APPROXIMATION OF QUANTUM GRAPH VERTEX COUPLINGS BY SCALED SCHRÖDINGER OPERATORS ON THIN BRANCHED MANIFOLDS

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Abstract. We discuss approximations of vertex couplings of quantum graphs using families of thin branched manifolds. We show that if a Neumann type Laplacian on such manifolds is amended by suitable potentials, the resulting Schrödinger operators can approximate non-trivial vertex couplings. The latter include not only the δ-couplings but also those with wavefunctions discontinuous at the vertex. We work out the example of the symmetric δ'-couplings and make a conjecture that the same method can be applied to all couplings invariant with respect to the time reversal. We conclude with a result that certain vertex couplings cannot be approximated by a pure Laplacian.

ec:intro

1. Introduction

The quantum graph models represent a simple and versatile tool to study numerous physical phenomena. The current state of art in this field is described in the recent proceedings volume [EKK+08] to which we refer for an extensive bibliography.

One of the big questions in this area is the physical meaning of quantum graph vertex coupling. The general requirement of self-adjointness admits boundary conditions containing a number of parameters, and one would like to understand how to choose these when a quantum graph model is applied to a specific physical situation. One natural idea is to approximate the graph in question by a family of "fat graphs", i.e. tube-like manifolds built around the graph "skeleton", equipped with a suitable second-order differential operator. Such systems have no ad hoc parameters and one can try to find what vertex couplings arise when the manifold is squeezed to the graph.

The question is by no means easy and the answer depends on the type of the operator chosen. If it is the Laplacian with Dirichlet boundary conditions one has to employ an energy renormalisation because the spectral threshold given by the lowest transverse eigenvalue blows up to infinity as the tube diameter tends to zero. If one chooses the reference point between the thresholds, the limiting boundary conditions are determined by the scattering on the respective "fat star" manifold [MV07]. If, on the other hand, the threshold energy is subtracted, the limit gives generically a decoupled graph, i.e. the family of edges with Dirichlet conditions at their endpoints [P05, MV07, DT06]. One can nevertheless get a non-trivial coupling in the limit if the tube network exhibits a threshold resonance [G08, ACF07], and moreover, using a more involved limiting process one can get also boundary conditions with richer spectral properties [CE07].

The case when the fat graph supports a Laplacian of Neumann type is better understood and the limit of all types of spectra as well as of resonances has been worked out [FW93, RS01, KuZ01, EP05, EP07, G08, EP08]. Moreover, convergence of resolvents etc. has been shown in [Sai00, P06, EP07]. Of course, no energy renormalisation is needed in this case. On the other hand, the limit yields only the simplest boundary conditions called free or Kirchhoff.

The aim of this paper is to show that one can do better in the Neumann case if the Laplacian is replaced by suitable families of Schrödinger operators with properly scaled

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potentials. Such approximations have been shown to work on graphs themselves [E96, ENZ01], the main idea here is to "lift" them to the tube-like manifolds.[1] First we will show that using potentials supported by the vertex regions of the manifold with the "natural" scaling, as ε^{-1} where ε is the tube radius parameter, we can get the so-called δ-coupling, the one-parameter family with the wavefunctions continuous everywhere, including at the vertex. Note that this suggests, in particular, that one cannot achieve such an approximation in a purely geometric way, with a curvature-induced potential of the type [DEK01], because the latter scales typically as ε^{-2}; we will say more on that in the concluding remarks. As main result in this case, we show the convergence of the spectra and the resolvents as the network branch widths shrink to zero. (cf. Theorems 3.3–3.7).

On the other hand, the δ-coupling is only a small part in the set of all admissible couplings; in a vertex joining n edges the boundary conditions contain n^2 parameters. Here we use the seminal idea of Cheon and Shigehara [CS98] applied to the graph case in [CE04] and generalised in [ET06, ET07]. For the sake of simplicity we are going to work out in this paper only the example of the so-called symmetric δ'-coupling, in short δ'_{s}, a one-parameter family which is a counterpart of δ, by using the result of [CE04] and "lifting" it to the manifold. We show that such a coupling is approximated with a potential in the vertex region together with potentials at the edges with compact supports approaching the vertex, all properly scaled, cf. Theorem 4.7. The speed with which the potentials are "coming together" must be slower than that of the squeezing. In particular, the approximating potentials have distances of order ε^α with $0 < \alpha < 1/13$, whereas the tube radius parameter is of order ε. The rate between the two we obtain is surely not optimal.

We are convinced that in the same way one can lift to the manifolds the more general limiting procedures devised in [ET07] which gives rise to a $\binom{n+1}{2}$-parameter family of boundary conditions, namely those which are invariant with respect to the time reversal. We refrain from working such a more general result, however, because such an extension would require a voluminous work of algebraic nature. In order not to burden this paper with a complicated notation and bulky calculations, we state the claim as a conjecture here with the intention to present the appropriate proofs in a later work.

Let us survey the contents of the paper. In the next section we define the graph and manifold models and provide necessary estimates. In Section 3 we prove the convergence in the δ-coupling case. For the sake of clarity we analyse first in detail the star-shaped graphs with a single vertex. The main result here is Theorem 3.4 which states the rate of resolvent convergence with an appropriate identification operator. As its corollaries we get in Theorems 3.5–3.6 convergence of different spectral components. Furthermore, the approximation bears a local character which allows us to extend the result to more complex graphs; the corresponding general result about graphs with δ-couplings is stated in Theorem 3.7. In Section 4 we turn to the δ'_{s}-coupling case; for simplicity we restrict ourselves to star graphs with a single vertex. The main result is again the resolvent convergence which is stated in Theorem 4.7. We conclude the paper with a short section in which we formulate the conjecture about the general case and discuss the approximations from both the mathematical and physical points of view.

2. The graph and manifold models

2.1. **Graph model.** Let us start with a star-shaped metric graph G having only one vertex v and $\deg v$ adjacent edges $e \in E$ of lengths $\ell_e \in (0, \infty]$, so we can think of $E = \{1, \dots, \deg v\}$. We identify the (metric) edge e with the interval $I_e := (0, \ell_e)$

[1]This is not the only possibility, another approach to approximation of non-trivial vertex conditions was proposed recently in [Pa07b, Pa07a].

oriented in such a way that 0 corresponds to the vertex v. Moreover, the metric graph G is given by the abstract space $G := \dot\bigcup_e \overline{I}_e/\sim$ where $\dot\cup$ denotes the disjoint union, and where the equivalence relation $\sim$ identifies the points $0 \in \overline{I}_e$ with the vertex v. The basic Hilbert space is $\mathsf{L}_2(G) := \bigoplus_{e\in E} \mathsf{L}_2(I_e)$ with norm given by

$$\|f\|^2 = \|f\|_G^2 = \sum_{e\in E} \int_0^{\ell_e} |f(s)|^2 \,\mathrm{d}s.$$

The decoupled Sobolev space of order k is defined as

$$\mathsf{H}^k_{\max}(G) := \bigoplus_{e\in E} \mathsf{H}^k(I_e)$$

together with its natural norm. Let $\underline{p} = \{p_e\}_e$ be a vector consisting of the weights $p_e > 0$ for $e \in E$. The Sobolev space associated to the weight $\underline{p}$ is given by

$$\mathsf{H}^1_{\underline{p}}(G) := \{\, f \in \mathsf{H}^1_{\max}(G) \,|\, \underline{f}(v) \in \mathbb{C}\underline{p} \,\}, \tag{2.1}$$ eq:sob1

where $\underline{f}(v) := \{f_e(0)\}_e \in \mathbb{C}^{\deg v}$ is the evaluation vector of f at the vertex v and $\mathbb{C}\underline{p}$ is the complex span of $\underline{p}$. We use the notation

$$\underline{f}(v) = f(v)\underline{p}, \qquad \text{i.e.,} \qquad f_e(0) = f(v)p_e \tag{2.2}$$ eq:eval.f

for all $e \in E$. In particular, if $\underline{p} = (1, \dots, 1)$, we arrive at the *continuous* Sobolev space $\mathsf{H}^1(G) := \mathsf{H}^1_{\underline{p}}(G)$. The standard Sobolev trace estimate

$$|g(0)|^2 \le a\|g'\|^2_{(0,\ell)} + \frac{2}{a}\|g\|^2_{(0,\ell)} \tag{2.3}$$ eq:sob.tr

for $g \in \mathsf{H}^1(0,\ell)$ and $0 < a \le \ell$ ensures that $\mathsf{H}^1_{\underline{p}}(G)$ is a closed subspace of $\mathsf{H}^1_{\max}(G)$, and therefore itself a Hilbert space. A simple consequence is the following claim.

m:sob.tr **Lemma 2.1.** *We have*

$$|f(v)|^2 \le |\underline{p}|^{-2}\Big(a\|f'\|_G^2 + \frac{2}{a}\|f\|_G^2\Big)$$

for $f \in \mathsf{H}^1_{\underline{p}}(G)$ and $0 < a \le \ell_0 := \min_{e\in E}\{\ell_e, 1\}$.

We define various Laplacians on the metric graph via their quadratic forms. Let us start with the (weighted) *free* Laplacian Δ_G defined via the quadratic form $\mathfrak{d} = \mathfrak{d}_G$ given by

$$\mathfrak{d}(f) := \|f'\|_G^2 = \sum_e \|f_e'\|^2_{I_e} \qquad \text{and} \qquad \operatorname{dom}\mathfrak{d} := \mathsf{H}^1_{\underline{p}}(G)$$

for a fixed $\underline{p}$ (the forms and the corresponding operators should be labelled by the weight $\underline{p}$, of course, but we drop the index, in particular, because we are most interested in the case $\underline{p} = (1, \dots, 1)$). Note that $\mathfrak{d}$ is a closed form since the norm associated to the quadratic form $\mathfrak{d}$ is precisely the Sobolev norm given by $\|f\|^2_{\mathsf{H}^1(G)} = \|f'\|_G^2 + \|f\|_G^2$.

The Laplacian with *δ-coupling of strength q* is defined via the quadratic form $\mathfrak{h} = \mathfrak{h}_{(G,q)}$ given by

$$\mathfrak{h}(f) := \|f'\|_G^2 + q(v)|f(v)|^2 \qquad \text{and} \qquad \operatorname{dom}\mathfrak{h} := \mathsf{H}^1_{\underline{p}}(G). \tag{2.4}$$ eq:def.qf.del

The δ-coupling is a "small" perturbation of the free Laplacian, namely we have:

lta.pert **Lemma 2.2.** *The form $\mathfrak{h}_{(G,q)}$ is relatively form-bounded with respect to the free form $\mathfrak{d}_G$ with relative bound zero, i.e., for any $\eta > 0$ there exists $C_\eta > 0$ such that*

$$|\mathfrak{h}(f) - \mathfrak{d}(f)| = |q(v)||f(v)|^2 \le \eta\,\mathfrak{d}(f) + C_\eta\|f\|_G^2.$$

Proof. It is again a simple consequence of Lemma 2.1. Since we need the precise behaviour of the constant C_η, we give a short proof here. From Lemma 2.1 we conclude that

$$|\mathfrak{h}(f) - \mathfrak{d}(f)| \le |q(v)| |\underline{p}|^{-2} \Big(a\mathfrak{d}(f) + \frac{2}{a} \|f\|_G^2 \Big).$$

for any $0 < a \le \ell_0$. Set $a := \min\{\eta |\underline{p}|^2 / |q(v)|, \ell_0\}$ and

$$C_\eta := 2 \max\Big\{ \frac{|q(v)|^2}{\eta |\underline{p}|^4}, \frac{|q(v)|}{\ell_0 |\underline{p}|^2} \Big\},$$

then the desired estimate follows. □

One can see that the norms associated to $\mathfrak{h}$ and $\mathfrak{d}$ are equivalent and, in particular, setting $\eta = 1/2$ in the above estimate yields:

or:delta.pert **Corollary 2.3.** *The quadratic form $\mathfrak{h}$ is closed and obeys the estimate*

$$\mathfrak{d}(f) \le 2(\mathfrak{h}(f) + C_{1/2} \|f\|_G^2).$$

The operator $H = H_{(G,q)}$ associated to $\mathfrak{h}$ acts as $(Hf)_e = -f_e''$ on each edge and a function f in its domain satisfies the conditions

$$\frac{f_{e_1}(0)}{p_{e_1}} = \frac{f_{e_2}(0)}{p_{e_2}} =: f(v) \qquad \text{and} \qquad \sum_e p_e f_e'(0) = q(v) f(v) \tag{2.5}$$ eq:vx.cc

for any pair (e_1, e_2) of edges meeting at the vertex v. We use the formal notation

$$H = H_{(G,q)} = \Delta_G + q(v)\delta_v. \tag{2.6}$$ eq:delta

Note that the free operator Δ_G, i.e., the operator with vanishing δ-coupling $q = 0$, is non-negative by definition and satisfies the so-called weighted *free* or *Kirchhoff* vertex conditions.

In order to compare the "free" quadratic form with the graph norm of H we need the following estimate:

lem:res.est **Lemma 2.4.** *We have*

$$\|f\|_{\mathsf{H}^1(G)}^2 = \mathfrak{d}(f) + \|f\|_G^2 \le 2 \max\{C_{1/2}, \sqrt{2}\} \|(H \mp \mathrm{i}) f\|_G^2$$

for $f \in \operatorname{dom} H \subset \operatorname{dom} \mathfrak{h} = \mathsf{H}^1_{\underline{p}}(G)$.

Proof. Using the estimate of Corollary 2.3, we obtain

$$\mathfrak{d}(f) + \|f\|^2 \le 2\big(\mathfrak{h}(f) + (C_{1/2} + 1)\|f\|^2\big) \le 2\big|\mathfrak{h}(f) + \|f\|^2\big| + 2C_{1/2}\|f\|^2.$$

Moreover, the first term can be estimated as

$$\begin{aligned} \big|\mathfrak{h}(f) + \|f\|^2\big|^2 \le 2\big(\mathfrak{h}(f)^2 + \|f\|^4\big) &= 2\big|\mathfrak{h}(f) - \mathrm{i}\|f\|^2\big| \big|\mathfrak{h}(f) + \mathrm{i}\|f\|^2\big| \\ &= 2\big|\langle f, (H \mp \mathrm{i}) f\rangle\big|^2 \le 2\|f\|^2 \|(H \mp \mathrm{i}) f\|^2. \end{aligned}$$

Finally, we apply the estimate $\|f\| \le \|(H \mp \mathrm{i}) f\|$ to obtain the result. □

Remark 2.5. Note that we have not said anything about the boundary conditions at the free ends of the edges of finite length if there are any. As we employ the Sobolev space $\mathsf{H}^1_{\underline{p}}(G)$ for the domain, we implicitly introduce Neumann conditions for the operator, $f_e'(\ell_e) = 0$. However, one can choose any other condition at the free ends, or to construct more complicated graphs by putting the star graphs together.

sec:mfd

2.2. **Manifold model of the "fat" graph.** Let us now define the other element of the approximation we are going to construct. For a given $\varepsilon \in (0, \varepsilon_0]$ we associate a connected d-dimensional manifold X_ε to the star graph G in the following way. To the edge $e \in E$ and the vertex v we ascribe the Riemannian manifolds

$$X_{\varepsilon,e} := I_e \times \varepsilon Y_e \qquad \text{and} \qquad X_{\varepsilon,v} := \varepsilon X_v, \tag{2.7}$$ eq:mfd.ed

respectively, where εY_e is a manifold Y_e (called *transverse manifold)* equipped with the metric $h_{\varepsilon,e} := \varepsilon^2 h_e$ (see Figure 1). More precisely, the so-called *edge neighbourhood* $X_{\varepsilon,e}$ and the *vertex neighbourhood* $\varepsilon X_{\varepsilon,v}$ carry the metrics $g_{\varepsilon,e} = \mathrm{d}^2 s + \varepsilon^2 h_e$ and $g_{\varepsilon,v} = \varepsilon^2 g_v$, where h_e and g_v are ε-independent metrics on Y_e and X_v, respectively. Omitting the scaling parameter ε in the notation conventionally means $\varepsilon = 1$, i.e., we denote by $X_e = X_{\varepsilon,e}$, $X_v = X_{\varepsilon,v}$, $Y_e = \varepsilon Y_e$ etc. the Riemannian manifolds with $\varepsilon = 1$ in the metric. For convenience, we will always use the ε-independent coordinates $(s,y) \in X_e = I_e \times Y_e$ and $x \in X_v$, so that the radius-type parameter ε only enters via the Riemannian metrics. Without loss of generality, we may assume that each cross-section Y_e is connected, otherwise we replace the edge e by as many edges as is the number of connected components.

We assume that for each edge e, the vertex neighbourhood $X_{\varepsilon,v}$ has a boundary component denoted by $\partial_e X_{\varepsilon,v}$. Note that $\partial_e X_{\varepsilon,v} = \varepsilon \partial_e X_v$ is *isometric* to the scaled transverse manifold εY_e. Fixing such an isometry and assuming that $X_{\varepsilon,v}$ has product structure (drawn in light grey in Figure 1) near each of the boundary components $\partial_e X_{\varepsilon,v}$, we identify the boundary component $\partial_v X_{\varepsilon,e} = \{0\} \times \varepsilon Y_e$ of the edge neighbourhood $X_{\varepsilon,e}$ with $\partial_e X_{\varepsilon,v}$. In this way, we obtain a smooth Riemannian manifold X_ε from the components

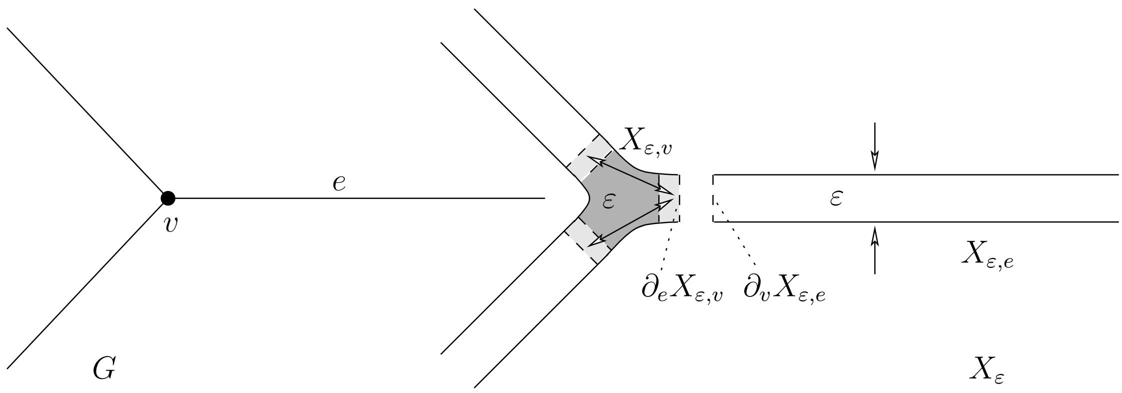

FIGURE 1. A star graph G with three edges and the associated manifold model X_ε with transversal manifolds Y_e being intervals. The vertex neighbourhood is drawn dark and light grey. The light grey regions have product structure, and for each edge, we identify the boundary component $\partial_e X_{\varepsilon,v}$ with $\partial_v X_{\varepsilon,e} = \{0\} \times \varepsilon Y_e$. fig:pot-appro

$X_{\varepsilon,e}$ ($e \in E$) and $X_{\varepsilon,v}$. Roughly speaking, the manifold X_ε consists of the number $\deg v$ of straight cylinders[2] with cross-section εY_e of radius ε attached to the central manifold $X_{\varepsilon,v} = \varepsilon X_v$.

The entire manifold X_ε may or may not have a boundary ∂X_ε, depending on whether there is at least one finite edge length $\ell_e < \infty$ or one transverse manifold Y_e has a non-empty boundary. In such a situation, we assume that $X_\varepsilon = \mathring{X}_\varepsilon \cup \partial X_\varepsilon$, i.e., $\partial X_\varepsilon \subset X_\varepsilon$. A particular case is represented by embedded manifolds which deserve a comment:

[2]The straightness here refers to the intrinsic geometry only. We do not assume in general that the manifolds X_ε are embedded, for instance, into a Euclidean space, see also Remark 2.6.

rem:long.err *Remark* 2.6. Note that the above setting contains the case of the ε-neighbourhood of an embedded graph $G \subset \mathbb{R}^2$, but only up to a longitudinal error of order of ε. The manifold X_ε itself does *not* form an ε-neighbourhood of a metric graph embedded in some ambient space, since the vertex neighbourhoods cannot be fixed in the ambient space unless one allows slightly shortened edge neighbourhoods. Nevertheless, introducing ε-independent coordinates also in the longitudinal direction simplifies the comparison of the Laplacian on the metric graph and the manifold, and the error made is of order $\mathrm{O}(\varepsilon)$, as we will see in Lemma 2.7 for a single edge.

The basic Hilbert space of the manifold model is

$$\mathsf{L}_2(X_\varepsilon) = \bigoplus_e \big(\mathsf{L}_2(I_e) \otimes \mathsf{L}_2(\varepsilon Y_e)\big) \oplus \mathsf{L}_2(\varepsilon X_v) \tag{2.8}$$ eq:lsqr.

with the norm given by

$$\|u\|^2_{X_\varepsilon} = \sum_{e\in E} \varepsilon^{d-1} \int_{X_e} |u|^2 \, \mathrm{d}y_e \, \mathrm{d}s + \varepsilon^d \int_{X_v} |u|^2 \, \mathrm{d}x_v,$$

where $\mathrm{d}x_e = \mathrm{d}y_e \, \mathrm{d}s$ and $\mathrm{d}x_v$ denote the Riemannian volume measures associated to the (unscaled) manifolds $X_e = I_e \times Y_e$ and X_v, respectively. In the last formula we have employed the appropriate scaling behaviour, $\mathrm{d}x_{\varepsilon,e} = \varepsilon^{d-1}\, \mathrm{d}y_e \, \mathrm{d}s$ and $\mathrm{d}x_{\varepsilon,v} = \varepsilon^d \, \mathrm{d}x_v$.

Denote by $\mathsf{H}^1(X_\varepsilon)$ the Sobolev space of order one, the completion of the space of smooth functions with compact support under the norm given by $\|u\|^2_{\mathsf{H}^1(X_\varepsilon)} = \|\mathrm{d}u\|^2_{X_\varepsilon} + \|u\|^2_{X_\varepsilon}$. As in the case of the metric graphs, we define the Laplacian Δ_{X_ε} on X_ε via its quadratic form

$$\mathfrak{d}_\varepsilon(u) := \|\mathrm{d}u\|^2_{X_\varepsilon} = \sum_{e\in E} \varepsilon^{d-1} \int_{X_e} \Big(|u'(s,y)|^2 + \frac{1}{\varepsilon^2} |\mathrm{d}_{Y_e} u|^2_{h_e} \Big) \, \mathrm{d}y_e \, \mathrm{d}s + \varepsilon^{d-2} \int_{X_v} |\,\mathrm{d}u|^2_{g_v} \, \mathrm{d}x_v, \tag{2.9}$$ eq:h.eps

where u' denotes the *longitudinal* derivative, $u' = \partial_s u$, and $\mathrm{d}u$ is the exterior derivative of u. As before, the form $\mathfrak{d}_\varepsilon$ is closed by definition. Adding a potential, we define the Hamiltonian H_ε as the operator associated with the form $\mathfrak{h}_\varepsilon = \mathfrak{h}_{(X_\varepsilon, Q_\varepsilon)}$ given by

$$\mathfrak{h}_\varepsilon = \|\mathrm{d}u\|^2_{X_\varepsilon} + \langle u, Q_\varepsilon u \rangle_{X_\varepsilon},$$

where the potential Q_ε has support only in the (unscaled) vertex neighbourhood X_v and

$$Q_\varepsilon(x) = \frac{1}{\varepsilon} Q(x), \tag{2.10}$$ eq:pot.e

where $Q = Q_1$ is a fixed bounded and measurable function on X_v. The reason for this particular scaling will become clear in the proof of Proposition 3.2. Roughly speaking, it comes from the fact that $\operatorname{vol} X_{\varepsilon,v}$ is of order ε^d, whereas the $(d–1)$-dimensional transverse volume $\operatorname{vol} Y_{\varepsilon,e}$ is of order ε^{d-1}. The operators H_ε and Δ_ε are associated to forms $\mathfrak{h}_\varepsilon$ and $\mathfrak{d}_\varepsilon$, respectively; note that $\Delta_\varepsilon = \Delta_{X_\varepsilon} \geq 0$ is the usual (Neumann) Laplacian on X_ε. As usual the Neumann boundary condition occurs only in the operator domain if $\partial X_\varepsilon \neq \emptyset$. We postpone for a moment the check that H_ε is relatively form-bounded with respect to Δ_{X_ε}, see Lemma 2.10 below.

Let us compare the two cylindrical neighbourhoods, $X_{\varepsilon,e} = I \times \varepsilon Y_e$ and $\widetilde{X}_{\varepsilon,e} = I_\varepsilon \times \varepsilon Y_e$, on edges of length $\ell > 0$ and $\ell_\varepsilon = (1-\varepsilon)\ell$, respectively. The result for the entire space X_ε then follows by combining the estimates on the edges and the fact that the potential is only supported on the vertex neighbourhoods. The verification of the δ_ε-quasi-unitary equivalence in the next lemma is straightforward; for a proof we refer to [P09, Prop. 5.3.10].[3]

[3] Note that we used a slightly different notation in [P06, App.], where *δ-quasi unitary equivalence* was called *δ-closeness*.

long.err **Lemma 2.7.** *Let* $\mathscr{H}_e := \mathsf{L}_2(X_{\varepsilon,e})$ *and* $\widetilde{\mathscr{H}_e} := \mathsf{L}_2(\widetilde{X}_{\varepsilon,e})$*. Moreover, define*

$$J_e \colon \mathscr{H}_e \longrightarrow \widetilde{\mathscr{H}_e} \qquad (J_e f)(\widetilde{s}, y) := f((1-\varepsilon)^{-1}\widetilde{s}, y),$$

$$J_e' \colon \widetilde{\mathscr{H}_e} \longrightarrow \mathscr{H}_e \qquad (J_e' u)(s, y) := u((1-\varepsilon)s, y).$$

Then the quadratic forms $\mathfrak{d}_\varepsilon(f) := \|f\|^2_{X_{\varepsilon,e}}$ *and* $\widetilde{\mathfrak{d}}_\varepsilon(u) := \|u\|^2_{\widetilde{X}_{\varepsilon,e}}$ *with* $\operatorname{dom}\mathfrak{d}_\varepsilon = \mathsf{H}^1(X_{\varepsilon,e})$ *and* $\operatorname{dom}\widetilde{\mathfrak{d}}_\varepsilon = \mathsf{H}^1(\widetilde{X}_{\varepsilon,e})$ *are* δ_ε*-quasi-unitarily equivalent with* $\delta_\varepsilon = 2\varepsilon/(1-\varepsilon)^{1/2}$*; namely, we have* $J_e'J_e = \mathrm{id}$*,* $J_eJ_e' = \mathrm{id}$*,* $\|J_e\| \le 1$*,* $\|J_e'\| \le 1 + \delta_\varepsilon$*,*

$$\|J_e' - J_e^*\| \le \delta_\varepsilon \qquad \text{and} \qquad \bigl|\widetilde{\mathfrak{d}}_\varepsilon(J_e f, u) - \mathfrak{d}_\varepsilon(f, J_e' u)\bigr| \le \delta_\varepsilon \|f\|_{\mathsf{H}^1(G)} \|u\|_{\mathsf{H}^1(X_\varepsilon)}.$$

In particular, we get

$$\|(\Delta_{\widetilde{X}_{\varepsilon,e}} + 1)^{-1} - J_e(\Delta_{X_{\varepsilon,e}} + 1)^{-1} J_e'\| \le 2\delta_\varepsilon = \mathrm{O}(\varepsilon).$$

For the verification of the quasi-unitary equivalence of the graph and manifold Hamiltonian in the next section, we need some more notation and estimates. The estimates are already provided in [EP05, P06], but we will also need a precise control of the edge length, when we approximate the δ_{s}'-coupling by δ-couplings in Section 4 below. Therefore, we present short proofs of the estimate here.

We first introduce the following averaging operators

$$\textstyle\fint_v u := \displaystyle\fint_{X_v} u \,\mathrm{d}x_v \qquad \text{and} \qquad \textstyle\fint_e u(s) := \displaystyle\fint_{Y_e} u(s, \cdot) \,\mathrm{d}y_e$$

for $u \in \mathsf{L}_2(X_\varepsilon)$, where

$$\fint_M u \,\mathrm{d}x := \frac{1}{\operatorname{vol} M} \int_M u \,\mathrm{d}x$$

denotes the *normalised* integral for $u \in \mathsf{L}_2(M)$ on the manifold M (for the existence of the trace $u(s, \cdot) \in \mathsf{L}_2(Y_e)$ for *all* $s \in I_e$, one needs an estimate similar to (2.12)).

In order to obtain the below Sobolev trace estimate below, we need a further decomposition of the vertex neighbourhood X_v. Recall that X_v has $(\deg v)$-many boundary components isometric to Y_e. We assume that each such boundary component has a collar neighbourhood $X_{v,e} = (0, \ell_e) \times Y_e$ of length ℓ_e. Note that the scaled vertex neighbourhood $X_{\varepsilon,v} = \varepsilon X_v$ is of order ε in *all* directions, so that the scaled collar neighbourhoods $X_{\varepsilon,v,e} := \varepsilon X_{v,e}$ are of length $\varepsilon\ell_e$. We can always assume that such a decomposition exists, by possibly using a different cut of the manifold X into X_v and X_e, the price being an additional longitudinal error of order ε (see Lemma 2.7). Similarly as in (2.3), one can get the following Sobolev trace estimates for the scaled manifolds:

$$\|u\|^2_{\partial_e X_{\varepsilon,v}} \le \varepsilon\widetilde{a}\|\mathrm{d}u\|^2_{X_{\varepsilon,v,e}} + \frac{2}{\varepsilon\widetilde{a}}\|u\|^2_{X_{\varepsilon,v,e}} \tag{2.11}$$ eq:sob.tr1

$$\|u\|^2_{\partial_v X_{\varepsilon,e}} \le a\|u'\|^2_{X_{\varepsilon,e}} + \frac{2}{a}\|u\|^2_{X_{\varepsilon,e}} \tag{2.12}$$ eq:sob.tr2

for $0 < a, \widetilde{a} \le \ell_e$ on the vertex and edge neighbourhood, respectively, where $u' = \partial_s u$ denotes the longitudinal derivative. The unscaled versions are obtained, of course, by setting $\varepsilon = 1$. Moreover, by the Cauchy-Schwarz inequality we get

$$\operatorname{vol} Y_e \bigl|\textstyle\fint_e u(0)\bigr|^2 \le \|u\|^2_{\partial_e X_v} = \|u\|^2_{\partial_v X_e}.$$

In the following lemma we compare the averaging over the boundary of X_v with the averaging over the whole space X_v:

m:av.int **Lemma 2.8.** *For* $u \in \mathsf{H}^1(X_v)$*, we have*

$$\operatorname{vol}\partial X_v \bigl|\textstyle\fint_{\partial X_v} u - \fint_v u\bigr|^2 \le \displaystyle\sum_{e \in E} \operatorname{vol}\partial_e X_v \bigl|\textstyle\fint_{\partial_e X_v} u - \fint_v u\bigr|^2 \le \Bigl(1 + \dfrac{2}{\ell_0 \lambda_2(v)}\Bigr)\|\mathrm{d}u\|^2_{X_v},$$

where $\ell_0 = \min_e\{\ell_e, 1\}$*, and where* $\lambda_2(v)$ *denotes the second (i.e., first non-zero) eigenvalue of the Neumann Laplacian on* X_v*; the latter is defined conventionally as the operator associated to the form* $\mathfrak{d}_v(u) := \|\mathrm{d}u\|^2_{X_v}$ *with the domain* $\operatorname{dom}\mathfrak{d}_v := \mathsf{H}^1(X_v)$*.*

Proof. Using the Cauchy-Schwarz inequality and the estimate (2.11) for each edge e with $\varepsilon = 1$ and $\widetilde{a} = \ell_0$, we obtain

$$\operatorname{vol}\partial X_v \big|\textstyle\fint_{\partial X_v} w\big|^2 = \displaystyle\sum_e \operatorname{vol}\partial_e X_v \big|\textstyle\fint_{\partial_e X_v} w\big|^2 \le \|w\|^2_{\partial X_v} \le \|\mathrm{d}w\|^2_{X_v} + \frac{2}{\ell_0}\|w\|^2_{X_v}. \tag{2.13}$$ eq:sob.t

We apply the above estimate to the function $w = P_v u := u - \fint_v u$ and observe that

$$\|w\|^2_{X_v} \le \frac{1}{\lambda_2(v)}\|\mathrm{d}w\|^2_{X_v} \tag{2.14}$$ eq:min-m

as one can check using the fact that $\mathrm{d}w = \mathrm{d}u$ and that P_v is the projection onto the orthogonal complement of the first eigenfunction $\mathbb{1}_v \in \mathsf{L}_2(X_v)$. □

We also need an estimate over the vertex neighbourhood. It will assure that in the limit $\varepsilon \to 0$, no family of normalised eigenfunctions $(u_\varepsilon)_\varepsilon$ with eigenvalues lying in a bounded interval can concentrate on $X_{\varepsilon,v}$.

lem:vx.est **Lemma 2.9.** *We have*

$$\|u\|^2_{X_{\varepsilon,v}} \le \varepsilon^2 C(v)\|\mathrm{d}u\|^2_{X_{\varepsilon,v}} + 4\varepsilon c_{\mathrm{vol}}\Big[a\|u'\|^2_{X_{\varepsilon,E}} + \frac{2}{a}\|u\|^2_{X_{\varepsilon,E}}\Big]$$

for $0 < a \le \ell_0 = \min_e\{\ell_e, 1\}$*, where* $C(v) := C(v,\ell_0) = 4\big[\frac{1}{\lambda_2(v)} + c_{\mathrm{vol}}\big(1 + \frac{2}{\ell_0\lambda_2(v)}\big)\big]$*,* $c_{\mathrm{vol}} := \operatorname{vol}X_v/\operatorname{vol}\partial X_v$ *and* $X_{\varepsilon,E} := \bigcup_e X_{\varepsilon,e}$ *denotes the union of all edge neighbourhoods.*

Proof. We start with the estimate

$$\|u\|^2_{X_{\varepsilon,v}} \le 2\varepsilon^d\Big(\big\|u - \textstyle\fint_v u\big\|^2_{X_v} + \big\|\textstyle\fint_v u\big\|^2_{X_v}\Big) \le 2\varepsilon^d\Big(\displaystyle\frac{2}{\lambda_2(v)}\|\mathrm{d}u\|^2_{X_v} + \operatorname{vol}X_v\big|\textstyle\fint_v u\big|^2\Big)$$

using (2.14) and the fact that $\fint_v u$ is constant. Moreover, the last term can be estimated by

$$\begin{aligned}\operatorname{vol}\partial X_v\big|\textstyle\fint_v u\big|^2 &\le 2\operatorname{vol}\partial X_v\Big(\big|\textstyle\fint_v u - \fint_{\partial X_v} u\big|^2 + \big|\textstyle\fint_{\partial X_v} u\big|^2\Big)\\ &\le 2\Big(1 + \frac{2}{\ell_0\lambda_2(v)}\Big)\|\mathrm{d}u\|^2_{X_v} + \sum_e \operatorname{vol}\partial_e X_v\big|\textstyle\fint_{\partial_e X_v} u\big|^2\end{aligned}$$

using Lemma 2.8. Since $\partial_e X_v$ is isometric to $\partial_v X_e = \{0\} \times Y_e$ by assumption, we can estimate the latter sum by

$$\sum_e \operatorname{vol}\partial_v X_e\big|\textstyle\fint_{\partial_e X_v} u\big|^2 \le \displaystyle\sum_e \|u\|^2_{\partial_v X_e} \le a\|u'\|^2_{X_E} + \frac{2}{a}\|u\|^2_{X_E}$$

due to (2.12) for $\varepsilon = 1$ and $0 < a \le \ell_0$ on each edge e. Here, $X_E := X_{1,E}$ is the union of the unscaled edge neighbourhoods. The desired estimate then follows from the scaling behaviour $\|\mathrm{d}u\|^2_{X_{\varepsilon,v}} = \varepsilon^{d-2}\|\mathrm{d}u\|^2_{X_v}$ and $\|w\|^2_{X_{\varepsilon,e}} = \varepsilon^{d-1}\|w\|^2_{X_e}$ for $w = u$ or $w = u'$ (where $u' = \partial_s u$ denotes the longitudinal derivative). □

We are now able to prove the relative (form-)boundedness of the Hamiltonian H_ε with respect to the Laplacian Δ_{X_ε} for the indicated class of potentials. It will be of particular importance to have a precise control of the constants ε_η and $\widetilde{C}_\eta$ in terms of the various parameters of our spaces, when we deal with the approximation of the δ'_{s}-coupling by δ-couplings with shrinking spacing $a = \varepsilon^\alpha$ in Section 4 below.

Lemma 2.10. *To a given $\eta \in (0,1)$ there exists $\varepsilon_\eta > 0$ such that the form $\mathfrak{h}_\varepsilon$ is relatively form-bounded with respect to the free form $\mathfrak{d}_\varepsilon$ with relative bound η for all $\varepsilon \in (0, \varepsilon_\eta]$, in other words, there exists $\widetilde{C}_\eta > 0$ such that*

$$|\mathfrak{h}_\varepsilon(u) - \mathfrak{d}_\varepsilon(u)| \le \eta\, \mathfrak{d}_\varepsilon(u) + \widetilde{C}_\eta \|u\|^2_{X_\varepsilon}$$

whenever $0 < \varepsilon \le \varepsilon_\eta$, where the constants ε_η and $\widetilde{C}_\eta$ are given by

$$\varepsilon_\eta := \frac{\eta}{\|Q\|_\infty C(v)} \quad \text{and} \quad \widetilde{C}_\eta := 8c_{\mathrm{vol}} \|Q\|_\infty \max\Big\{ \frac{4c_{\mathrm{vol}}\|Q\|_\infty}{\eta}, \frac{1}{\ell_0} \Big\} \tag{2.15}$$

and fulfil $\varepsilon_\eta = \mathrm{O}(\ell_0)$ and $\widetilde{C}_\eta = \mathrm{O}(\ell_0^{-1})$ as $\ell_0 \to 0$.

Proof. The potential $Q_\varepsilon = \varepsilon^{-1} Q$ is by assumption supported on the vertex neighbourhood X_v, therefore we have

$$\begin{aligned} |\mathfrak{h}_\varepsilon(f) - \mathfrak{d}_\varepsilon(f)| &\le \frac{\|Q\|_\infty}{\varepsilon} \|u\|^2_{X_{\varepsilon,v}} \\ &\le \|Q\|_\infty \big(\varepsilon C(v) \|\mathrm{d}u\|^2_{X_{\varepsilon,v}} + 4ac_{\mathrm{vol}} \|u'\|^2_{X_{\varepsilon,E}} \big) + \frac{8\|Q\|_\infty c_{\mathrm{vol}}}{a} \|u\|^2_{X_{\varepsilon,E}} \end{aligned}$$

using Lemma 2.9, for $0 < a \le \ell_0$. Choosing $a = \min\{\ell_0, \eta(4c_{\mathrm{vol}}\|Q\|_\infty)^{-1}\}$ and $0 < \varepsilon \le \varepsilon_\eta$ with ε_η as above, we can estimate the quadratic form contributions by

$$\eta \big(\|\mathrm{d}u\|^2_{X_{\varepsilon,v}} + \|u'\|^2_{X_{\varepsilon,E}} \big) \le \eta \|\mathrm{d}u\|^2_{X_\varepsilon}.$$

The expression for $\widetilde{C}_\eta$ then follows by evaluating the coefficient of the remaining norm. □

We need to estimate the "free" quadratic form against the form associated with the Hamiltonian:

Corollary 2.11. *The quadratic form $\mathfrak{h}_\varepsilon$ is closed. Moreover, setting $\eta = 1/2$, we get the estimate*

$$\mathfrak{d}_\varepsilon(u) \le 2\big(\mathfrak{h}_\varepsilon(u) + \widetilde{C}_{1/2} \|u\|^2_{X_\varepsilon}\big)$$

which holds provided $0 < \varepsilon \le \varepsilon_{1/2}$.

As in Lemma 2.4, we can prove the following estimate in order to compare the "free" quadratic form with the graph norm of H_ε:

Lemma 2.12. *We have*

$$\|u\|^2_{\mathsf{H}^1(X_\varepsilon)} = \mathfrak{d}_\varepsilon(u) + \|u\|^2_{X_\varepsilon} \le 2 \max\{\widetilde{C}_{1/2}, \sqrt{2}\} \|(H_\varepsilon \mp \mathrm{i})u\|^2_{X_\varepsilon}$$

for $u \in \operatorname{dom} H_\varepsilon \subset \operatorname{dom} \mathfrak{h}_\varepsilon = \mathsf{H}^1(X_\varepsilon)$ and $0 < \varepsilon \le \varepsilon_0$.

3. Approximation of δ-couplings

After this preliminaries we can pass to our main problems. The first one concerns approximation of a δ-coupling by Schrödinger operators with scaled potentials supported by the vertex regions. For the sake of simplicity most part of the discussion will be done for the situation with a single vertex as described in Section 2.

quasi.unitary

3.1. **Quasi-unitary identification operators.** First, we need some notation how to compare operators and forms acting in different Hilbert spaces. We say that the quadratic forms $\mathfrak{h}$ and $\mathfrak{h}_\varepsilon$ are *δ_ε-quasi-unitarily equivalent w.r.t. the free first order scale*[4] if there are identification operators

$$J \colon \mathscr{H} \longrightarrow \mathscr{H}_\varepsilon, \quad J^1 \colon \mathscr{H}^1 \longrightarrow \mathscr{H}^1_\varepsilon \quad \text{and} \quad J'^1 \colon \mathscr{H}^1_\varepsilon \longrightarrow \mathscr{H}^1,$$

eq:closeness

called *δ_ε-quasi-unitary* if

$$\|Jf - J^1 f\|^2 \le \delta_\varepsilon^2 \|f\|^2_{\mathsf{H}^1(G)}, \qquad \|J^* u - J'^1 u\|^2 \le \delta_\varepsilon^2 \|u\|^2_{\mathsf{H}^1(X_\varepsilon)}, \tag{3.1a}$$

eq:j1

$$J^* J f = f, \qquad \|JJ^* u - u\|^2 \le \delta_\varepsilon^2 \|u\|^2_{\mathsf{H}^1(X_\varepsilon)}, \tag{3.1b}$$

eq:j.inv

$$\bigl|\mathfrak{h}(J'^1 u, f) - \mathfrak{h}_\varepsilon(u, J^1 f)\bigr| \le \delta_\varepsilon \|u\|_{\mathsf{H}^1(X_\varepsilon)} \|f\|_{\mathsf{H}^1(G)}. \tag{3.1c}$$

eq:j.com

Here,

$$\mathscr{H} := \mathsf{L}_2(G), \qquad \mathscr{H}^1 := \mathsf{H}^1(G), \qquad \mathscr{H}_\varepsilon := \mathsf{L}_2(X_\varepsilon), \qquad \mathscr{H}^1_\varepsilon := \mathsf{H}^1(X_\varepsilon). \tag{3.2}$$

eq:space

The attribute *free first order scale* refers to the fact that we use the first order space $\mathscr{H}^1 := \mathsf{H}^1(G)$ with norm using the free Laplacian, and similarly on the manifold. Note that the attribute *δ_ε-quasi-unitary* refers to the fact that we have a quantitative generalisation of unitary operators. In particular, if $\delta_\varepsilon = 0$, then a δ_ε-quasi-unitary operator is just unitary. A general spectral theory for quasi-unitary equivalent operators is developed in a simple form in [P06, App.] and in a more elaborated version in [P09, Ch. 4].

We need a relation between the different constants of the graph and the manifold model introduced above. Specifically, we set

$$p_e := (\operatorname{vol}_{d-1} Y_e)^{1/2} \qquad \text{and} \qquad q(v) = \int_{X_v} Q \, \mathrm{d}x_v. \tag{3.3}$$

eq:def.p

Let us now fix the quasi-unitary operators by a natural choice: Let $J \colon \mathscr{H} \longrightarrow \mathscr{H}_\varepsilon$ be given by

$$Jf := \varepsilon^{-(d-1)/2} \bigoplus_{e \in E} (f_e \otimes \mathbb{1}_e) \oplus 0 \tag{3.4}$$

eq:def.j

with respect to the decomposition (2.8). Here $\mathbb{1}_e$ is the normalised eigenfunction of Y_e associated to the lowest (zero) eigenvalue, i.e. $\mathbb{1}_e(y) = (\operatorname{vol}_{d-1} Y_e)^{-1/2}$. Roughly speaking, we extend a function constantly in its transversal direction on the edge neighbourhoods and set it zero on the vertex neighbourhood.

In order to relate the Sobolev spaces of order one we correct the error made at the vertex neighbourhood by fixing the function to be constant there. Namely, we define $J^1 \colon \mathscr{H}^1 \longrightarrow \mathscr{H}^1_\varepsilon$ by

$$J^1 f := \varepsilon^{-(d-1)/2} \Bigl(\bigoplus_{e \in E} (f_e \otimes \mathbb{1}_e) \oplus f(v) \mathbb{1}_v \Bigr), \tag{3.5}$$

eq:j.1

where $\mathbb{1}_v$ is the constant function on X_v with value 1. Note that the latter operator is well defined:

$$(J^1 f)_e(0, y) = \varepsilon^{-(d-1)/2} p_e^{-1} f_e(0) = \varepsilon^{-(d-1)/2} f(v) = (J^1 f)_v(x)$$

for any $x \in X_v$ due to (3.3) and (2.2). In particular, the function $J^1 f$ matches along the different components of the manifold, thus $J^1 f \in \mathsf{H}^1(X_\varepsilon)$. Moreover, $f(v)$ is defined for $f \in \mathsf{H}^1(G)$ (see Lemma 2.1).

[4]We use a slightly different notation w.r.t. the monograph [P09, Ch. 4] and the appendix of [P06], in order to simplify matters here.

The mapping in the opposite direction is given by the adjoint, $J^*\colon \mathscr{H}_\varepsilon \longrightarrow \mathscr{H}$, which means that we average a function in transversal direction, i.e.,

$$(J^*u)_e(s) = \varepsilon^{(d-1)/2} p_e \fint_e u(s). \tag{3.6}$$

eq:j.

Furthermore, we modify J^* on the first order spaces to an operator $J'^1\colon \mathscr{H}^1_\varepsilon \longrightarrow \mathscr{H}^1$ given by

$$(J'^1_e u)(s) := \varepsilon^{(d-1)/2} p_e \Big[\fint_e u(s) + \chi_e(s)\Big(\fint_v u - \fint_e u(0)\Big)\Big], \tag{3.7}$$

eq:j.1.

which differs from $J^* f$ only by a correction near the vertices. Here χ_e is a Lipschitz continuous cut-off function on the edge I_e such that $\chi_e(0) = 1$ and $\chi_e(\ell_e) = 0$. If we choose the function χ_e to be piecewise affine linear with $\chi_e(0) = 1$, $\chi_e(\ell_0) = 0$ and $\chi_e(\ell_e) = 0$, then $\|\chi_e\|^2_{I_e} = \ell_0/3 \le \ell_0$ and $\|\chi'_e\|^2_{I_e} = \ell_0^{-1}$. Moreover, $(J'^1_e u)_e(0) = \varepsilon^{(d-1)/2} p_e \fint_v u$ so that $f := J'^1 u$ satisfies $\underline{f}(0) \in \mathbb{C}\underline{p}$, and therefore $f \in \mathsf{H}^1_{\underline{p}}(G)$, i.e., $J'^1 u$ indeed maps into the right space. Note that by construction of the manifold, we have $\fint_{\partial_e X_v} u = \fint_e u(0)$.

loseness

3.2. **Quasi-unitary equivalence.**

In this subsection, we will verify the conditions (3.1) of quasi-unitary equivalence. We start this subsection with a lower bound on the operators H and H_ε in terms of the model parameters; for the definitions of the constants $C_{1/2}$, $\varepsilon_{1/2}$ and $\widetilde{C}_{1/2}$ see Lemma 2.2 and Lemma 2.10. Note that $\widetilde{C}_{1/2}$ still depends on $\|Q\|_\infty$ and ℓ_0.

lower.bd

Lemma 3.1. *For $\varepsilon \in (0, \varepsilon_{1/2}]$ the operators H_ε and H are bounded from below by $\lambda_0 := -\widetilde{C}_{1/2}$. Moreover, if all lengths are finite, i.e. $\ell_e < \infty$, and $q(v) \le 0$, then we have*

$$\inf \sigma(H) \le \frac{q(v)}{\operatorname{vol} X_E} \qquad \text{and} \qquad \inf \sigma(H_\varepsilon) \le \frac{q(v)}{\operatorname{vol} X_E + \varepsilon \operatorname{vol} X_v},$$

where $X_E := \bigcup_e X_e$ is the union of the edge neighbourhoods.

Proof. Due to (3.3) we have $|\underline{p}|^2 = \operatorname{vol} \partial X_v$ and $|q(v)| = \big|\int_{X_v} Q \,\mathrm{d}x_v\big| \le \|Q\|_\infty \operatorname{vol} X_v$ so that

$$C_{1/2} \le \max\Big\{4c^2_{\mathrm{vol}}\|Q\|^2_\infty, \frac{2c_{\mathrm{vol}}\|Q\|_\infty}{\ell_0}\Big\} \le \widetilde{C}_{1/2} = \max\Big\{64c^2_{\mathrm{vol}}\|Q\|^2_\infty, \frac{8c_{\mathrm{vol}}\|Q\|_\infty}{\ell_0}\Big\}, \tag{3.8}$$

eq:c.1-2

where we recall that $c_{\mathrm{vol}} = \operatorname{vol} X_v / \operatorname{vol} \partial X_v$. The spectral estimates then follow by inserting suitable test functions into the Rayleigh quotients $\mathfrak{h}(f)/\|f\|^2$ and $\mathfrak{h}_\varepsilon(u)/\|u\|^2$. For f, we choose the edgewise constant function $f_e(x) = p_e$. Note that $f \in \mathsf{H}^1_{\underline{p}}(G)$. On the manifold, we choose the constant $u := J^1 f = \varepsilon^{(d-1)/2}\mathbb{1}$. The upper bound on the infimum on the spectrum follows by the relation $\ell_e p_e^2 = \operatorname{vol} X_e$ using (3.3). □

Now we are in position to demonstrate that the two Hamiltonians are quasi-unitary equivalent in the sense of (3.1), i.e., we estimate the expressions with the identification operators and the forms $\mathfrak{h}$, $\mathfrak{h}_\varepsilon$ in terms of the "free" quadratic forms $\mathfrak{d}$ and $\mathfrak{d}_\varepsilon$. The precise dependence of the error δ_ε on the model parameters will be needed in Section 4.

loseness

Proposition 3.2. *The quadratic forms $\mathfrak{h}_\varepsilon$ and $\mathfrak{h}$ are δ_ε-quasi-unitary equivalent w.r.t. free first order scale and the identification operators J, J^1, J'^1 given above, where $\delta_\varepsilon = \mathrm{O}(\varepsilon^{1/2})$ as $\varepsilon \to 0$. In particular, δ_ε is given explicitly by*

$$\delta_\varepsilon^2 := \max\Big\{\frac{8\varepsilon c_{\mathrm{vol}}}{\ell_0}, \frac{\varepsilon^2}{\lambda_2(E)}, \varepsilon^2 C(v), \frac{2\varepsilon}{\ell_0}\Big(1 + \frac{2}{\ell_0\lambda_2(v)}\Big), \frac{4\varepsilon c_{\mathrm{vol}}\|Q\|^2_\infty}{\ell_0\lambda_2(v)}\Big\}. \tag{3.9}$$

eq:def.delta

Here, $\ell_0 = \min_e\{1, \ell_e\}$, $\lambda_2(E) := \min_e \lambda_2(e)$ and $c_{\mathrm{vol}} = \operatorname{vol} X_v / \operatorname{vol} \partial X_v$. Moreover, $\lambda_2(e)$ and $\lambda_2(v)$ denote the second (first non-vanishing) eigenvalue of the (Neumann-)Laplacian on Y_e and X_v, respectively, and $C(v)$ was defined in Lemma 2.9.

Proof. The first condition in (3.1a) is here

$$\|Jf - J^1 f\|^2_{X_\varepsilon} = \varepsilon \operatorname{vol} X_v |f(v)|^2 \le \varepsilon c_{\mathrm{vol}} \Big(\|f'\|^2_G + \frac{2}{\ell_0} \|f\|^2_G \Big)$$

using Lemma 2.1 with $a = \ell_0 \le 1$ and the fact that $|\underline{p}|^2 = \operatorname{vol} \partial X_v$ due to (3.3). Next we need to show the second estimate in (3.1a). In our situation, we have

$$\|J^* u - J'^1 u\|^2_G = \varepsilon^{d-1} \sum_{e \in E} \|\chi_e\|^2_{I_e} p_e^2 \Big| \fint_v u - \fint_e u(0) \Big|^2 \le \varepsilon \Big(1 + \frac{2}{\ell_0 \lambda_2(v)} \Big) \|\mathrm{d} u\|^2_{X_{\varepsilon,v}} \qquad (3.10)$$ eq:j.sca

using Lemma 2.8. Moreover, the first equation in (3.1b) is easily seen to be fulfilled. The second estimate in (3.1b) is more involved. Here, we have

$$\|JJ^* u - u\|^2 = \sum_e \|u - \fint_e u\|^2_{X_{\varepsilon,e}} + \|u\|^2_{X_{\varepsilon,v}}.$$

The first term can be estimated as in (2.14) by

$$\big\|u - \fint_e u\big\|^2_{X_{\varepsilon,e}} = \int_{I_e} \big\|u(s) - \fint_e u(s)\big\|^2_{Y_e} \, \mathrm{d}s \le \frac{1}{\lambda_2(e)} \int_{I_e} \|\mathrm{d}_{Y_e} u(s)\|^2_{Y_e} \, \mathrm{d}s = \frac{\varepsilon^2}{\lambda_2(e)} \|\mathrm{d}_{Y_e} u\|^2_{X_{\varepsilon,e}},$$

where $u(s) := u(s, \cdot)$. The second term can be estimated by Lemma 2.9. In particular, for the inequality in (3.1b), the first, second and third term in the definition of δ_ε are sufficient.

Let us finally prove (3.1c) in our model. Note that this estimate differs from the ones given in [P06] by the absence of the potential term $Q_\varepsilon = \varepsilon^{-1} Q$ there. In our situation, we have

$$\begin{aligned} &\big|\mathfrak{h}(J'^1 u, f) - \mathfrak{h}_\varepsilon(u, J^1 f)\big|^2 \\ &\qquad \le 2\varepsilon^{d-1} \Big[\Big| \sum_e p_e \Big(\fint_v \overline{u} - \fint_e \overline{u}(0) \Big) \langle \chi_e', f' \rangle_{I_e} \Big|^2 + \big| q(v) \fint_v \overline{u} - \langle Qu, \mathbb{1}_v \rangle_{X_v} \big|^2 |f(v)|^2 \Big]. \end{aligned}$$

Note that the derivative terms cancel on the edges due to the product structure of the metric and the fact that $\mathrm{d}_{Y_e} \mathbb{1}_e = 0$ and the vertex contribution vanishes due to $\mathrm{d}_{X_v} \mathbb{1}_v = 0$. The first term can be estimated as before in (3.10) up to an additional factor $2\ell_0^{-1}$. For the second term, we use our definition $q(v) = \int_{X_v} Q \, \mathrm{d}x_v$ and the fact that $q(v) \fint_v \overline{u} = \langle u, \fint_v Q \mathbb{1}_v \rangle_{X_v}$ to conclude

$$\begin{aligned} \big| q(v) \fint_v \overline{u} - \langle Qu, \mathbb{1}_v \rangle_{X_v} \big|^2 &= \big| \big\langle u, \fint_v Q - Q \big\rangle_{X_v} \big|^2 \\ &= \big| \langle u, P_v Q \rangle_{X_v} \big|^2 = \big| \langle P_v u, Q \rangle_{X_v} \big|^2 \le \frac{1}{\lambda_2(v)} \|\mathrm{d}u\|^2_{X_v} \|Q\|^2_{X_v} \end{aligned}$$

where $P_v u := u - \fint_v u$ is the projection onto the orthogonal complement of $\mathbb{1}_v$. The last estimate follows from (2.14). Collecting the error terms for the sesquilinear form estimate, we see that the forth and fifth term in the definition of δ_ε are necessary as lower bound on δ_ε, using also Lemma 2.1 for the estimate on $|f(v)|^2$, and $\|Q\|^2_{X_v} \le \operatorname{vol} X_v \|Q\|^2_\infty$. ☐

Now we can prove our main result on the approximation of a δ-coupling in the manifold model. We say that the graph and manifold Hamiltonians H and H_ε are $\widetilde{\delta}_\varepsilon$*-quasi-unitarily equivalent w.r.t. the natural scale of Hilbert spaces* generated by H and H_ε or simply $\widetilde{\delta}_\varepsilon$-*quasi-unitarily equivalent*, if there is an identification operator $J \colon \mathsf{L}_2(G) \longrightarrow \mathsf{L}_2(X_\varepsilon)$ such that $J^* J = \mathrm{id}$,

$$\big\|(\mathrm{id} - JJ^*) R^\pm_\varepsilon\big\| \le \widetilde{\delta}_\varepsilon \quad \text{and} \quad \big\|JR^\pm - R^\pm_\varepsilon J\big\| \le \widetilde{\delta}_\varepsilon, \qquad (3.11)$$ eq:q-u.c

where $\|\cdot\|$ denotes the operator norm, and where $R^\pm := (H \mp \mathrm{i})^{-1}$ and $R^\pm_\varepsilon := (H_\varepsilon \mp \mathrm{i})^{-1}$ denote the resolvents, respectively. The resolvent estimates are supposed to hold for both signs; the deviation $\widetilde{\delta}_\varepsilon \ge 0$ from being unitarily equivalent will be specified in the next theorem. We use the resolvent in the points $z = \pm\mathrm{i}$ since in Section 4, the lower bound λ_0 on H_ε will depend on ε and may tend to $-\infty$ as $\varepsilon \to 0$. Recall the definition of $\widetilde{C}_{1/2}$, $\varepsilon_{1/2}$ (see (2.15)) and $\lambda_0 := -\widetilde{C}_{1/2}$.

loseness **Theorem 3.3.** *For $\varepsilon \in (0, \varepsilon_{1/2}]$, the operators H_ε and H are $\widetilde{\delta}_\varepsilon$-quasi-unitarily equivalent with $\widetilde{\delta}_\varepsilon = 10\delta_\varepsilon \max\{\widetilde{C}_{1/2}, \sqrt{2}\} = \mathrm{O}(\varepsilon^{1/2})$, where δ_ε is given in* (3.9)*.*

Proof. The first norm estimate in (3.11) follows from (3.1b) shown in Proposition 3.2. The second norm estimate can be seen as follows: Let $\widetilde{f} \in \mathsf{L}_2(G)$, $\widetilde{u} \in \mathsf{L}_2(X_\varepsilon)$. Setting $f := R^\pm \widetilde{f} \in \operatorname{dom} H$ and $u := R_\varepsilon^\mp \widetilde{u} \in \operatorname{dom} H_\varepsilon$, we have

$$\begin{aligned}\langle \widetilde{u}, (JR^\pm - R_\varepsilon^\pm J)\widetilde{f}\rangle &= \langle \widetilde{u}, Jf\rangle - \langle u, J\widetilde{f}\rangle \\ &= \langle \widetilde{u}, (J - J^1)f\rangle + \big(\mathfrak{h}_\varepsilon(u, J^1 f) - \mathfrak{h}(J'^1 u, f)\big) + \langle (J'^1 - J^*)u, \widetilde{f}\rangle \\ &\qquad - \mathrm{i}\big(\langle u, (J^1 - J)f\rangle + \langle (J'^1 - J^*)u, f\rangle\big),\end{aligned}$$

and therefore

$$\big|\langle \widetilde{u}, (JR^\pm - R_\varepsilon^\pm J)\widetilde{f}\rangle\big| \le 10\delta_\varepsilon \max\{\widetilde{C}_{1/2}, \sqrt{2}\}\|\widetilde{f}\|\|\widetilde{u}\|$$

using the estimates (3.1) shown in Proposition 3.2 together with Lemmata 2.4 and 2.12, and the fact that $C_{1/2} \le \widetilde{C}_{1/2}$. □

Once we have the estimates of the quasi-unitary equivalence in (3.11), we can extend the estimates to other functions of the operators. This is done in detail in [P06, App. A] or more evolved in [P09, Ch. 4] (see also Remark 4.8).

thm:res **Theorem 3.4.** *We have*

$$\|J(H - z)^{-1} - (H_\varepsilon - z)^{-1}J\| = \mathrm{O}(\varepsilon^{1/2}), \tag{3.12a}$$

$$\|J(H - z)^{-1}J^* - (H_\varepsilon - z)^{-1}\| = \mathrm{O}(\varepsilon^{1/2}) \tag{3.12b}$$

for $z \notin [\lambda_0, \infty)$. The error depends only on δ_ε, given in (3.9)*, and on z. Moreover, we can replace the function $\varphi(\lambda) = (\lambda - z)^{-1}$ by any measurable, bounded function converging to a constant as $\lambda \to \infty$ and being continuous in a neighbourhood of $\sigma(H)$.*

The following spectral convergence is also a consequence of the $\mathrm{O}(\varepsilon^{1/2})$-quasi-unitary equivalence (see e.g. [P06, Thm. A.13] or [P09, Sec. 4.3]). For details of the uniform convergence of sets, i.e. the convergence in Hausdorff-distance sense we refer to [HN99, App. A] or [P09, App. A.1].

thm:spec **Theorem 3.5.** *The spectrum of H_ε converges to the spectrum of H uniformly on any finite energy interval. The same is true for the essential spectrum.*

Proof. The spectral convergence is a direct consequence of the quasi-unitary equivalence, see the theory developed in [P06, App.] and [P09, Ch. 4]. □

For the discrete spectrum we have the following result:

isc.spec **Theorem 3.6.** *For any $\lambda \in \sigma_{\mathrm{disc}}(H)$ there exists a family $\{\lambda_\varepsilon\}_\varepsilon$ with $\lambda_\varepsilon \in \sigma_{\mathrm{disc}}(H_\varepsilon)$ such that $\lambda_\varepsilon \to \lambda$ as $\varepsilon \to 0$. Moreover, the multiplicity is preserved. If λ is a simple eigenvalue with normalised eigenfunction φ, then there exists a family of simple normalised eigenfunctions $\{\varphi_\varepsilon\}_\varepsilon$ of H_ε (ε small) such that*

$$\|J\varphi - \varphi_\varepsilon\|_{X_\varepsilon} \to 0$$

as $\varepsilon \to 0$.

We remark that the convergence of higher-dimensional eigenspaces is also valid, however, it requires some technicalities which we skip here.

To summarise, we have shown that the δ-coupling with weighted entries can be approximated by a geometric setting and a potential located on the vertex neighbourhood.

Let us briefly sketch how to extend the above convergence results Theorems 3.3–3.6 to more complicated — even to non-compact — graphs. Denote by G a metric graph, given by the underlying discrete graph (V, E, ∂) with $\partial\colon E \longrightarrow V \times V$, $\partial e = (\partial_- e, \partial_+ e)$ denoting the initial and terminal vertex, and the length function $\ell\colon E \longrightarrow (0, \infty)$, such that each edge e is identified with the interval $I_e = (0, \ell_e)$ (for simplicity, we assume here that all length are finite, i.e., $\ell_e < \infty$). Let X_ε be the corresponding approximating manifold constructed from the building blocks $X_{\varepsilon,e} = I_e \times \varepsilon Y_e$ and $X_{\varepsilon,v} = \varepsilon X_v$ as in Section 2.2. For more details, we refer to [EP05, P06, EP08, P09]. Since a metric graph can be constructed from a number of star graphs with identified end points of the free ends, we can define global identification operators. We only have to assure that the global error we make is still uniformly bounded:

m:non-compact **Theorem 3.7.** *Assume that G is a metric graph and X_ε the corresponding approximating manifold constructed according to G. If*

$$\inf_{v\in V} \lambda_2(v) > 0, \quad \sup_{v\in V} \frac{\operatorname{vol} X_v}{\operatorname{vol} \partial X_v} < \infty, \quad \sup_{v\in V} \|Q\restriction_{X_v}\|_\infty < \infty, \quad \inf_{e\in E} \lambda_2(e) > 0, \quad \inf_{e\in E} \ell_e > 0,$$

then the corresponding Hamiltonians $H = \Delta_G + \sum_v q(v)\delta_v$ and $H_\varepsilon = \Delta_{X_\varepsilon} + \sum_v \varepsilon^{-1} Q\restriction_{X_v}$ are $\widetilde{\delta}_\varepsilon$-quasi-unitarily equivalent, where the error $\widetilde{\delta}_\varepsilon = \mathrm{O}(\varepsilon^{1/2})$ depends only on the above mentioned global constants.

4. Approximation of the δ'_{s}-couplings

sec:delta'

The main aim of this section is to show how the symmetrised δ'-coupling, or δ'_{s}, can be approximated using manifold model discussed above. To this aim we shall use a result of [CE04] by which a δ'_{s}-coupling can be approximated by means of several δ-couplings on the same metric graph, located close to the vertex and "lift" this approximation to the manifold. For the sake of simplicity we will again consider the star-shape setting with a single vertex. We believe, however, that the method we use can be directly generalised to more complicated graphs but also, what is equally important, to other vertex couplings, once they can be approximated by combinations of δ-couplings on the graph, possibly with an addition of extra edges — see [ET06, ET07].

Let thus G be a star graph as in Section 2 where we denote the vertex in the centre by v_0 and where we label the $n = \deg v$ edges by $e = 1, \dots, n$. Again for simplicity, we assume that all the (unscaled) transverse volumes $p_e^2 = \operatorname{vol} Y_e$ are the same; without loss of generality we may put $\operatorname{vol} Y_e = 1$. Moreover, we assume that all lengths are finite, i.e. $\ell_e < \infty$, and equal, so we may put $\ell_e = 1$. First we recall the definition of the δ'_{s}-coupling: the operator H^β, formally written as $H^\beta = \Delta_G + \beta\delta'_{v_0}$, acts as $(H^\beta f)_e = -f''_e$ on each edge for functions f in the domain

$$\operatorname{dom} H^\beta := \Big\{\, f \in \mathsf{H}^2_{\max}(G) \;\Big|\; \forall e_1, e_2\colon f'_{e_1}(0) = f'_{e_2}(0) =: f'(0),\ \sum_e f_e(0) = \beta f'(0), \\ \forall e\colon f'_e(\ell_e) = 0 \Big\}. \qquad (4.1)$$ eq:h.bet

For the sake of definiteness we imposed here Neumann conditions at the free ends of the edges, however, the choice is not substantial; we could use equally well Dirichlet or any other boundary condition. The corresponding quadratic form is given as

$$\mathfrak{h}^\beta(f) = \sum_e \|f_e'\|^2 + \frac{1}{\beta}\Big|\sum_e f_e(0)\Big|^2, \qquad \operatorname{dom}\mathfrak{h}^\beta = \mathsf{H}^1_{\max}(G)$$

if $\beta \neq 0$ and

$$\mathfrak{h}^\beta(f) = \sum_e \|f_e'\|^2, \qquad \operatorname{dom}\mathfrak{h}^\beta = \Big\{\, f \in \mathsf{H}^1_{\max}(G) \,\Big|\, \sum_e f_e(0) = 0 \,\Big\}$$

if $\beta = 0$; the condition $f \in H^0$ is obviously dual to the free (or Kirchhoff) vertex coupling — see, e.g., [Ku04, Sec. 3.2.3].

The (negative) spectrum of H^β is easily found:

c.delta' **Lemma 4.1.** *If $\beta \geq 0$ then $H^\beta \geq 0$. On the other hand, if $\beta < 0$ then H^β has exactly one negative eigenvalue $\lambda = -\kappa^2$ where κ is the solution of the equation*

$$\cosh\kappa + \frac{\beta\kappa}{\deg v}\sinh\kappa = 0. \tag{4.2}$$

eq:kappa.beta

Proof. The non-negativity of H^β follows from the quadratic form expression for $\beta > 0$ and $\beta = 0$. We make the ansatz

$$f_e(s) = \cosh\kappa(1-s)$$

fulfilling automatically the Neumann condition at $s = 1$ and the continuity condition at $s = 0$ since $f_e'(0) = -\kappa\sinh\kappa$ is independent of e. The remaining condition at zero leads to the above relation of κ and β, showing in another way that if $\beta \geq 0$ there cannot exist a negative eigenvalue. □

The main idea of the approximation of a δ_{s}'-coupling by Schrödinger operators on a manifold is to employ a combination of δ-couplings in an operator one may call an *intermediate Hamiltonian* $H^{\beta,a}$, and then to use the approximations for δ-couplings given in the previous section.

In order to define $H^{\beta,a}$, we first modify the (discrete) structure of the graph G inserting additional vertices v_e of degree 2 on the edge e with the distance $a \in (0,1)$ from the central vertex v_0 (see Figure 2). Each edge e is splitted into two edges e_a and e_1. We denote the metric graph with the additional vertices v_e and splitted edges by G_a, i.e., $V(G_a) = \{v_0\} \cup \{\, v_e \,|\, e = 1, \dots, n \,\}$, $E(G_a) = \{\, e_a, e_1 \,|\, e = 1, \dots n \,\}$ and $\ell_{e_a} = a$, $\ell_{e_1} = 1 - a$. This metrically equivalent graph G_a will be needed when associating the corresponding manifold. As vertex conditions on the additional vertices v_e we use the unweighted free conditions.

Remark 4.2. It is useful to note that the Laplacians Δ_G and Δ_{G_a} associated to the metric graphs G and G_a are unitarily equivalent. Indeed, introducing additional vertices of degree two with (unweighted) free conditions does not change the original quadratic form $\mathfrak{d}_G$ with the domain $\mathsf{H}^1(G) = \operatorname{dom}\mathfrak{d}$ associated to the free operator $\Delta_G = H_{(G,0)}$. Figuratively speaking, the free operator does not see these vertices of degree two. We just have to change the coordinate on the edge e, i.e. we can either use the original coordinate $s \in (0, \ell_e)$ on the edge e or we can split the edge e into two edges e_a and e_1 of length $\ell_{e_a} = a$ and $\ell_{e_1} = \ell_e - a = 1 - a$ with the corresponding coordinates.

The core of the approximation lies in a suitable, a-dependent choice of the parameters of these δ-couplings. Writing the operator in terms of the formal notation introduced in (2.6), we put

$$H^{\beta,a} := \Delta_G + b(a)\delta_{v_0} + \sum_e c(a)\delta_{v_e}, \qquad b(a) = -\frac{\beta}{a^2}, \qquad c(a) = -\frac{1}{a},$$

to be the *intermediate* Hamiltonian. Notice that the strength of the central δ-coupling depends on β while the added δ-interactions are attractive, the sole parameter being the distance a. The operator can be defined via its quadratic form

$$\mathfrak{h}^{\beta,a}(f) := \sum_e \|f_e'\|^2 - \frac{\beta}{a^2}|f(0)|^2 - \frac{1}{a}\sum_e |f_e(a)|^2, \qquad \operatorname{dom}\mathfrak{h}^a = \mathsf{H}^1(G),$$

where $\mathsf{H}^1(G) = \mathsf{H}^1_{\underline{p}}(G)$ with $\underline{p} = (1,\dots,1)$, i.e. the functions $f \in \mathsf{H}^1(G)$ are distinguished by being continuous at v_0, $f_{e_1}(0) = f_{e_2}(0) =: f(0)$.

The next theorem shows that the intermediate Hamiltonian converges indeed to the δ_{s}'-coupling with the strength β on the star-shaped graph:

thm:delta' **Theorem 4.3** (Cheon, Exner)**.** *We have*

$$\|(H^{\beta,a} - z)^{-1} - (H^\beta - z)^{-1}\| = \mathrm{O}(a)$$

as $a \to 0$ for $z \notin \mathbb{R}$, where $\|\cdot\|$ denotes the operator norm on $\mathsf{L}_2(G)$.[5]

Note that the choice of the parameters $b(a)$ $c(a)$ of the δ-interactions as functions of the distance a follows from a careful analysis of the resolvents of $H^{\beta,a}$ and H^β. Each of these is highly singular as $a \to 0$, however, in the difference all the singularities cancel leaving us with a vanishing expression. Needless to say, that such a limiting process is highly non-generic.

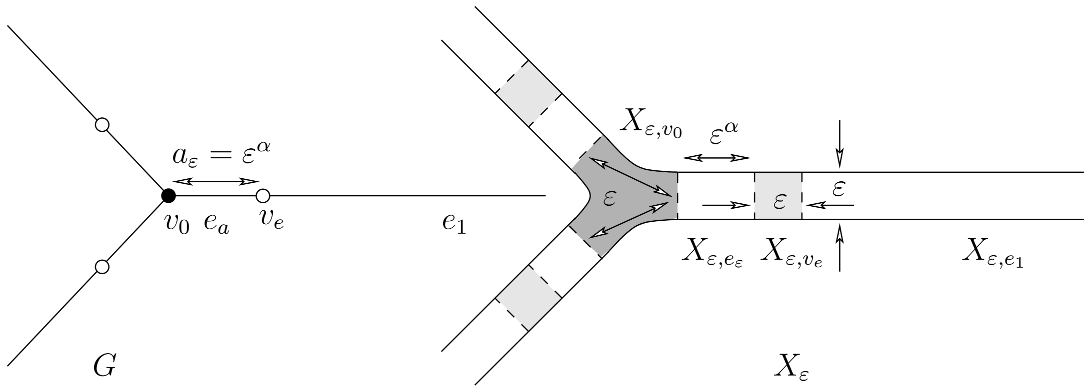

FIGURE 2. The intermediate graph picture used in the δ_{s}'-approximation and the corresponding manifold model. fig:pot-

Let us now consider the manifold model approaching the intermediate Hamiltonian $H^{\beta,a}$ in the limit $\varepsilon \to 0$ with $a = a_\varepsilon = \varepsilon^\alpha$ and $0 < \alpha < 1$ to be specified later on. Let X_ε be a manifold model of the graph G as shown in Figure 2. For the additional vertices of degree two we choose the vertex neighbourhoods as a part of the cylinder of length ε and distance of order of a_ε from the central vertex v_0. The edge e_{a_ε} now has the length $a_\varepsilon = \varepsilon^\alpha$ depending on ε. The "free" edge e_1 joining v_e with the free end point at $s = 1$ is again ε-depending, namely it has the length $1 - a_\varepsilon = 1 - \varepsilon^\alpha$. By the argument given in Lemma 2.7 we can deal with this error and assume that this edge again has length one, the price being an extra error of order $\mathrm{O}(\varepsilon^\alpha)$, affecting neither the final result nor the quantitative error estimate. Next we have to choose the potentials in the vicinity of the vertices $v = v_0$ and $v = v_e$. The simplest option is to assume that they are constant,

$$Q_{\varepsilon,v}(x) := \frac{1}{\varepsilon} \cdot \frac{q_\varepsilon(v)}{\operatorname{vol} X_v}, \qquad x \in X_v$$

[5]The claim made in [CE04] is only that the norm tends to zero, however, the rate with which it vanishes is obvious from the proof. We remove the superfluous $\deg v$ from the definition of $H^{\beta,a}$ in that paper. It should also be noted that the proof in [CE04] is given for star graphs with semi-infinite edges but the argument again modifies easily to the finite-length situation we consider here.

so that $\int_{X_v} Q_{\varepsilon,v}\,\mathrm{d}x = \varepsilon^{-1} q_\varepsilon(v)$ (see (2.10) and (3.3)), where we put

$$q_\varepsilon(v_0) := b(\varepsilon^\alpha) = -\beta\varepsilon^{-2\alpha} \qquad \text{and} \qquad q_\varepsilon(v_e) := c(\varepsilon^\alpha) = -\varepsilon^{-\alpha}.$$

The corresponding manifold Hamiltonian and the respective quadratic form are then given by

$$H_\varepsilon^\beta = \Delta_{X_\varepsilon} - \varepsilon^{-1-2\alpha} \frac{\beta}{\operatorname{vol} X_{v_0}} \mathbb{1}_{X_{v_0}} - \varepsilon^{-1-\alpha} \sum_{e \in E} \mathbb{1}_{X_{v_e}} \tag{4.3}$$ eq:h.beta.eps

and

$$\mathfrak{h}_\varepsilon^\beta(u) = \|\mathrm{d}u\|^2_{X_\varepsilon} - \varepsilon^{-1-2\alpha} \frac{\beta}{\operatorname{vol} X_{v_0}} \|u\|^2_{X_{\varepsilon,v_0}} - \varepsilon^{-1-\alpha} \sum_{e \in E} \|u\|^2_{X_{\varepsilon,v_e}},$$

respectively. Note that the unscaled vertex neighbourhood X_{v_e} of the added vertex v_e has volume 1 by construction.

Before proceeding to the approximation itself, let us first make some comments about the lower bounds of the operators $H^{\beta,a}$ and their manifold approximations H_ε^β:

er.bd.gr **Lemma 4.4.** *If $\beta < 0$, then the spectrum of $H^{\beta,a}$ is uniformly bounded from below as $a \to 0$, in other words, there is a constant $C > 0$ such that*

$$\inf \sigma(H^{\beta,a}) \geq -C \quad \textit{as} \quad a \to 0.$$

If $\beta \geq 0$, on the other hand, then the spectrum of $H^{\beta,a}$ is asymptotically unbounded from below,

$$\inf \sigma(H^{\beta,a}) \to -\infty \quad \textit{as} \quad a \to 0.$$

Note that although we know the limit spectrum as $a \to 0$ (see Lemma 4.1), the resolvent convergence of Theorem 4.3 does not necessarily imply the uniform boundedness from below of $H^{\beta,a}$ (see Remark 4.10).

Proof. Let $\beta < 0$. Then an eigenfunction on the (original) edge e has the form

$$f_e(s) = \begin{cases} A\cosh(\kappa s) + B_e \sinh(\kappa s), & 0 \leq s \leq a \\ C_e \cosh(\kappa(1-s)), & a \leq s \leq 1. \end{cases}$$

for $\kappa > 0$, the corresponding eigenvalue being $\lambda = -\kappa^2$. The Neumann condition $f_e'(1) = 0$ at $s = 1$ is automatically fulfilled, as well as the continuity at $s = 0$ for the different edges e, since $f_e(0) = A$ is independent of e. The continuity in $s = a$ and the jump condition in the derivative lead to non-trivial coefficients A, B_e and C_e if and only if B_e and C_e are independent of e and if

$$\frac{\beta}{a^2}\bigl(\sinh(\kappa a)\cosh\kappa(1-a) - a\kappa\cosh\kappa\bigr) + n\kappa\bigl(\kappa a \sinh\kappa - \cosh(\kappa a)\cosh\kappa(1-a)\bigr) = 0$$

with associated eigenvalue $\lambda = -\kappa(a)^2$ of multiplicity one. It can be seen that $\kappa(a)$ is bounded, and that the above equation reduces to (4.2) as $a \to 0$.

For the second part, assume that $\beta \geq 0$. It is sufficient to calculate the Rayleigh quotient for the constant test function $f = \mathbb{1} \in \mathsf{H}^1(G)$ which yields

$$\frac{\mathfrak{h}^{\beta,a}(f)}{\|f\|^2} = -\frac{1}{n}\Bigl(\frac{\beta}{a^2} + \frac{1}{a}\Bigr)$$

being of order $\mathrm{O}(a^{-2})$ if $\beta < 0$ and of order $\mathrm{O}(a^{-1})$ if $\beta = 0$, negative in both cases; recall that $n = \deg v$. $\square$

Similarly, we expect the same behaviour for the operators on the manifold.

r.bd.mfd **Lemma 4.5.** *If $\beta \geq 0$, then the spectrum of H_ε^β is asymptotically unbounded from below, i.e.,*

$$\inf \sigma(H_\varepsilon^\beta) \to -\infty \quad \textit{as} \quad \varepsilon \to 0.$$

Proof. Again, we plug the constant test function $u = \mathbb{1}$ into the Rayleigh quotient and obtain

$$\frac{\mathfrak{h}^\beta_\varepsilon(u)}{\|u\|^2} = -\frac{\beta\varepsilon^{-2\alpha} + \varepsilon^{-\alpha}}{n(1+\varepsilon+\varepsilon^\alpha) + \varepsilon \operatorname{vol} X_{v_0}}$$

which obviously tends to $-\infty$ as $\varepsilon \to 0$. □

rem:sp.bdd *Remark* 4.6. As for a counterpart to the first claim in Lemma 4.4, the proof of the uniform boundedness from below as $\varepsilon \to 0$ for $\beta < 0$ seems to need quite subtle estimates to compare the effect of the two competing potentials on X_{ε,v_0} and X_{ε,v_e} having strength proportional to $|\beta|\varepsilon^{-2\alpha}$ and $\varepsilon^{-\alpha}$, respectively. Since the positive contribution $Q_{\varepsilon,v_0} = |\beta|\varepsilon^{-1-2\alpha}$ is more singular than the negative contributions $Q_{\varepsilon,v_e} = -\varepsilon^{-1-\alpha}$, we expect that the threshold of the spectrum remains bounded as $\varepsilon \to 0$.

We can now prove our second main result. For the δ'_{s}-coupling Hamiltonian H_β and the approximating operator H^β_ε defined in (4.1) and (4.3), respectively, we make the following claim.

hm:res.delta' **Theorem 4.7.** *Assume that $0 < \alpha < 1/13$, then H^β_ε and H^β are $\overline{\delta}_\varepsilon$-quasi-unitarily equivalent, i.e., $J^*J = \mathrm{id}$,*

$$\big\|(\mathrm{id} - JJ^*)(H^\beta_\varepsilon \mp \mathrm{i})^{-1}\big\| \le \overline{\delta}_\varepsilon \quad \text{and} \quad \big\|(H^\beta_\varepsilon \mp \mathrm{i})^{-1}J - J(H^\beta \mp \mathrm{i})^{-1}\big\| \le \overline{\delta}_\varepsilon,$$

where $\overline{\delta}_\varepsilon = \mathrm{O}(\varepsilon^{\min\{\alpha,(1-13\alpha)/2\}})$ depends on the quantities in (3.9), and where J is the same identification operator as in Section 3.

Proof. Denote by $H^{\beta,\varepsilon} = H^{\beta,a_\varepsilon}$ the ε-depending intermediate Hamiltonian on the metric graph with δ-potentials of strength depending on ε as defined before. For the corresponding graph and manifold model, the lower bound to lengths depends now on ε, specifically, $\ell_0 = a_\varepsilon = \varepsilon^\alpha$. Moreover, from the definition of the constants $C_{1/2} \le \widetilde{C}_{1/2}$ and $\varepsilon_{1/2}$ in (2.15) and from Proposition 3.2, we conclude that

$$\widetilde{C}_{1/2} = \widetilde{C}_{1/2}(\varepsilon) = \mathrm{O}(\varepsilon^{-4\alpha}), \qquad \varepsilon_{1/2} = \varepsilon_{1/2}(\varepsilon) = \mathrm{O}(\varepsilon^{3\alpha}) \qquad \text{and} \qquad \delta_\varepsilon = \mathrm{O}(\varepsilon^{(1-5\alpha)/2}).$$

Note that the dominant term in the error δ_ε (see (3.9)) is the last one containing the potential. The first convergence follows now immediately from Proposition 3.2 together with Lemma 2.12. Moreover, from Theorem 3.3 it follows that

$$\big\|(H^\beta_\varepsilon - \mathrm{i})^{-1}J - J(H^{\beta,\varepsilon} - \mathrm{i})^{-1}\big\| \le 10\delta_\varepsilon \max\{\widetilde{C}_{1/2}(\varepsilon), \sqrt{2}\} = \mathrm{O}(\varepsilon^{(1-13\alpha)/2}).$$

so that Theorem 4.3 yields the sought conclusion. Note that the exponent of ε in $\delta_\varepsilon \widetilde{C}_{1/2}(\varepsilon)$ is $(1-5\alpha)/2 - 4\alpha = (1-13\alpha)/2 > 0$ provided $\alpha < 1/13$. □

We can now proceed and state results as in Theorems 3.4–3.7 for the δ'_{s}-approximation; we will mention some exemplary results in the following theorem.

rem:q-u-e *Remark* 4.8. Note that in [P06, App.] or [P09, Ch. 4], we considered only non-negative operators (covering, as usual, operators bounded *uniformly* from below by a suitable shift). In our present situation, we can only guarantee the resolvent convergence at *non-real* points like $z = \pm\mathrm{i}$. Nevertheless, the arguments in [P06] or [P09] can be used to conclude the convergence of suitable functions of operators as well as the convergence of the dimension of spectral projections etc.

Note that the spectrum of H^β and H^β_ε here is purely discrete.

Theorem 4.9. *We have*

$$\|J(H^\beta - z)^{-1} - (H^\beta_\varepsilon - z)^{-1}J\| = \mathrm{O}(\varepsilon^{1/2}), \tag{4.4a}$$

$$\|J(H^\beta - z)^{-1}J^* - (H^\beta_\varepsilon - z)^{-1}\| = \mathrm{O}(\varepsilon^{1/2}) \tag{4.4b}$$

for $z \notin \mathbb{R}$. The error depends on the quantities in (3.9) *and on z. Moreover, we can replace the function $\varphi(\lambda) = (\lambda - z)^{-1}$ by any measurable, bounded function converging to a constant as $\lambda \to \infty$ and being continuous in a neighbourhood of $\sigma(H^\beta)$.*

For any $\lambda \in \sigma(H^\beta)$ there exists a family $\{\lambda_\varepsilon\}_\varepsilon$ with $\lambda_\varepsilon \in \sigma(H_\varepsilon^\beta)$ such that $\lambda_\varepsilon \to \lambda$ as $\varepsilon \to 0$. Moreover, the multiplicity is preserved. Finally, the eigenfunctions of H_ε^β converge to eigenfunctions of H^β in the sense of Theorem 3.6.

:sp.bdd2 *Remark* 4.10. Note that the asymptotic lower unboundedness of H_ε^β (and of the intermediate operator $H^{\beta,\varepsilon}$) for $\beta \geq 0$ described in Lemmata 4.4 and 4.5 is not a contradiction to the fact that the limit operator H^β is non-negative. For example, the spectral convergence of an analogue of Theorem 3.5 holds only for *compact* intervals $I \subset \mathbb{R}$. In particular, $\sigma(H^\beta) \cap I = \emptyset$ implies that

$$\sigma(H_\varepsilon^\beta) \cap I = \emptyset \qquad \text{and} \qquad \sigma(H^{\beta,\varepsilon}) \cap I = \emptyset$$

provided $\varepsilon > 0$ is sufficiently small. This spectral convergence means that the negative spectral branches of H_ε^β all have to tend to $-\infty$.

5. Concluding remarks

ec:concl

5.1. **Other vertex couplings.** Let us first comment on possible extension of the results derived above to more general vertex couplings. As we have mentioned in the introduction, the result of [CE04] based on the seminal idea of [CS98] allows for extensions worked out in [ET07]. Considering again a star graph with n edges, we have specifically

- a family of couplings obtained as the limit of the star with *two* additional δ-vertices added at each edge. The first is at the distance a^3 from the central vertex with the coupling constant $-a^{-3} + \beta_e a^{-2}$ at the e-th edge, the other at the distance $a + a^3$ with the coupling $-a^{-1} + \gamma_e$. In the central vertex we have a δ-coupling of the strength ηa^{-4}. The real numbers β_e, γ_e and η are coupled by one condition, so the limit yields a $2n$-parameter family of couplings; the norm resolvent convergence is established in this case;
- an $\binom{n+1}{2}$ family of couplings covering generically all boundary conditions with *real* coefficients can be obtained similarly if we use one δ-vertex at each edge at the distance d from the centre and the graph is amended by links of length of order of d connecting the additional vertices with another δ-coupling in the middle — see [ET07] for a detailed description. In this case the convergence was established for the boundary conditions.

The proposed approximation is now the following. We replace the graph by a network with a fat edge width ε and the δ-couplings by constant potentials of the appropriated strength at the segment of fat edge of length ε. We call the corresponding Schrödinger operator H_ε^ω, where ω stands now for the appropriate family of parameters, and by H^ω the corresponding limiting operator on the graph itself.

en.coupl **Conjecture 5.1.** *If $a = \varepsilon^\alpha$ holds in the above setting with $\alpha > 0$ sufficiently small then the claim analogous to Theorem 4.7 is valid with the same identification operator J.*

5.2. **Purely geometric approximations.** One way to provide a *geometric* approximation would be to let the particle live on a "sleeve-type" manifold X_ε — physically one can imagine a nanotube network — being subject to a curvature-induced potential such as considered in [DEK01]. A trouble with this idea, however, is that the potential would naturally scale as ε^{-2} in the limit which does not fit into the approximation scheme discussed here, and a more elaborate approach has to be sought.

5.3. **Physical realisation of the approximations.** Let us finally make a few remarks on the meaning of the obtained approximations. Since the non-trivial coupling comes from particularly chosen potentials on the thin tube network a natural question is in which way we can control them. We have seen above that there are topological and analytic obstructions for certain purely geometric approximations.

However, there are other ways how to realise the potentials in question physically. Thinking of the network as of a model of a semiconductor system, one can certainly use a local variation of the material parameters. Doping the network locally changes the Fermi energy at the spot creating effectively a potential well or barrier. From the practical point of view, indeed, the applicability is limited because our approximations need potentials which get stronger with the diminishing tube width ε.

Another, and more exciting way, is to use external fields. It is a common practise in experiment with nanosystems to add "gates", or local electrodes, to which a voltage can be applied. In this way one can produce local potentials fitting into our approximation scheme, without material restrictions. This opens an rather intriguing possibility of creating quantum graphs with the vertex coupling controllable by an experimentalist (see e.g. [BG08] for some numerical simulations).

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