# AHARONOV–BOHM RING TOUCHING A QUANTUM WIRE: HOW TO MODEL IT AND TO SOLVE THE INVERSE PROBLEM

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An explicitly solvable model of the gated Aharonov–Bohm ring touching a quantum wire is constructed and investigated. The inverse spectral and scattering problems are discussed. It is shown that the Titchmarsh–Weyl matrix function associated with the boundary vertices determines a unique electric potential on the graph even though the graph contains a loop. This system gives another family of isospectral quantum graphs.

Keywords: quantum graphs, inverse problems.

### 1. Introduction

Transport, scattering and spectral properties of small rings connected by wires are a subject of current interest of both physicists and mathematicians. Theoretical studies of such systems are connected with the investigation of different exactly solvable models. It is commonly accepted to use the so-called (metric) quantum graphs — Schrödinger operators on metric graphs — in modelling such devices. The main subject of this article is the quantum system depicted in Fig. 1. It is formed by a one-dimensional wire coupled to an Aharonov–Bohm ring.

This system has already been considered in [28], where the scattering matrix for the system and the resistance were calculated using heuristic arguments. The main interest of the authors [28] was concentrated on the dependence of explicit physical quantities on the magnetic potential, or more precisely, on the flux of the magnetic field through the loop.

The first aim of the current article is to present a rigorous exactly solvable model for this system. We are going to show how heuristic arguments can be used to pick appropriate matching conditions at the vertex connecting the loop to the wire. This is precisely the area where physical and mathematical arguments have to

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Fig. 1. Graph  $\Gamma$ . A bounded wire with an Aharonov–Bohm ring attached.

be taken into account simultaneously resulting in a mathematically rigorous model reflecting physical intuition.

This article also has a pure mathematical goal. We discuss the corresponding inverse problem with the Titchmarsh–Weyl matrix function (TW-matrix) playing the role of spectral data. This problem was studied in the case of trees (graphs without cycles) and it was proven that the potential and matching conditions are uniquely determined by the TW-matrix [1, 2, 5, 6, 10-14, 16, 29, 30]. It was realized that if the graph has a loop, the inverse potential problem in general is not uniquely solvable even in the case of the so-called standard matching conditions<sup>1</sup> at the vertices. If the graph has a cycle with several contact points, then the inverse problem may be solved by considering magnetic Schrödinger operators and spectral data dependent on the fluxes of the magnetic field through the cycle [18, 19]. This approach does not work if the graph has a loop (like the graph  $\Gamma$  on Fig. 1) and the matching conditions are standard. It appears that the system under investigation is described by matching conditions different from the standard ones and these conditions have certain special properties that makes it possible to solve the inverse problem. Both inverse problems to reconstruct the matching conditions and the potential are studied. On the other hand, the presented exactly solvable model gives another counterexample showing that the inverse problem to reconstruct the metric graph in general does not have a unique solution.

To use the TW-matrix is natural from the physical point of view, since it is directly related to graph's scattering matrix. On the other hand, since the TW-matrix is of Nevanlinna type (analytic function with positive imaginary part in the upper halfplane), its entries are not independent. One might prefer to reduce the set of spectral data considering just few entries of the TW-matrix, but we refrain from doing this in order to treat different boundary points on an equal basis.

We would like to mention that V. Yurko investigated a slightly different inverse problem for differential operators on graphs, namely, how to recover the potential from the spectra of different self-adjoint operators associated with the same differential expression [29–35]. One can see our two approaches as natural continuations of the classical methods developed to solve the inverse problem on a compact interval. In these methods the inverse problem is solved using Dirichlet–Dirichlet and Dirichlet–

<sup>&</sup>lt;sup>1</sup>By standard matching conditions we mean the conditions that the function is continuous and the sum of normal derivatives at the vertex is equal to zero.

Neumann spectra (corresponds to Yurko's approach) and Titchmarsh–Weyl function (corresponds to our approach). These two problems are entirely connected and the connection between the corresponding sets of spectral data is clear in the case of one compact interval. On the other hand, this connection is far from being straightforward in the case of graphs with cycles. We note that Yurko considered the case of arbitrary compact graphs (with several cycles) but with just standard matching conditions at internal vertices.

## 2. Description of the model

This section is devoted to the construction of the self-adjoint operator modelling the gated Aharonov–Bohm ring touching a quantum wire. This system has already been discussed in [28] and we are going to use already developed physical intuition in our construction. This operator will be studied in the following sections using rigorous mathematical methods, which require that the model is formulated precisely as well as all conditions on the parameters.

As we already mentioned the model will be constructed using quantum graphsordinary differential operators on metric graphs. Every such operator is determined by the triple consisting of:

1) metric graph,

- 2) differential operator acting on the edges,
- 3) matching and boundary conditions at internal and external vertices.

All three components of the triple are described in the following subsections.

### 2.1. Metric graph

The metric graph  $\Gamma$  is formed by three edges  $[x_1, x_2], [x_3, x_4]$  and  $[x_5, x_6]$  connected together as shown in Fig. 1, i.e. the edge  $[x_1, x_2]$  forms a loop attached to the other two edges. The end points form three vertices  $v_1 = \{x_1, x_2, x_4, x_6\}, v_2 = \{x_3\}, v_3 = \{x_5\}$ . The vertex  $v_1$  is internal whereas  $v_2$  and  $v_3$  are boundary vertices. The metric graph  $\Gamma$  is determined by three parameters—the lengths of the edges. The edges are considered as subintervals of  $\mathbb{R}$ . In what follows we are going to consider functions on  $\Gamma$  and the corresponding Hilbert space

$$L_2(\Gamma) = L_2([x_1, x_2]) \oplus L_2([x_3, x_4]) \oplus L_2([x_5, x_6]).$$
(1)

Having in mind the physical experiment, we are going to model, it might be useful to consider the graph  $\Gamma$  as the wire  $[x_3, x_5] = [x_3, x_4] \cup [x_6, x_5]$  (the points  $x_4$  and  $x_6$  identified) with the loop  $[x_1, x_2]$  attached to it at the internal point  $x_4 \sim x_6$ .

### 2.2. Differential operator

The magnetic Schrödinger operator is defined by two real potentials, electric (square integrable) and magnetic (continuous) respectively,

$$q \in L_2(\Gamma), \qquad a \in C(\Gamma), \qquad q(x), a(x) \in \mathbb{R},$$
 (2)

as follows,

$$L_{q,a} = \left(i\frac{d}{dx} + a(x)\right)^2 + q(x).$$
(3)

The domain of the differential operator contains all functions from the Sobolev space  $W_2^2(\Gamma \setminus \{v_1, v_2, v_3\})$ , so that the range belongs to the Hilbert space.

The magnetic potential a on every edge can be eliminated by the elementary unitary transformation described below, but it cannot always be lifted up to the whole graph  $\Gamma$  due to the loop. Spectral properties of the operator do not depend on the particular form of the magnetic potential, but are determined by the integral  $\Phi = \int_{x_1}^{x_2} a(x) dx$ , which gives the flux of the magnetic field through the loop.

### 2.3. The matching and boundary conditions

The role of these conditions is to make the differential operator self-adjoint and to connect together different edges respecting the geometry of  $\Gamma$ . Note that the differential operator  $L_{q,a}$  given by (3) does not reflect in which way the edges are connected to each other.

The boundary vertices  $v_2 = \{x_3\}$  and  $v_3 = \{x_5\}$  are used to approach the system. To solve the inverse problem the dynamical response operator associated with the boundary points will be used. Therefore the corresponding boundary conditions can be chosen arbitrarily. We are going to assume the Dirichlet boundary conditions

$$\begin{cases} \psi(x_3) = 0, \\ \psi(x_5) = 0. \end{cases}$$
(4)

Let us now discuss appropriate matching conditions for the unique internal vertex  $v_1 = \{x_1, x_2, x_4, x_6\}$ . We are going not only to take into account which end points are joined at this vertex, but also the space arranging of the corresponding edges as it is shown in Fig. 1.

Any Hermitian matching condition can be written in the form [22, 2]

$$i(S-I)\begin{pmatrix}\psi(x_1)\\\psi(x_2)\\\psi(x_4)\\\psi(x_6)\end{pmatrix} = (S+I)\begin{pmatrix}\partial\psi(x_1)\\\partial\psi(x_2)\\\partial\psi(x_4)\\\partial\psi(x_6)\end{pmatrix},$$
(5)

where  $\psi(x_j)$  and  $\partial \psi(x_j)$  are the boundary values of the function and its extended derivative at the end points. The limits are taken from inside of the corresponding intervals and the extended derivatives are defined by

$$\partial \psi = \begin{cases} \frac{d}{dx} \psi(x_j) - ia(x_j) \psi(x_j), & x_j \text{ is a left end point,} \\ -\frac{d}{dx} \psi(x_j) + ia(x_j) \psi(x_j), & x_j \text{ is a right end point.} \end{cases}$$
(6)

S is the vertex scattering matrix for the energy  $k^2 = 1$ . The entries of the 4×4 matrix S will be denoted by  $s_{ij}$ , where the indices i, j run over 1, 2, 4, 6 corresponding to the end points glued together at the vertex  $v_1$ . We assume that the system is in the ballistic regime. Then the geometry of the system suggests that the transition probabilities  $x_1 \rightarrow x_2$  and  $x_1 \rightarrow x_6$  are much greater than  $x_1 \rightarrow x_1$  and  $x_1 \rightarrow x_4$ . The other transition probabilities have similar properties. Therefore we shall assume that the entries  $s_{11}, s_{14}, s_{22}, s_{26}, s_{41}, s_{44}, s_{62}$ , and  $s_{66}$  in S are equal to zero whereas all other entries do not vanish.

The standard Schrödinger equation with zero magnetic potential is time reversal invariant. The corresponding eigenfunctions may be chosen real. It is natural to require that the model operator possesses the same property, i.e. it is time reversal invariant. This holds true only if any function  $\psi$  satisfies matching conditions (5) if and only if  $\overline{\psi}$  satisfies the same conditions. This is true only if the matrix S parameterizing the matching conditions is symmetric  $S^t = S$ .

We are not going to discuss the impact of the spectral characteristics of the vertex scattering matrix upon the spectral properties of the system. This motivates the decision to restrict our studies to the case where the matrix S in (5) determines the vertex scattering matrix which is independent of the energy

$$S_v(k) = S. \tag{7}$$

The vertex scattering matrix corresponding to the matching conditions (5) is given by

$$S_v(k) = \frac{(k+1)S + (k-1)I}{(k-1)S + (k+1)I}, \qquad k \neq 0,$$

which implies that it is energy independent if and only if the spectrum of S consists of  $\pm 1$ , hence S is Hermitian.

We shall also assume that the matching conditions are properly connecting, i.e. the matrix S is irreducible. This means that the set of end points  $\{x_1, x_2, x_4, x_6\}$  cannot be divided into two (or more) classes, so that the matching conditions do not connect the boundary values at the points belonging to different classes, in other words that the matrix S cannot be transformed into block-diagonal form by permutations.

Let us list all introduced requirements on the matrix S appearing in the matching conditions (5). From the physical point of view these requirements are:

1) The Schrödinger operator with zero magnetic potential is time reversal invariant.

2) The vertex scattering matrix is energy independent.

3) The matrix S is consistent with the space arrangement of the system.

4) The matching conditions are properly connecting.

These conditions can be reformulated using mathematical language as follows:

- 1) The matrix S is symmetric.
- 2) The matrix S is Hermitian.
- 3) The entries  $s_{12}$ ,  $s_{16}$ ,  $s_{21}$ ,  $s_{24}$ ,  $s_{42}$ ,  $s_{46}$ ,  $s_{61}$ , and  $s_{64}$  are all different from zero and

all other entries vanish,

$$s_{11} = s_{14} = s_{22} = s_{26} = s_{41} = s_{44} = s_{62} = s_{66} = 0.$$
 (8)

4) The matrix S is irreducible.

The set of matrices S satisfying these conditions is characterised by the following lemma.

LEMMA 1. The set of unitary  $4 \times 4$  matrices S satisfying conditions 1)–4) is given by

$$S = \begin{pmatrix} 0 & \alpha & 0 & \beta \\ \alpha & 0 & \sigma\beta & 0 \\ 0 & \sigma\beta & 0 & -\sigma\alpha \\ \beta & 0 & -\sigma\alpha & 0 \end{pmatrix},$$
(9)

where  $\sigma = \pm 1$  and  $\alpha, \beta \in \mathbb{R}$  are subject to

$$\alpha^2 + \beta^2 = 1 \tag{10}$$

and

$$\alpha \neq 0 \neq \beta. \tag{11}$$

*Proof*: Every symmetric Hermitian matrix has real entries. Every such matrix satisfying condition 3) has the form

$$S = \begin{pmatrix} 0 & \alpha & 0 & \beta \\ \alpha & 0 & \gamma & 0 \\ 0 & \gamma & 0 & \delta \\ \beta & 0 & \delta & 0 \end{pmatrix}, \qquad \alpha, \beta, \gamma, \delta \in \mathbb{R}.$$

The unitarity of S implies that

$$\alpha^{2} + \gamma^{2} = \beta^{2} + \delta^{2} = \alpha^{2} + \beta^{2} = \gamma^{2} + \delta^{2} = 1,$$
  
$$\alpha\beta + \gamma\delta = \alpha\gamma + \beta\delta = 0.$$

The parameters  $\alpha$  and  $\beta$  can be chosen arbitrarily subject to (10). Since  $\gamma^2 = \beta^2$ , the parameter  $\gamma$  is determined up to a sign

$$\gamma = \sigma \beta, \qquad \sigma = \pm 1.$$

The parameter  $\delta$  is now uniquely determined,  $\delta = -\sigma \alpha$ . To satisfy condition 4) we have to assume (11). It is clear that every S given by (9) satisfies all required conditions.

The transition probabilities between the end points are given by the squares of the corresponding entries in the matrix S. The transition probabilities  $x_1 \rightarrow x_2$ 

and  $x_1 \rightarrow x_6$  are equal to  $\alpha^2$  and  $\beta^2 = 1 - \alpha^2$ , respectively. If  $\alpha = \pm 1/\sqrt{2}$  then these probabilities are equal. Our calculations imply that in this case the transition probabilities  $x_2 \rightarrow x_1$  and  $x_2 \rightarrow x_4$  are also equal. Similar relations hold even if the probabilities are not pairwise equal.

Weak and strong couplings. It might be interesting to discuss the extreme cases where either  $\alpha$  or  $\beta$  is equal to zero<sup>2</sup>. The corresponding matrices are of the form

$$S = \begin{pmatrix} 0 & \pm 1 & 0 & 0 \\ \pm 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \pm 1 \\ 0 & 0 & \pm 1 & 0 \end{pmatrix} \quad \text{and} \quad S = \begin{pmatrix} 0 & 0 & 0 & \pm 1 \\ 0 & 0 & \pm 1 & 0 \\ 0 & \pm 1 & 0 & 0 \\ \pm 1 & 0 & 0 & 0 \end{pmatrix}$$

where the signs can be chosen arbitrarily with the only requirement that S is symmetric. The matching conditions corresponding to the first matrix are suitable to describe the system presented below rather than the system given on Fig. 1.



Fig. 2. Graph  $\Gamma_1$ . Quantum wire and ring disconnected.

The second matrix describes the system where the point  $x_1$  is connected to  $x_6$  and  $x_2$  to  $x_4$ , i.e. the system without any loop (or more precisely, the loop can be unwinded by pulling away the end points).

Summing up we see that the cases  $\alpha = 0$  or  $\beta = 0$  correspond to systems with different geometry—the corresponding geometric graphs differ from the graph  $\Gamma$ .

### 2.4. Definition of the operator

Let us put together all components of the triple determining the quantum graph modelling the system under investigation.

DEFINITION 1. The self-adjoint operator  $L_{q,a}$  is defined by the differential expression (3) on the domain of functions from the Sobolev space  $W_2^2(\Gamma \setminus \{x_j\}_{j=1}^6)$ 

<sup>&</sup>lt;sup>2</sup>Note that the corresponding matrices S are reducible and therefore these cases are excluded from our studies.

satisfying the Dirichlet boundary conditions (4) and the matching conditions (5) with the matrix S given by (9).

The self-adjointness of the operator  $L_{q,a}$  can be proven by first showing that it is symmetric (by integration by parts) and that the range of  $L_{q,a} - i$  coincides with the Hilbert space  $L_2(\Gamma)$ . The introduced quantum graph depends on the following parameters:

- the lengths  $l_j = x_{2j} x_{2j-1}$ , j = 1, 2, 3, of the three edges forming the metric graph  $\Gamma$ ,
- two real potentials: electric  $q \in L_2(\Gamma)$  and magnetic  $a \in C(\Gamma)$ ,
- three parameters determining the matrix S: two real numbers  $\alpha, \beta \in \mathbb{R}$  subject to  $\alpha^2 + \beta^2 = 1$  and the sign parameter  $\sigma = \pm 1$ .

In what follows we are going to indicate the dependence of the operator just on the functional parameters q and a, having in mind all other parameters.

## 3. Titchmarsh-Weyl matrix function

### 3.1. Definition of the Titchmarsh-Weyl matrix function

Following the general theory [18] let us introduce the Titchmarsh–Weyl matrix function (TW-matrix) associated with the graph  $\Gamma$ . It is a straightforward analog of the classical Titchmarsh–Weyl function for the one-dimensional Schrödinger equation. Consider any solution  $\psi$  to the eigenfunction differential equation

$$\left(i\frac{d}{dx} + a(x)\right)^2 \psi(x) + q(x)\psi(x) = \lambda\psi(x), \qquad x \in (x_{2j-1}, x_{2j}), \quad j = 1, 2, 3, \quad (12)$$

with Im  $\lambda \neq 0$  satisfying the matching conditions (5) (but not necessarily the boundary conditions (4)). Every such solution is uniquely determined by the values  $\psi(x_3), \psi(x_5)$ , since otherwise the self-adjoint operator  $L_{q,a}$  would have an unreal eigenvalue. Then the 2 × 2 matrix function

$$M_{\Gamma}(\lambda, \Phi) : \begin{pmatrix} \psi(x_3) \\ \psi(x_5) \end{pmatrix} \mapsto \begin{pmatrix} \partial \psi(x_3) \\ \partial \psi(x_5) \end{pmatrix}$$
(13)

is the *Titchmarsh–Weyl matrix function* (*TW-matrix*) for the magnetic Schrödinger operator  $L_{q,a}$  on the metric graph  $\Gamma$ . It is a Nevanlinna 2 × 2 matrix function having singularities at the spectrum of  $L_{q,a}$ .

The definition of the TW-matrix is connected with the choice of the boundary conditions at the vertices  $v_2$  and  $v_3$ : different boundary conditions will lead to a slight modification of  $M_{\Gamma}$ . The TW-matrix given by (13) corresponding to the Dirichlet boundary conditions (4) can also be viewed as a Dirichlet-to-Neumann map.

In what follows we are going to use the TW-matrix associated with the kernel ker  $\Gamma$  of the graph  $\Gamma$ . The kernel of a graph is obtained by pruning it, i.e. by

cutting away the boundary edges (see [18]). The kernel of the graph  $\Gamma$  consists of the loop  $[x_1, x_2]$  with the two contact points  $x_4$  and  $x_6$  attached to it.



Fig. 3. The kernel of the graph  $\Gamma$ .

The TW-matrix  $M_{\ker\Gamma}(\lambda, \Phi)$  associated with ker  $\Gamma$  is uniquely defined by

$$M_{\ker\Gamma}(\lambda, \Phi) : \begin{pmatrix} \psi(x_4) \\ \psi(x_6) \end{pmatrix} \mapsto - \begin{pmatrix} \partial \psi(x_4) \\ \partial \psi(x_6) \end{pmatrix}, \qquad \text{Im } \lambda \neq 0, \tag{14}$$

where as before  $\psi$  is any solution to the eigenfunction differential equation (12). Note that formula (14) compared with (13) contains an extra sign, which is introduced in order to ensure that  $M_{\ker\Gamma}(\lambda)$  is a Nevanlinna matrix function.

#### 3.2. Calculation of the TW-matrix

In this subsection we are going to calculate the TW-matrix for the kernel of the quantum graph  $\Gamma$ .

LEMMA 2. The TW-matrix for the kernel of graph  $\Gamma$  is given by

$$M_{\ker\Gamma}(\lambda, \Phi) = \frac{1}{(1-\alpha^2)t_{12}(\lambda)} \begin{pmatrix} 2\alpha\cos\Phi - (\alpha^2 t_{11}(\lambda) + t_{22}(\lambda)) & \sigma(e^{i\Phi} + \alpha^2 e^{-i\Phi}) - \sigma\alpha\operatorname{Tr} T(\lambda) \\ \sigma(\alpha^2 e^{i\Phi} + e^{-i\Phi}) - \sigma\alpha\operatorname{Tr} T(\lambda) & 2\alpha\cos\Phi - (t_{11} + \alpha^2 t_{22}) \end{pmatrix},$$
(15)

where  $T = \{t_{ij}\}_{i,j=1}^2$  is the transfer matrix for the magnetic potential-free Schrödinger equation on the interval  $[x_1, x_2]$  and  $\Phi = \int_{x_1}^{x_2} a(x) dx$  is the flux of the magnetic field through the ring.

*Proof*: The boundary values of the function  $\psi$  satisfy the matching conditions (5) with the matrix S given by (9). The matrix S is both unitary and Hermitian, which implies that

$$S=P_1-P_{-1},$$

where  $P_{\pm 1}$  are orthogonal spectral projectors on the eigensubspaces of S corresponding to the eigenvalues  $\pm 1$ . Hence the matching conditions (5) can be written in the

form [17]:

$$P_{-1} \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \psi(x_4) \\ \psi(x_6) \end{pmatrix} = 0, \qquad P_1 \begin{pmatrix} \partial \psi(x_1) \\ \partial \psi(x_2) \\ \partial \psi(x_4) \\ \partial \psi(x_4) \\ \partial \psi(x_6) \end{pmatrix} = 0.$$
(16)

The corresponding eigensubspaces are two-dimensional and the matching conditions take the form

$$\begin{aligned}
-\psi(x_1) + \alpha \psi(x_2) &+ \beta \psi(x_6) = 0, \\
\alpha \psi(x_1) - \psi(x_2) + \sigma \beta \psi(x_4) &= 0, \\
\partial \psi(x_1) + \alpha \partial \psi(x_2) &+ \beta \partial \psi(x_6) = 0, \\
\alpha \partial \psi(x_1) + \partial \psi(x_2) + \sigma \beta \partial \psi(x_4) &= 0.
\end{aligned}$$
(17)

Consider now the eigenfunction equation (12) on the interval  $[x_1, x_2]$ . The magnetic potential a(x) can be eliminated by the following unitary transformation,

$$\hat{\psi}(x) = \exp\left(-i\int_{x_1}^x a(y)dy\right)\psi(x), \qquad x \in [x_1, x_2].$$

The function  $\hat{\psi}$  satisfies the equation

$$-\frac{d^2}{dx^2}\hat{\psi}(x) + q(x)\hat{\psi}(x) = \lambda\hat{\psi}(x)$$
(18)

instead of (12). If  $T(\lambda) = \{t_{ij}(\lambda)\}_{i,j=1}^2$  is the transfer matrix for the Schrödinger equation with zero magnetic potential (18),

$$T(\lambda)\begin{pmatrix}\hat{\psi}(x_1)\\\hat{\psi}'(x_1)\end{pmatrix} = \begin{pmatrix}\hat{\psi}(x_2)\\\hat{\psi}'(x_2)\end{pmatrix},$$

then the boundary values of  $\psi$  are connected by

$$\begin{cases} \psi(x_2) = e^{i\Phi} t_{11}(\lambda)\psi(x_1) + e^{i\Phi} t_{12}(\lambda)\partial\psi(x_1), \\ \partial\psi(x_2) = -e^{i\Phi} t_{21}(\lambda)\psi(x_1) - e^{i\Phi} t_{22}(\lambda)\partial\psi(x_1). \end{cases}$$
(19)

Eqs. (17) and (19) form a linear system of 6 equations on 8 variables  $\psi(x_1), \psi(x_2), \psi(x_4), \psi(x_6), \partial \psi(x_1), \partial \psi(x_2), \partial \psi(x_4), \partial \psi(x_6)$  and can be written as

280

follows:

$$\begin{pmatrix} -1 & \alpha \\ \alpha & -1 \end{pmatrix} \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \end{pmatrix} = \begin{pmatrix} 0 & -\beta \\ -\sigma\beta & 0 \end{pmatrix} \begin{pmatrix} \psi(x_4) \\ \psi(x_6) \end{pmatrix},$$
$$\begin{pmatrix} 1 & \alpha \\ \alpha & 1 \end{pmatrix} \begin{pmatrix} \partial\psi(x_1) \\ \partial\psi(x_2) \end{pmatrix} = \begin{pmatrix} 0 & -\beta \\ -\sigma\beta & 0 \end{pmatrix} \begin{pmatrix} \partial\psi(x_4) \\ \partial\psi(x_6) \end{pmatrix},$$
$$\begin{pmatrix} e^{i\Phi}t_{12} & 0 \\ e^{i\Phi}t_{22} & 1 \end{pmatrix} \begin{pmatrix} \partial\psi(x_1), \\ \partial\psi(x_2) \end{pmatrix} = \begin{pmatrix} -e^{i\Phi}t_{11} & 1 \\ -e^{i\Phi}t_{21} & 0 \end{pmatrix} \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \end{pmatrix}.$$
(20)

Eliminating  $\psi(x_1), \psi(x_2), \ \partial \psi(x_1), \partial \psi(x_2)$  we calculate the TW-matrix  $M_{\ker \Gamma}(\lambda)$  given by (15). To simplify the expression one has to take into account that:

det 
$$T(\lambda) = 1^1$$
,  $\sigma^2 = 1$ ,  $\beta^2 = 1 - \alpha^2$ .

The calculated TW-matrix is determined by the electric potential (via the transfer matrix T), the flux of the magnetic field  $\Phi$  and  $\alpha$  and  $\sigma$  parameterizing the matrix S. It does not depend on the parameter  $\beta$ , which is determined by  $\alpha$  up to a sign.

### 4. Solution of the inverse problem

This section is devoted to the solution of the inverse problem for the quantum graph operator  $L_{q,a}$ . The TW-matrix is going to play the role of spectral data. To solve the inverse problem one has to recover all components of the triple: the metric graph, the differential operator and the matching conditions. In the following section it will be shown that the scattering matrix for our model has the zero reflection coefficient if all potentials are zero. It follows that the metric graph is not always uniquely determined by the TW-matrix. For this reason we are going to discuss just how to recover the potential in the Schrödinger operator and the parameters determining the matching conditions.

The TW-matrix for the kernel is determined by the transfer matrix T for the magnetic potential-free Schrödinger equation on the loop, the flux  $\Phi$  of the magnetic field and the parameters  $\alpha$  and  $\sigma$  from the matrix S. It follows that the precise form of the magnetic potential a cannot be recovered as well as the parameter  $\beta = \pm \sqrt{1-a^2}$  is determined up to a sign.

THEOREM 1. Let  $L_{q,a}$  be a magnetic Schrödinger operator on the metric graph  $\Gamma$  with the real square integrable potential  $q \in L_2(\Gamma)$  and the real continuous magnetic potential  $a \in C(\Gamma)$  with the domain determined by the matching conditions (5) and the Dirichlet boundary conditions (4). Assume that the TW-matrix function is known for the zero magnetic potential as well as for a certain nonzero magnetic

<sup>&</sup>lt;sup>1</sup>The determinant of  $T(\lambda)$  is one, since it is a transfer matrix for the Schrödinger operator with zero magnetic potential.

potential with  $\Phi = \pi$ , where  $\Phi = \int_{x_1}^{x_2} a(x) dx$  is the total flux of the magnetic field through the ring.

Then these spectral data determine a unique electric potential q on the graph  $\Gamma$  as well as unique parameters  $\alpha$  and  $\sigma$  in the matching conditions (5). In other words, the scattering matrix S (9) from (5) is determined up to one sign parameter.

**Proof:** Consider first the magnetic potential-free Schrödinger equation and the corresponding TW-matrix. In [1] it was shown that this matrix function is in one-to-one correspondence with the dynamical response operator and therefore determines a unique potential q on all boundary edges. In the case of graph  $\Gamma$  this means that the TW-matrix for zero magnetic potential determines the electric potential q on the edges  $[x_3, x_4]$  and  $[x_5, x_6]$ .

Our next step is to reduce the inverse problem for the graph  $\Gamma$  to the inverse problem for its kernel. Let us establish the relation between the corresponding TW-matrices. If the magnetic potential is equal to zero on the boundary edges, then these TW-matrices are in one-to-one correspondence. Let the function  $\psi$  be the unique solution of (12) satisfying matching conditions (5) and prescribed boundary values  $\psi(x_3), \psi(x_5)$ . The TW-matrix for  $\Gamma$  determines  $\partial \psi(x_3), \partial \psi(x_5)$ . Solving the Cauchy problems for the equation

$$-\psi''(x) + q(x)\psi(x) = \lambda\psi(x),$$

on the intervals  $[x_3, x_4]$  and  $[x_5, x_6]$  one determines the boundary values  $\psi^0(x_4)$ ,  $\partial \psi^0(x_4)$ ;  $\psi^0(x_6)$ ,  $\partial \psi^0(x_6)$  in the case of zero magnetic potential (remember that the potential q on  $[x_3, x_4]$  and  $[x_5, x_6]$  is already known). If the magnetic potential is different from zero, then the corresponding boundary values are

$$\begin{cases} \psi(x_4) = e^{i\Phi_2}\psi^0(x_4), \\ \partial\psi(x_4) = e^{i\Phi_2}\partial\psi^0(x_4), \end{cases} \begin{cases} \psi(x_6) = e^{i\Phi_3}\psi^0(x_6), \\ \partial\psi(x_6) = e^{i\Phi_3}\partial\psi^0(x_6). \end{cases}$$

where  $\Phi_j = \int_{x_{2j-1}}^{x_{2j}} a(x)dx$ , j = 2, 3. Let us denote by  $M_{\ker\Gamma}^0$  the 2 × 2 matrix connecting  $\psi^0(x_4), \psi^0(x_6)$  with  $\partial \psi^0(x_4), \partial \psi^0(x_6)$ ,

$$M^0_{\ker \Gamma}: \begin{pmatrix} \psi^0(x_4) \\ \psi^0(x_6) \end{pmatrix} \mapsto - \begin{pmatrix} \partial \psi^0(x_4) \\ \partial \psi^0(x_6) \end{pmatrix}.$$

It allows us to calculate the TW-matrix for the kernel

$$M_{\ker\Gamma}(\lambda, \Phi) = \begin{pmatrix} e^{i\Phi_2} & 0\\ 0 & e^{i\Phi_3} \end{pmatrix} M_{\ker\Gamma}^0 \begin{pmatrix} e^{i\Phi_2} & 0\\ 0 & e^{i\Phi_3} \end{pmatrix}^{-1}.$$

Observe that only the diagonal of the TW-matrix is uniquely determined, since the phases  $\Phi_2$ ,  $\Phi_3$  remain undetermined. In what follows we are going to show that the diagonal of the TW-matrix for the kernel determines the potential on the loop.

Consider the difference

$$(M_{\ker \Gamma}(\lambda, 0))_{11} - (M_{\ker \Gamma}(\lambda, \pi))_{11} = \frac{4\alpha}{1 - \alpha^2} \frac{1}{t_{12}(\lambda)}.$$

Taking into account the asymptotics of the analytic function (see e.g. [25, 26])

$$t_{12}(\lambda) \sim \frac{\sin k l_1}{k}, \qquad k \to \infty,$$

both the function  $t_{12}$  and the ratio  $r \equiv \frac{1-\alpha^2}{\alpha} = \frac{1}{\alpha} - \alpha$  are determined by the difference. Every r determines a unique  $\alpha$  from the interval (-1, 1). The functions  $t_{11}$  and  $t_{22}$  can be calculated now as

$$t_{11}(\lambda) = \frac{1}{1+\alpha^2} \left( 2\alpha + t_{12}(\lambda)(\alpha^2 (M_{\ker\Gamma}(\lambda,0))_{11} - (M_{\ker\Gamma}(\lambda,0))_{22}), \\ t_{22}(\lambda) = \frac{1}{1+\alpha^2} \left( 2\alpha + t_{12}(\lambda)(\alpha^2 (M_{\ker\Gamma}(\lambda,0))_{22} - (M_{\ker\Gamma}(\lambda,0))_{11}) \right).$$
(21)

The functions  $t_{12}$  and  $t_{22}$  determine the unique potential q on the interval  $[x_1, x_2]$  [8, 9, 24–26].

The sign parameter  $\sigma$  can be determined from the TW-matrix in the case of zero magnetic potential<sup>1</sup>,

$$\sigma = \frac{(1 - \alpha^2) t_{12}(\lambda) \left( M_{\ker \Gamma}(\lambda, 0) \right)_{12}}{1 + \alpha^2 - \alpha \operatorname{Tr} T(\lambda)}.$$
(22)

Thus we have determined the potential q on the whole  $\Gamma$  as well as parameters  $\alpha$  and  $\sigma$  appearing in the matching conditions.

We would like to underline that our approach gives an explicit procedure to reconstruct the potential. The main difference to the inverse problem for trees is that potential on the loop is not reconstructed locally but on the whole loop at once.

Since the TW-matrix for the kernel does not depend on the sign of the parameter  $\beta$ , it is more or less clear that this sign cannot be determined from the general TW-matrix. One may consider the following unitary transformation in  $L_2(\Gamma)$ ,

$$(Uf)(x) = \begin{cases} -f(x), & x \in (x_1, x_2), \\ f(x), & x \in (x_3, x_4) \cup (x_5, x_6). \end{cases}$$
(23)

The Schrödinger operator  $U^{-1}L_{q,a}U$  is determined by the same differential expression as the operator  $L_{q,a}$ , the Dirichlet conditions at the boundary vertices and by matching conditions (5) with the parameters  $\alpha, -\beta, \sigma$  instead of  $\alpha, \beta, \sigma$ . The TW-matrices for these two Schrödinger operators are identical.

<sup>&</sup>lt;sup>1</sup>Note that the right-hand side has to be independent of  $\lambda$ .

Extending the set of spectral data by adding the TW-matrix for a few other values of the magnetic flux  $\Phi$  will not allow us to calculate the unique matrix S from the matching conditions.

It is clear that a similar result can be proven if the TW-matrices are known for two other values of the magnetic flux, not necessarily  $\Phi = 0, \pi$ . We needed the TW-matrix for zero magnetic field ( $\Phi = 0$ ) in order to be able to calculate  $\sigma$ . It also appears natural to use  $\Phi = \pi$  since this value of the magnetic flux can easily be identified by examining experimental data.

If the matching conditions at the vertex  $v_1$  are known, then the potential can be reconstructed without considering TW-matrices depending on the magnetic flux.

THEOREM 2. Let  $L_q$  be a magnetic potential-free Schrödinger operator on the metric graph  $\Gamma$  with the real square integrable potential  $q \in L_2(\Gamma)$  with the domain determined by the matching conditions (5) and the Dirichlet boundary conditions (4). Assume that the parameters  $\sigma$ ,  $\alpha$  and  $\beta$  appearing in the matrix S parameterizing the matching conditions are known.

Then the TW-matrix function determines a unique potential q on the graph  $\Gamma$ .

*Proof*: During the proof of Theorem 1 we already showed that the TW-matrix for zero magnetic potential determines a unique electric potential q on the boundary edges as well as the TW-matrix associated with the kernel of the graph.

In the case of zero magnetic potential  $\Phi = 0$  the formulae (20) give the following expression for the TW-matrix

$$\begin{split} M_{\ker\Gamma}(\lambda, 0) \\ &= -\frac{1}{\sigma\beta^2} \binom{\alpha\beta}{\sigma\beta} \frac{\beta}{\sigma\alpha\beta} \frac{1}{t_{12}(\lambda)} \binom{-t_{11}(\lambda)}{1} \frac{1}{1-\alpha^2} \binom{\sigma\alpha\beta}{\sigma\beta} \frac{\beta}{\alpha\beta}, \end{split}$$

which implies directly that

$$\frac{1}{t_{12}(\lambda)} \begin{pmatrix} -t_{11}(\lambda) & 1\\ 1 & -t_{22}(\lambda) \end{pmatrix} = \frac{1}{1-\alpha^2} \begin{pmatrix} \sigma \alpha & -1\\ -\sigma & \alpha \end{pmatrix} M_{\ker\Gamma}(\lambda, 0) \begin{pmatrix} \sigma \alpha & -\sigma\\ -1 & \alpha \end{pmatrix}.$$
 (24)

Formula (24) allows one to calculate the functions  $t_{11}$ ,  $t_{12}$  and  $t_{22}$  and therefore to reconstruct the whole transfer matrix  $T(\lambda)$ . It determines a unique potential q even on the loop.

The last theorem shows that the potential on the loop may be reconstructed even without considering the dependence of the spectral data on the magnetic flux. This is due to a very special form of the matching conditions at the vertex connecting the loop to the one-dimensional wire. Both spectral subspaces for the matrix S corresponding to the eigenvalues  $\pm 1$  have dimension 2. We used this property to calculate the transformed transfer matrix T using (24). The reconstruction procedure is again explicit.

### 5. The scattering problem

This section is devoted to a brief discussion of the scattering problem associated with the Aharonov–Bohm ring attached to the infinite wire (see Fig. 4).



Fig. 4. Graph  $\Gamma_2$ . An infinite wire with an Aharonov–Bohm ring attached.

We assume for simplicity that both electric and magnetic potentials q and a, respectively, are equal to zero on the infinite wire. The operator is determined by the same differential expression (3) and the same matching conditions (5) with points  $0^{\pm}$  substituting the points  $x_4$  and  $x_6$ , respectively. Every generalized eigenfunction restricted to the infinite wire is a linear combination of incoming and outgoing waves

$$\psi(k^2, x) = \begin{cases} b_1 e^{ikx} + a_1 e^{-ikx}, & x < 0, \\ a_2 e^{ikx} + b_2 e^{-ikx}, & x > 0. \end{cases}$$
(25)

The  $2 \times 2$  matrix S(k) connecting the amplitudes of incoming and outgoing waves,

 $\mathbb{S}(k): \binom{b_1}{b_2} \mapsto \binom{a_1}{a_2}, \tag{26}$ 

is the scattering matrix for the quantum graph  $\Gamma_2$ . It is in one-to-one correspondence with the TW-matrix for the kernel

$$\mathbb{S}(k) = \frac{ikI - M_{\ker\Gamma}(k^2, \Phi)}{ikI + M_{\ker\Gamma}(k^2, \Phi)}.$$
(27)

It follows that the scattering matrix known for two different values of the magnetic flux can play the role of spectral data (instead of the TW-matrix).

The calculated scattering matrix has another important property: if the potential q on the loop is equal to zero, then the reflection coefficients in the matrix S (i.e. the coefficients  $S_{11}$  and  $S_{22}$ ) are identically equal to zero. Really, let us calculate the entry  $S_{11}$ 

$$\mathbb{S}_{11} = \frac{-1}{\det(ik+M_{\ker\Gamma})} \left(k^2 + ik((M_{\ker\Gamma})_{11} - (M_{\ker\Gamma})_{22}) + \det M_{\ker\Gamma}\right).$$

Standard straightforward calculations in the case of zero potential q give the transfer matrix

$$T(\lambda) = \left(\begin{array}{c} \cos kl_1 & \sin kl_1/k \\ -k\sin kl_1 & \cos kl_1 \end{array}\right).$$

It follows that

$$k^{2} + ik((M_{\ker\Gamma})_{11} - (M_{\ker\Gamma})_{22}) + \det M_{\ker\Gamma} = 0,$$

i.e.  $\mathbb{S}_{11} = 0$ . Similar calculations prove that  $\mathbb{S}_{22} = 0$ .

It follows that if the contact vertex between the wire and the ring is not placed at the origin (as for the graph  $\Gamma_2$ ), then its position cannot be determined from the scattering matrix. Similarly, for the graph  $\Gamma$  the lengths of the edges  $[x_3, x_4]$  and  $[x_5, x_6]$  are not determined by the TW-matrix in the case of zero electric potential q.

### 6. Conclusions

A mathematically rigorous model of the quantum system consisting of a wire connected to an Aharonov–Bohm ring is developed. The corresponding TW-matrix and scattering matrix are calculated. Both matrices depend on the flux  $\Phi$  of the magnetic field through the ring. A special form of the matching conditions at the contact vertex allows us to determine a unique electric potential q on the whole graph, whereas geometric parameters of the graph are not always uniquely determined. This example shows that the inverse problem for quantum graphs even with loops may have a unique solution, provided that the matching conditions are different from standard. It might be interesting to characterize all matching conditions leading to a unique solution to the inverse problem. Our example of graphs with equal TW-matrices is important for studies of isospectral graphs [3, 4, 7, 15, 20, 21, 23, 27].

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