### Vertex couplings in quantum graphs

Ondřej Turek

(Joint work with T. Cheon and P. Exner)

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Formulation of boundary conditions

## Motivation

- Over time, technologies allow to produce tinier and tinier objects, and to make use of them in applications.
- In particular, various structures made from thin wires can be produced:



⇒ A natural question arises: How does a particle behave on such a structure? Vertex couplings in quantum graphs

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## Motivation

- Over time, technologies allow to produce tinier and tinier objects, and to make use of them in applications.
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⇒ A natural question arises: How does a particle behave on such a structure? Vertex couplings in quantum graphs

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Formulation of boundary conditions

If the thickness is sufficiently small (a few nm), one can neglect the real thickness of the wires



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ightarrow quantum mechanics on graphs.



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- ► If the thickness is sufficiently small (a few nm), one can neglect the real thickness of the wires → quantum mechanics on graphs.
- ... reduction from 3-dimensional QM to 1-dimensional QM - a huge simplification!



 Quantum graphs are <u>models</u> for structures made from thin wires. Vertex couplings in quantum graphs

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Approximations of strongly singular vertex couplings

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Quantum graph (rigorously)

Quantum graph is a pair  $(\Gamma, H_{\Gamma})$ ,

where

- Γ is a metric graph,
- ► H<sub>Γ</sub> is a <u>Hamiltonian</u> on Γ.



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Let the graph  $\Gamma$  have N edges:

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Let the graph **Γ** have *N* edges:



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Let the graph  $\Gamma$  have N edges:

Let the graph  $\Gamma$  have N edges:



• wavefunction of a free particle on  $\Gamma$ :  $\Psi = \begin{pmatrix} \Psi^{\mu} \\ \vdots \\ e^{i/\mu} \end{pmatrix}$ 

Hamiltonian:

$$H_{\Gamma} \left( \begin{array}{c} \psi_1 \\ \vdots \\ \psi_N \end{array} \right) = \left( \begin{array}{c} -\psi_1'' \\ \vdots \\ -\psi_N'' \end{array} \right)$$

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& <u>boundary conditions</u> at the vertices.

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Let the graph  $\Gamma$  have N edges:



• wavefunction of a free particle on  $\Gamma$ :  $\Psi = \begin{pmatrix} \psi_1 \\ \vdots \\ z/\psi_2 \end{pmatrix}$ 

$$H_{\Gamma} \left( \begin{array}{c} \psi_1 \\ \vdots \\ \psi_N \end{array} \right) = \left( \begin{array}{c} -\psi_1'' \\ \vdots \\ -\psi_N'' \end{array} \right)$$

& <u>boundary conditions</u> at the vertices.

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Formulation of boundary conditions

# Boundary vectors (at a vertex of degree n)



$$\Psi(0) := \begin{pmatrix} \psi_1(0_+) \\ \vdots \\ \psi_n(0_+) \end{pmatrix}$$

(limits of values)

$$\Psi'(0):=\left(egin{array}{c} \psi_1'(0_+) \ dots \ dots \ \psi_n'(0_+) \end{array}
ight)$$

(limits of derivatives)

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# Boundary vectors (at a vertex of degree n)



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(limits of derivatives)

### Boundary conditions

B. c. connect  $\Psi(0)$  and  $\Psi'(0)$  so that  $H_{\Gamma}$  is self-adjoint.

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### Boundary conditions in a vertex of degree n

(I) The b. c. have to connect the boundary vectors

$$\left(\begin{array}{c}\psi_1(0_+)\\\vdots\\\psi_n(0_+)\end{array}\right) \quad \text{and} \quad \left(\begin{array}{c}\psi_1'(0_+)\\\vdots\\\psi_n'(0_+)\end{array}\right)$$

(II) so that the Hamiltonian is self-adjoint.

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### Boundary conditions in a vertex of degree n

(I) The b. c. have to connect the boundary vectors

$$\begin{pmatrix} \psi_1(0_+) \\ \vdots \\ \psi_n(0_+) \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \psi'_1(0_+) \\ \vdots \\ \psi'_n(0_+) \end{pmatrix}$$

(II) so that the Hamiltonian is self-adjoint.

As to (I): How to connect the boundary values?

Usually in the way

 $A\Psi(0)+B\Psi'(0)=0\,,$ 

where A, B are complex matrices  $n \times n$ .

As to (II): When is the Hamiltonian self-adjoint?► (to be answered on the next slide)

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# Self-adjointness (Kostrykin & Schrader 1999)

Let us consider for simplicity a graph with 1 vertex, i.e. a *star graph*. Boundary conditions in its vertex:

$$A\Psi(0) + B\Psi'(0) = 0.$$
 (1)

Hamiltonian: denoted  $H_{\Gamma}$ .

**Theorem** (K & S 1999):  $H_{\Gamma}$  is self-adjoint *iff* 

i.  $\operatorname{rank}(A|B) = n$ , ii.  $AB^*$  is self-adjoint.



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# Self-adjointness (Kostrykin & Schrader 1999)

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**Theorem** (K & S 1999):  $H_{\Gamma}$  is self-adjoint *iff* 

i. rank(A|B) = n, ii.  $AB^*$  is self-adjoint.

Any pair (A, B) satisfying i and ii thus determines (via (1)) certain vertex coupling:

$$(A, B) \mapsto$$
 vertex coupling

**Small problem:** Many different pairs (A, B) define the same coupling.



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# Why " $(A, B) \mapsto$ vertex coupling" is not one-to-one

If the pair (A, B) is replaced by (CA, CB) for <u>any regular</u>  $C \in \mathbb{C}^{n,n}$ , the "new" b. c.

 $CA\Psi(0) + CB\Psi'(0) = 0$ 

are identical to

 $A\Psi(0)+B\Psi'(0)=0.$ 

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(Easy to see.)

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# Why " $(A, B) \mapsto$ vertex coupling" is not one-to-one

If the pair (A, B) is replaced by (CA, CB) for <u>any regular</u>  $C \in \mathbb{C}^{n,n}$ , the "new" b. c.

 $CA\Psi(0) + CB\Psi'(0) = 0$ 

are identical to

$$A\Psi(0)+B\Psi'(0)=0.$$

(Easy to see.)

Sometimes it is useful to have a one-to-one correspondence

 $(A, B) \longleftrightarrow$  vertex coupling.

How to make the pair (A, B) unique?

By letting them satisfy <u>additional suitable constraint</u>.

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Constraint of Harmer and Kostr. & Schr. (2000)

$$A = U - I, \quad B = i(U + I)$$

where U is a unitary matrix  $n \times n$ . The b.c. can be written in the form

$$(U-I)\Psi(0) + i(U+I)\Psi'(0) = 0.$$

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Constraint of Harmer and Kostr. & Schr. (2000)

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where U is a unitary matrix  $n \times n$ . The b.c. can be written in the form

$$(U-I)\Psi(0) + i(U+I)\Psi'(0) = 0.$$

### Advantages:

- (2) looks simple,
- we see immediately that the family of vertex couplings in a vertex of degree n has n<sup>2</sup> real parameters (because U(n) has n<sup>2</sup> real parameters).

### **Disadvantages:**

- Elements of U often do not look simple,
- a unitary matrix "hides" its parameters.

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(2)

## Constraint of Cheon, Exner and Turek (2010)

### where

• 
$$m = \operatorname{rank}(B)$$

- S is a self-adjoint matrix  $m \times m$ ,
- T is a general complex matrix  $m \times (n m)$ ,

► 
$$I^{(m)}$$
,  $I^{(n-m)}$  are identity matrices  $m \times m$ ,  
 $(n-m) \times (n-m)$ .

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Constraint of Cheon, Exner and Turek (2010) We call the constrained b. c. "*ST*-form":

$$\begin{pmatrix} I^{(m)} & T \\ \hline 0 & 0 \end{pmatrix} \Psi'(0) = \begin{pmatrix} S & 0 \\ \hline -T^* & I^{(n-m)} \end{pmatrix} \Psi(0) \quad (3)$$

### Disadvantages:

- The structure of (3) is complicated and depends on rank(B),
- ► (3) does not allow arbitrary numbering of the edges.

### Advantages:

- The elements of S and T represent the coupling parameters in a straightforward way,
- ► A and B contain many zero elements.

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# One more form

• PQRS-form - the "symmetrized" ST-form

$$\begin{pmatrix} I^{(p+q-n)} & 0 & P \\ \hline R & I^{(n-p)} & Q+RP \\ \hline 0 & 0 & 0 \end{pmatrix} \Psi'(0) = \\ = \begin{pmatrix} S & -SR^* & 0 \\ \hline 0 & 0 & 0 \\ \hline -P^* & -Q^* & I^{(n-q)} \end{pmatrix} \Psi(0)$$

where

▶ 
$$p,q \in \mathbb{N}_0, p+q \leq n$$
,

- S is a self-adjoint matrix  $p \times p$ ,
- ► I<sup>(p+q-n)</sup>, I<sup>(n-p)</sup>, I<sup>(n-q)</sup> are identity matrices of the given sizes,
- P, Q, R are general complex matrices of the corresponding sizes.

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# Another unique formulation of b.c. (Kuchment)

**Theorem** (Kuchment 2004): There is an orthogonal projector P in  $\mathbb{C}^n$ , Q = Id - P and a self-adjoint operator L in  $Q\mathbb{C}^n$  such that the b. c. can be written as

$$P\Psi(0) = 0$$
 (4a)  
 $Q\Psi'(0) + LQ\Psi(0) = 0.$  (4b)

**Remark.** The formulation (4) is in some sense related to the ST-form.

### Advantages:

Useful for certain calculations.

### **Disadvantages:**

- ► (4) contains 2n equations (the form  $A\Psi(0) + B\Psi'(0) = 0$  has only *n* equations),
- coupling parameters are again "hidden".

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Example:  $\delta$ -coupling with parameter  $\alpha \in \mathbb{R}$ 

- the most common type of a point interaction
- is expressed by the following two requirements:
- 1. continuity in the vertex

$$\psi_j(0) = \psi_k(0) =: \psi(0) \quad \forall j, k \in \{1, \dots, n\}$$

2. sum of the derivatives is proportional to the value  $\psi(0)$ 

$$\sum_{j=1}^n \psi_j'(\mathbf{0}) = \alpha \cdot \boldsymbol{\psi}(\mathbf{0})$$

**Remark.** Terminology for n = 2:  $\delta$ -coupling  $\delta$ -interaction

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 $\delta$ -coupling expressed by Harmer and Kostr.&Schr.

$$(U-I)\Psi(0) + i(U+I)\Psi'(0) = 0$$

$$\begin{pmatrix} \frac{2}{n+i\alpha} - 2 & \frac{2}{n+i\alpha} - 1 & \frac{2}{n+i\alpha} - 1 & \cdots & \frac{2}{n+i\alpha} - 1 \\ \frac{2}{n+i\alpha} - 1 & \frac{2}{n+i\alpha} - 2 & \frac{2}{n+i\alpha} - 1 & \cdots & \frac{2}{n+i\alpha} - 1 \\ \frac{2}{n+i\alpha} - 1 & \frac{2}{n+i\alpha} - 1 & \frac{2}{n+i\alpha} - 2 & \cdots & \frac{2}{n+i\alpha} - 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{2}{n+i\alpha} - 1 & \frac{2}{n+i\alpha} - 1 & \frac{2}{n+i\alpha} - 1 & \cdots & \frac{2}{n+i\alpha} - 2 \end{pmatrix} \Psi(0) +$$

. . .

$$+i \begin{pmatrix} \frac{2}{n+i\alpha} & \frac{2}{n+i\alpha}+1 & \frac{2}{n+i\alpha}+1 & \cdots & \frac{2}{n+i\alpha}+1\\ \frac{2}{n+i\alpha}+1 & \frac{2}{n+i\alpha} & \frac{2}{n+i\alpha}+1 & \cdots & \frac{2}{n+i\alpha}+1\\ \frac{2}{n+i\alpha}+1 & \frac{2}{n+i\alpha}+1 & \frac{2}{n+i\alpha} & \cdots & \frac{2}{n+i\alpha}+1\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ \frac{2}{n+i\alpha}+1 & \frac{2}{n+i\alpha}+1 & \frac{2}{n+i\alpha}+1 & \cdots & \frac{2}{n+i\alpha} \end{pmatrix} \Psi'(0) = 0$$

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 $\delta$ -coupling expressed in the ST-form

$$\left(\begin{array}{c|c} I^{(m)} & T \\ \hline 0 & 0 \end{array}\right) \Psi'(0) = \left(\begin{array}{c|c} S & 0 \\ \hline -T^* & I^{(n-m)} \end{array}\right) \Psi(0)$$

$$\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix} \Psi'(0) = \begin{pmatrix} \alpha & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -1 & 0 & 0 & \cdots & 1 \end{pmatrix} \Psi(0)$$
$$m = \operatorname{rank}(B) = 1, \quad S = (\alpha), \quad T = \begin{pmatrix} 1 & 1 & \cdots & 1 \end{pmatrix}$$

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 $\delta\text{-coupling}$  expressed by Kuchment

$$P\Psi(0)=0 \ Q\Psi'(0)+LQ\Psi(0)=0$$

$$\frac{1}{\sqrt{n(n-1)}} \begin{pmatrix} 1-n & 1 & \cdots & 1\\ 1 & 1-n & \cdots & 1\\ \vdots & \vdots & \ddots & \vdots\\ 1 & 1 & \cdots & 1-n \end{pmatrix} \Psi(0) = 0$$
$$\begin{pmatrix} \frac{1}{\sqrt{n}} & \cdots & \frac{1}{\sqrt{n}}\\ \vdots & \vdots\\ \frac{1}{\sqrt{n}} & \cdots & \frac{1}{\sqrt{n}} \end{pmatrix} \Psi'(0) + \begin{pmatrix} -\frac{\alpha}{\sqrt{n}} & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & -\frac{\alpha}{\sqrt{n}} \end{pmatrix} \Psi(0) = 0$$

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Problem: What is the physical meaning of vertex couplings?

 δ coupling (δ potential) may be considered as a limit of regular potentials

n=2 (the line):

0

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 $\Rightarrow \delta$  potential is well understood.

Other couplings ?

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# The problem

How to construct (approximate) a singular coupling in a vertex of degree n



using only  $\delta$  potentials and vector potentials (i.e. only well understood objects)?

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1. Take *n* disjoint half lines.



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2. Connect the endpoints by short lines of the length d.



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3. Place a  $\delta$  potential at each half line endpoint.



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4. Place a  $\delta$  potential at the center of each short line.



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5. Place a constant vector potential on (some) short lines.



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### Limit process

6. Now take this system...



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### Limit process

7. ... and squeeze the central part...



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### Limit process

8. ... more and more.



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### What turned out

The limit yields a singular vertex coupling - any requested...



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## Supposing that...

... supposing that the strengths of the  $\delta$  potentials



are properly set and tuned during the squeezing process

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## Supposing that...

and the strengths of the vector potentials



are properly set and tuned during the squeezing process.

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## Supposing that...

and the strengths of the vector potentials



are properly set and tuned during the squeezing process.

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# The role of the *ST*-form

The *ST*-form

$$\begin{pmatrix} I^{(m)} & \mathbf{T} \\ 0 & 0 \end{pmatrix} \Psi'(0) = \begin{pmatrix} \mathbf{S} & \mathbf{0} \\ -\mathbf{T}^* & I^{(n-m)} \end{pmatrix} \Psi(0)$$

- positions of zeros in S and T determine which half lines have to be connected
- values in S and T determine parameters of the δ-couplings
- ► (mainly) phases of entries of S, T determine strengths of the vector potentials

**Remark**: If S and T are real (time-reversible vertex coupling), no added vector potential is necessary.

**Remark:** Parameters of  $\delta$ 's and potential strengths depend on d. Vertex couplings in quantum graphs

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H<sup>Ad</sup> - Hamiltonian of the approximated system

 $H_d^{Ag}$  - Hamiltonian of the approximating system





The aim is to compare the resolvents

 $R_{H^{Ad}}(k^2)$  and  $R_{H^{Ag}}(k^2)$ ,

but they act on different Hilbert spaces:

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H<sup>Ad</sup> - Hamiltonian of the approximated system

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but they act on different Hilbert spaces:

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Therefore we identify  $R_{H^{Ad}}(k^2)$  with

$$R_{H^{Ad}_d}(k^2) := R_{H^{Ad}}(k^2) \oplus \mathbf{0}\,,$$

where 0 is the zero operator acting on  $L^2(G')$ .



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Therefore we identify  $R_{H^{Ad}}(k^2)$  with

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where 0 is the zero operator acting on  $L^{2}(G')$ .

### Theorem

Let us assume the notation introduced before. Then

$$\lim_{d\to 0_+} \left\| R_{H_d^{A_g}}(k^2) - R_{H_d^{A_d}}(k^2) \right\| = 0.$$

**Remark.** Roughly speaking,  $H_d^{Ag}$  converges to  $H^{Ad}$  in the norm-resolvent sense as  $d \rightarrow 0$ .

**Proof:** Long and technical, using Krein's formula.

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