

Our second goal is to study the asymptotic behaviour as $\varepsilon\to 0$ of the rank 1 perturbation of the free Hamiltonian of the form

$$\mathscr{B}_\varepsilon := -\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\mu(\varepsilon)}{\varepsilon^3}\langle\cdot,V_\varepsilon\rangle_\Gamma V_\varepsilon(x).$$

In Section 3 we formulate the problem rigorously and state the results giving rise to new quantum-graph vertex couplings; the proofs and discussion are also given there.

2.1. Metric graphs. We begin with recalling a few basic notions from the theory of differential equations on graphs. A metric graph $G = (V, E)$ is identified with finite sets $V = V(G)$ of vertices and $E = E(G)$ of edges, the latter being isomorphic to (finite or semi-infinite) segments of the real line. A map $\psi\colon G \to \mathbb{C}$ is said to be a function on the graph and its restriction to the edge $e \in E(G)$ will be denoted by ψ_e. Each edge has a natural parametrization; if G is embedded into $\mathbb{R}^3$ it is given by the arc length of the curve representing the edge. A differentiation is always related to this natural length parameter. Vertices are endpoints of the corresponding edges; we denote by $\psi_e'(a)$ the limit value of the derivative at the point $a \in V(G)$ taken conventionally in the outward direction, i.e., away from the vertex. The integral $\int_G \psi\,\mathrm{d}x$ of ψ over G is the sum of integrals over all edges, the measure being the natural Lebesgue measure. Using this notion we can introduce the Hilbert space $L^2(G)$ with the scalar product $\langle\psi_1, \psi_2\rangle_G = \int_G \psi_1\overline{\psi}_2\,\mathrm{d}x$, and furthermore, the Sobolev space $H^2(G)$ on the graph with the norm $\|\psi\|_{H^2(G)} = (\|\psi\|_{L^2(G)} + \|\psi''\|_{L^2(G)})^{1/2}$. Observe that neither the function belonging to $H^2(G)$ nor its derivative need be continuous at the graph vertices. We say that a function ψ satisfies the Kirchhoff conditions at the vertex $a \in V(G)$ if ψ is continuous at this vertex and $\sum_e \psi_e'(a) = 0$ holds, where the sum is taken over all the edges incident in a; in the particular case when there is only one such edge e the Kirchhoff conditions at the "hanging" vertex a reduce to the usual Neumann condition, $\psi_e'(a) = 0$. The symbol $K(G)$ shall denote the set of functions on G obeying the Kirchhoff conditions at each graph vertex.

2.2. Perturbed and limit quantum-graph models. We focus on noncompact star-shaped graphs Γ consisting of 3 semi-infinite edges γ_1, γ_2, and γ_3 connected at a single vertex denoted by a. In that case $E(\Gamma) = \{\gamma_1, \gamma_2, \gamma_3\}$ and without loss of generality we may identify each γ_i with the halfline $[0, \infty)$. Our consideration will need neighborhoods of the vertex; if a_i stands for an arbitrary but fixed point of γ_i, we introduce the compact star graph Ω with vertices $V(\Omega) = \{a\} \cup \{a_i\}_{i=1}^n$. We will use the symbol a_i for both the vertex and its distance from a.

Given a star graph Γ, we introduce the family of Schrödinger operators $\mathscr{A}_\varepsilon$ on $L^2(\Gamma)$ with the domain $\mathfrak{D}(\mathscr{A}_\varepsilon) = H^2(\Gamma) \cap K(\Gamma)$, where the real-valued potential Q is integrable and has a compact support supposed to be the graph Ω constructed above. The function $\lambda(\cdot)$ in the above expression is supposed to be real-valued for real ε and holomorphic in the vicinity of the origin. In addition, it satisfies the condition: $\lambda(\varepsilon) = 1 + \varepsilon\lambda + \mathcal{O}(\varepsilon^2)$ as $\varepsilon \to 0$, where λ is a real number. In this section we will describe the convergence of $\mathscr{A}_\varepsilon$ as $\varepsilon \to 0$ in the norm-resolvent topology.

To state the results, we need one more notion. We shall say that a potential Q admits a zero-energy resonance of order m if there are m linearly independent (resonant) solutions to the Neumann problem

$$-\psi'' + Q\psi = 0 \quad \text{on } \Omega,\ \psi \in K(\Omega). \tag{2.1}$$

If $m > 0$, the construction we are going to present below requires a particular basis in the space of solutions of the problem (2.1).

Lemma 2.1. *Suppose that the problem* (2.1) *has* m $(= 0, 1, 2)$ *linearly independent solutions, then one can choose them as real-valued functions* $\psi_1, \ldots, \psi_m$ *satisfying* $\psi_i(a_j) = \delta_{ij}$ *for* $i, j = 1, \ldots, m$*, where* δ_{ij} *is the Kronecker symbol.*

For notational convenience, we introduce two sets via $\mathfrak{m} := \{1, \ldots, m\}$ and $\mathfrak{n} := \{1, 2, 3\} \setminus \mathfrak{m}$, respectively, adopting the convention that $\mathfrak{m}$ is empty for $m = 0$. To describe the outcome of the limiting process we need the following quantities: $\theta_{ij} := \psi_i(a_j)$ for $i \in \mathfrak{m}$, $j \in \mathfrak{n}$ and $q_{ij} := \int_\Gamma Q\psi_i\psi_j\,\mathrm{d}x$ for $i, j \in \mathfrak{m}$. Using them, we define the limit operator $\mathscr{A}$ as the one acting via $\mathscr{A}\psi := -\psi''$ on functions $\psi \in H^2(\Gamma)$ that obey the matching conditions

$$\begin{aligned} &\psi_j(0) - \sum_{i\in\mathfrak{m}} \theta_{ij}\psi_i(0) = 0, \quad j \in \mathfrak{n},\\ &\psi_i'(0) + \sum_{j\in\mathfrak{n}} \theta_{ij}\psi_j'(0) - \lambda \sum_{j\in\mathfrak{m}} q_{ij}\psi_j(0) = 0, \quad i \in \mathfrak{m}. \end{aligned} \tag{2.2}$$

R e m a r k 2.1. (a) In the generic case the potentials Q from the described class admit no zero-energy resonance, corresponding to Dirichlet decoupled edges, $\psi_j(0) = 0$.

(b) If $m = 1$, then the matching conditions (2.2) contain 4 parameters since $q_{ij} = q_{ji}$, while for $m = 2$ the number of parameters is 6.

(c) If λ is nonzero, the limit operator $\mathscr{A}$ may have a discrete spectrum in $(-\infty, 0)$.

Our first main result says that the Schrödinger operators $\mathscr{A}_\varepsilon$ approach $\mathscr{A}$ as $\varepsilon \to 0$ in the norm-resolvent topology with a particular convergence rate:

Theorem 2.1. $\mathscr{A}_\varepsilon \to \mathscr{A}$ *holds as* $\varepsilon \to 0$ *in the norm resolvent sense, and morever, for any fixed* $\zeta \in \mathbb{C} \setminus \mathbb{R}$ *there is a constant* C *such that*

$$\|(\mathscr{A}_\varepsilon - \zeta)^{-1} - (\mathscr{A} - \zeta)^{-1}\|_{\mathcal{B}(L^2(\Gamma))} \leqslant C\sqrt{\varepsilon}, \quad \varepsilon \in (0, 1].$$

The proof of the theorem is given in [8] for an arbitrary finite number of edges. A particular situation when λ is zero was treated in [15] for the star graphs with

3 edges. In the case $\lambda = 0$ the conditions (2.2) do not couple function values and derivatives, and as a result, the matching conditions of the limit operator are scale-invariant. This means, in particular, that $\mathscr{A}$ has no eigenvalues and $\sigma(H) = [0, \infty)$. Another manifestation of the scale-invariant character is that the scattering matrix, which we discussed in [14], is independent of energy. Observe that if the zero-energy resonance is of order 1, then the scale-invariant matching conditions with $\theta_{12} = \theta_{13} = 1$ lead to the δ-coupling with the parameter $\alpha = 0$, i.e., to the Kirchhoff coupling. For $m = 2$, the scale-invariant matching conditions are a generalization of the standard δ_s'-coupling with the parameter $\beta = 0$. In both the situations the model contains 2 parameters.

2.3. A bit of history. Šeba was seemingly the first to investigate the limit of $\mathscr{A}_\varepsilon$ for vertices connecting two edges, which is equivalent to generalized point interaction on the line [2], with the conclusion that the limit is trivial describing disconnected edges [16]. Recalling that the Schrödinger operators are quantum mechanical Hamiltonians for a particle on the line, one would have to conclude that, in dimension 1, the barrier $\varepsilon^{-2}Q(\cdot/\varepsilon)$ is asymptotically opaque, i.e., that the particle cannot tunnel through it in the limit $\varepsilon \to 0$. Note that the author considered $\lambda(\cdot)$ being constant. Later it was pointed out, however, that such a claim holds only generically and a nontrivial limit may exist when the potential Q has a zero-energy resonance—cf. [7] and subsequent papers of its authors. In [7] the numerical analysis of exactly solvable models of (1.1) with piece-wise constant Q of compact support was performed. Namely, the authors demonstrated that for resonant Q, the limiting value of the transmission coefficient $T_\varepsilon(k)$ of the operator $\mathscr{A}_\varepsilon$ is different from zero; in certain cases, the limit operator was defined via the matching conditions in its domain

$$\psi(+0) = \theta\psi(-0), \quad \theta\psi'(+0) = \psi'(-0). \tag{2.3}$$

The coupling conditions of the form (2.3) also appear in [13] in a realization of the pseudo-Hamiltonian $-\mathrm{d}^2/\mathrm{d}x^2 + \alpha\delta'(x)$ by means of the distribution theory over discontinuous test functions. In the paper [11], eigenvalue and eigenfunction asymptotics as $\varepsilon \to 0$ were studied for the full-line Schrödinger operators given by the differential expression $-\mathrm{d}^2/\mathrm{d}x^2 + \varepsilon^{-2}Q(x/\varepsilon) + q(x)$, where Q is regular and of compact support and q is unbounded at infinity. The eigenfunctions were shown to satisfy in the limit the Dirichlet condition $\psi(0) = 0$ in the non-resonant case and the interface condition (2.3) in a resonant case, thus again exhibiting the zero-energy dichotomy (see also [10] for the convergence of the corresponding Hamiltonians).

One has to stress, however, that the role of zero-energy resonances in the limit was in fact known before; one can find it in the analysis of the behaviour of $\mathscr{A}_\varepsilon$ on the line and its many-dimensional analogues, which has been discussed in literature in connection with the one-dimensional low-energy scattering [5] (see also [1], [6], [12] for discussion of zero-energy resonances and further references). It is also worth mentioning here that the low-energy scattering theory for Schrödinger operators in dimensions one and two is more complicated than in dimension three, which is connected with, respectively, the square root and logarithmic singularities the Green function of the free Hamiltonian then possesses. The above result was further generalized, in particular, to combinations of potentials with different scaling [9], which can be regarded as a realization of $\mathscr{A}_\varepsilon$ with nonconstant coupling function $\lambda(\cdot)$.

3. Vertex couplings obtained from $\mathscr{B}_\varepsilon$

In this section we consider the family of Schrödinger operators

$$\mathscr{B}_\varepsilon := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mu(\varepsilon)}{\varepsilon^3}\langle\cdot, V_\varepsilon\rangle_\Gamma V_\varepsilon(x), \quad \mathfrak{D}(\mathscr{B}_\varepsilon) = H^2(\Gamma)\cap K(\Gamma)$$

with $V_\varepsilon(x) := V(x/\varepsilon)$, where the real-valued potential V belongs to the Faddeev-Marchenko class and has zero mean, i.e., $\int_\Gamma V = 0$. The function $\mu(\cdot)$ in the above expression is real-valued for real ε and holomorphic in the vicinity of the origin, and satisfies the condition $\mu(\varepsilon) = \mu + \varepsilon\mu_1 + \mathcal{O}(\varepsilon^2)$ as $\varepsilon \to 0$, where μ and μ_1 are real numbers. We will investigate convergence of $\mathscr{B}_\varepsilon$ as $\varepsilon \to 0$ and find out which coupling conditions appear in the domain of the corresponding limit operator.

To describe the main result we introduce the quantities $\vartheta_i := \int_0^\infty x_i V(x_i)\,\mathrm{d}x_i$ for $i = 1,2,3$ and $A := \sum_{i=1}^{3}\int_0^\infty\int_0^\infty(|x_i - y_i|/2 - x_i)V(x_i)V(y_i)\,\mathrm{d}x_i\,\mathrm{d}y_i$. We thus define the limit operator $\mathscr{B}$ as the one acting as the negative second derivative on each edge γ_i on functions $\psi \in H^2(\Gamma)$ that obey the matching conditions

$$\frac{\psi_1(0)-\psi_2(0)}{\vartheta_1-\vartheta_2} = \frac{\psi_1(0)-\psi_3(0)}{\vartheta_1-\vartheta_3} = \beta\sum_{i=1}^{3}\vartheta_i\psi_i'(0), \quad \sum_{i=1}^{3}\psi_i'(0) = 0, \tag{3.1}$$

where $\beta = (\mu_1 A^2)^{-1}$ if $\mu = 1/A$, otherwise β is zero, i.e., the limit operator coincides with the Hamiltonian of the free particle $\mathscr{H}$. We start with the description of the Green function for the limit operator and then we will compare it with the one of $\mathscr{B}_\varepsilon$.

Lemma 3.1. *The resolvent of $\mathscr{B}$ is an integral operator with the kernel*

$$\Xi_k(x_i,y_j) = G_k(x_i,y_j) + \Lambda_{ij}(k^2)\mathrm{e}^{\mathrm{i}k(x_i+y_j)}, \quad i,j = 1,2,3, \tag{3.2}$$

with $k^2 \in \varrho(\mathscr{B})$ *and* $\Im k > 0$. *Here*

$$G_k(x_i, y_j) = \frac{\mathrm{i}}{2k}\Big[\delta_{ij}\mathrm{e}^{\mathrm{i}k|x_i-y_j|} + \Big(\frac{2}{3} - \delta_{ij}\Big)\mathrm{e}^{\mathrm{i}k(x_i+y_j)}\Big] \tag{3.3}$$

is the integral kernel of the resolvent of the free Hamiltonian $\mathscr{H}$, *and*

$$\Lambda(k^2) = \frac{\mathrm{i}\beta}{3(3\mathrm{i}+2\beta kd)}\begin{pmatrix} 4n_1+n_2+n_3 & n_3-2(n_1+n_2) & n_2-2(n_1+n_3) \\ n_3-2(n_1+n_2) & n_1+4n_2+n_3 & n_1-2(n_2+n_3) \\ n_2-2(n_1+n_3) & n_1-2(n_2+n_3) & n_1+n_2+4n_3 \end{pmatrix}$$

with $2d := \sum_{1\leqslant i<j\leqslant 3}(\vartheta_i-\vartheta_j)^2$, $n_1 := (\vartheta_1-\vartheta_2)(\vartheta_1-\vartheta_3)$, $n_2 := (\vartheta_2-\vartheta_1)(\vartheta_2-\vartheta_3)$ *and* $n_3 := (\vartheta_1-\vartheta_3)(\vartheta_2-\vartheta_3)$.

P r o o f. By using Krein's formula the sought Green's function is given via (3.2). To find the matrix Λ, we substitute (3.2) into the matching conditions (3.1). $\square$

Theorem 3.1. *As* $\varepsilon \to 0$, *the family of Hamiltonians* $\mathscr{B}_\varepsilon$ *converges to* $\mathscr{B}$ *in the norm-resolvent sense.*

P r o o f. To compare the resolvents of $\mathscr{B}_\varepsilon$ and $\mathscr{B}$, fix $k := \mathrm{i}\varkappa$ belonging to the resolvent sets of both operators; this can be achieved e.g. with $\varkappa > 0$ large enough. We start with the following observation. The resolvent $(\mathscr{B}_\varepsilon + \varkappa^2)^{-1}$ is an integral operator in $L^2(\Gamma)$ which has the kernel of the following form (see [3]):

$$(\mathscr{B}_\varepsilon + \varkappa^2)^{-1}(x_i, y_j) = G_{\mathrm{i}\varkappa}(x_i, y_j) - \zeta_\varepsilon((\mathscr{H}+\varkappa^2)^{-1}V_\varepsilon)(x_i)((\mathscr{H}+\varkappa^2)^{-1}V_\varepsilon)(y_j),$$

with $G_{\mathrm{i}\varkappa}$ of (3.3) and with the constant $\zeta_\varepsilon := (\varepsilon^3/\mu(\varepsilon) + \langle(\mathscr{H}+\varkappa^2)^{-1}V_\varepsilon, V_\varepsilon\rangle_\Gamma)^{-1}$.

Consider first the asymptotic behavior of ζ_ε as ε vanishes. Using the Taylor expansion of $\mathrm{e}^{-\varepsilon\varkappa(x_i+y_i)}$, together with the fact that V has compact support and zero mean, one easily derives the asymptotic formula

$$\langle(\mathscr{H}+\varkappa^2)^{-1}V_\varepsilon, V_\varepsilon\rangle_\Gamma = -A\varepsilon^3 + \varkappa B\varepsilon^4 + \mathcal{O}(\varepsilon^5),$$

where $B = -\frac{2}{3}(\vartheta_1^2+\vartheta_2^2+\vartheta_3^2-\vartheta_1\vartheta_2-\vartheta_1\vartheta_3-\vartheta_2\vartheta_3)$. We thus conclude that

$$\zeta_\varepsilon = \frac{-\beta}{\varepsilon^4(1-\varkappa\beta B)} + \mathcal{O}\Big(\frac{1}{\varepsilon^3}\Big), \quad \varepsilon \to 0.$$

Similar arguments give the following asymptotics of the function $(\mathscr{H}+\varkappa^2)^{-1}V_\varepsilon$:

$$((\mathscr{H}+\varkappa^2)^{-1}V_\varepsilon)(x_i) = -\varepsilon^2\,\mathrm{e}^{-\varkappa x_i}\Big[\sum_{j=1}^{3}\Big(\frac{1}{3}-\delta_{ij}\Big)\vartheta_j + \mathcal{O}(\varepsilon)\Big], \quad \varepsilon \to 0.$$

Combining the above formulas results in

$$(\mathscr{B}_\varepsilon + \varkappa^2)^{-1}(x_i, y_j) = G_{\mathrm{i}\varkappa}(x_i, y_j) + \mathrm{e}^{-\varkappa(x_i+y_j)}(\Lambda_{ij}(-\varkappa^2) + \mathcal{O}(\varepsilon)), \quad \varepsilon \to 0.$$

In view of the above relation, the kernel $(\mathscr{B}_\varepsilon + \varkappa^2)^{-1}(x_i, y_j)$ converges to the kernel $\Xi_{\mathrm{i}\varkappa}(x_i, y_j)$ in $L^2(\Gamma)$, and so the corresponding operators converge in the Hilbert-Schmidt norm. Thus $\{\mathscr{B}_\varepsilon\}_{\varepsilon \geqslant 0}$ approximates $\mathscr{B}$ in the norm-resolvent topology. $\square$

In [16] the author studied the family $\mathscr{B}_\varepsilon$ in dimension one; he proved that in the strong resolvent limit one gets the well-known δ'-coupling: $\psi'(-0) = \psi'(+0)$, $\psi(+0) - \psi(-0) = \beta\psi'(0)$. It was the first attempt to realize the physical meaning of this coupling and its connection with the pseudo-Hamiltonian $-\mathrm{d}^2/\mathrm{d}x^2 + \beta\langle\cdot, \delta'(x)\rangle\delta'(x)$. In the case of graphs two generalizations of this coupling are known: $\psi_1'(0) = \psi_2'(0) = \psi_3'(0)$, $\sum\limits_{i=1}^{3} \psi_i(0) = \beta\psi'(0)$ and $\sum\limits_{i=1}^{3} \psi_i'(0) = 0$, $\psi_i(0) - \psi_j(0) = (\beta/3)(\psi_i'(0) - \psi_j'(0))$ for $i, j = 1, 2, 3$. Using Šeba's approach, we introduce a new (physically motivated) definition of the δ'-coupling on the graph given by (3.1). Interestingly enough, although Šeba proved the strong resolvent convergence, we give the proof of the norm resolvent one, which is more suitable from the viewpoint of the quantum-mechanical approximations.

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