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A model of an electron in a quantum graph interacting with a two-level system

A. A. Boitsev, I. Y. Popov

ITMO University, Kronverkskiy, 49, St. Petersburg, 197101, Russia

boitsevanton@gmail.com, popov1955@gmail.com

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A model of an electron in a quantum graph interacting with a two-level system is considered. The operator describing the model has the form of sum of tensor products. Self-adjoint extensions and a scattering matrix are written in terms of a boundary triplet, corresponding to the considered symmetric operator. Diagrams of reflection are calculated and numerical results are discussed .

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1. Introduction

Electron transport in nanostructures under the action of a magnetic field attracts great attention during last decades. The reason is observation of many interesting effects found applications in nanoelectronics. One of such intriguing problems is that of Aharonov-Bohm oscillations in quantum transport [1–3]. Several models were suggested to describe the phenomenon. One of the most effective in the field is the quantum graph model (see, e.g., [4–7]). An excellent review of the state of the art in quantum graph theory is presented in [8].

We are interested in the case when the system (quantum graph) with an Aharonov-Bohm ring interacts with another system having two energy levels. In this case, the operator of the whole system has the form of a sum of tensor products:

$$S := A_{\mathfrak{H}} \otimes I_{\mathfrak{T}} + I_{\mathfrak{H}} \otimes T_{\mathfrak{T}},$$

where self-adjoint operators A and T act in Hilbert spaces $\mathfrak{H}$ and $\mathfrak{T}$, respectively. It is well known that such operators describe the interaction of two quantum systems. Extension technique for such operators is widely discussed in [9]. We introduce a model for an electron in a quantum graph interacting with a two-level system. Such an operator also preserves a tensor structure described above. The first operator A stands for the quantum graph and the second operator T, which is, actually, a 2×2 matrix, describes the two-level system.

In the following, we investigate the considered operator using boundary triplets approach and the results from [9]. Scattering matrix is obtained and the diagrams of the argument of the reflection coefficient (scattering phase) are constructed. The scattering has a resonance character.

2. Preliminaries

2.1. Linear relations

A linear relation Θ in $\mathcal{H}$ is a closed linear subspace of $\mathcal{H} \oplus \mathcal{H}$. The set of all linear relations in $\mathcal{H}$ is denoted by $\widetilde{\mathcal{C}}(\mathcal{H})$. We denote also by $\mathcal{C}(\mathcal{H})$ the set of all closed linear (not necessarily densely defined) operators in $\mathcal{H}$. Identifying each operator $T \in \mathcal{C}(\mathcal{H})$ with its graph $\mathrm{gr}\,(T)$, we regard $\mathcal{C}(\mathcal{H})$ as a subset of $\widetilde{\mathcal{C}}(\mathcal{H})$.

The role of the set $\widetilde{\mathcal{C}}(\mathcal{H})$ in extension theory becomes clear from Proposition 2.3. However, its role in the operator theory is substantially motivated by the following circumstances: in contrast to $\mathcal{C}(\mathcal{H})$, the set $\widetilde{\mathcal{C}}(\mathcal{H})$ is closed with respect to taking inverse and adjoint relations Θ^{-1} and Θ^*. The latter is given by: $\Theta^{-1} = \{\{g, f\} : \{f, g\} \in \Theta\}$ and

$$\Theta^* = \left\{ \begin{pmatrix} k \\ k' \end{pmatrix} : (h', k) = (h, k') \text{ for all } \begin{pmatrix} h \\ h' \end{pmatrix} \in \Theta \right\}. \tag{1}$$

A linear relation Θ is called symmetric if $\Theta \subset \Theta^*$ and self-adjoint if $\Theta = \Theta^*$.

2.2. Boundary triplets and proper extensions

Let us briefly recall some basic facts regarding boundary triplets. Let S be a densely defined closed symmetric operator with equal deficiency indices $n_{\pm}(S) := \dim(\mathfrak{N}_{\pm i})$, $\mathfrak{N}_z := \ker(S^* - z)$, $z \in \mathbb{C}_{\pm}$, acting on some separable Hilbert space $\mathfrak{H}$.

Definition 2.1.
(i) *A closed extension* $\widetilde{S}$ *of* S *is called proper if* $\operatorname{dom}(S) \subset \operatorname{dom}(\widetilde{S}) \subset \operatorname{dom}(S^*)$.
(ii) *Two proper extensions* $\widetilde{S}'$, $\widetilde{S}$ *are called disjoint if* $\operatorname{dom}(\widetilde{S}') \cap \operatorname{dom}(\widetilde{S}) = \operatorname{dom}(S)$ *and transversal if in addition* $\operatorname{dom}(\widetilde{S}') + \operatorname{dom}(\widetilde{S}) = \operatorname{dom}(S^*)$.

We denote by $\mathrm{Ext_S}$ the set of all proper extensions of S completed by the non-proper extensions S and S^* is denoted. For instance, any self-adjoint or maximal dissipative (accumulative) extension is proper.

Definition 2.2 ([10]). A triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$, where $\mathcal{H}$ is an auxiliary Hilbert space and $\Gamma_0, \Gamma_1 : \operatorname{dom}(S^*) \to \mathcal{H}$ are linear mappings, is called a boundary triplet for S^* if the "abstract Green's identity":

$$(S^*f, g) - (f, S^*g) = (\Gamma_1 f, \Gamma_0 g) - (\Gamma_0 f, \Gamma_1 g), \;\; f, g \in \operatorname{dom}(S^*). \tag{2}$$

is satisfied and the mapping $\Gamma := (\Gamma_0, \Gamma_1)^{\top} : \operatorname{dom}(S^*) \to \mathcal{H} \oplus \mathcal{H}$ is surjective, i.e. $\operatorname{ran}(\Gamma) = \mathcal{H} \oplus \mathcal{H}$.

A boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ for S^* always exists whenever $n_+(S) = n_-(S)$. Note also that $n_{\pm}(S) = \dim(\mathcal{H})$ and $\ker(\Gamma_0) \cap \ker(\Gamma_1) = \operatorname{dom}(S)$.

With any boundary triplet Π, one associates two canonical self-adjoint extensions $S_j := S^* \restriction \ker(\Gamma_j)$, $j \in \{0, 1\}$. Conversely, for any extension $S_0 = S_0^* \in \mathrm{Ext_S}$ there exists a (non-unique) boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ for S^* such that $S_0 := S^* \restriction \ker(\Gamma_0)$.

Using the concept of boundary triplets one can parameterize all proper extensions of A in the following way.

Proposition 2.3 ([11, 12]). *Let* $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ *be a boundary triplet for* S^*. *Then the mapping:*

$$\mathrm{Ext_S} \ni \widetilde{\mathrm{S}} \to \Gamma \mathrm{dom}\,(\widetilde{\mathrm{S}}) = \{(\Gamma_0 \mathrm{f}, \Gamma_1 \mathrm{f})^{\top} : \; \mathrm{f} \in \mathrm{dom}\,(\widetilde{\mathrm{S}})\} =: \Theta \in \widetilde{\mathcal{C}}(\mathcal{H}) \tag{3}$$

establishes a bijective correspondence between the sets $\mathrm{Ext_S}$ *and* $\widetilde{\mathcal{C}}(\mathcal{H})$. *We write* $\widetilde{S} = S_\Theta$ *if* $\widetilde{S}$ *corresponds to* Θ *by* (3). *Moreover, the following holds:*
(i) $S_\Theta^* = S_{\Theta^*}$, *in particular,* $S_\Theta^* = S_\Theta$ *if and only if* $\Theta^* = \Theta$.
(ii) S_Θ *is symmetric (self-adjoint) if and only if* Θ *is symmetric (self-adjoint).*
(iii) *The extensions* S_Θ *and* S_0 *are disjoint (transversal) if and only if there is a closed (bounded) operator* B *such that* $\Theta = \operatorname{gr}(B)$. *In this case* (3) *takes the form:*

$$S_\Theta := S_{\operatorname{gr}(B)} = S^* \restriction \ker(\Gamma_1 - B\Gamma_0). \tag{4}$$

In particular, $S_j := S^* \restriction \ker(\Gamma_j) = S_{\Theta_j}$, $j \in \{0, 1\}$, where $\Theta_0 := \begin{pmatrix} \{0\} \\ \mathcal{H} \end{pmatrix}$ and $\Theta_1 := \begin{pmatrix} \mathcal{H} \\ \{0\} \end{pmatrix} = \operatorname{gr}(\mathbb{O})$ where $\mathbb{O}$ denotes the zero operator in $\mathcal{H}$. Note also that $\widetilde{\mathcal{C}}(\mathcal{H})$ contains the trivial linear relations $\{0\} \times \{0\}$ and $\mathcal{H} \times \mathcal{H}$ parameterizing the extensions S and S^*, respectively, for any boundary triplet Π.

2.3. Gamma field and Weyl function

It is well known that Weyl function is an important tool in the direct and inverse spectral theory of Sturm-Liouville operators. In [11, 12] the concept of Weyl function was generalized to the case of an arbitrary symmetric operator S with $n_+(S) = n_-(S) \leqslant \infty$. Following [11] we briefly recall basic facts on Weyl functions and γ-fields associated with a boundary triplet Π.

Definition 2.4 ([11, 12]). Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for S^* and $S_0 = S^* \restriction \ker(\Gamma_0)$. The operator valued functions $\gamma(\cdot) : \rho(S_0) \to [\mathcal{H}, \mathcal{H}]$ and $M(\cdot) : \; \rho(S_0) \to [\mathcal{H}]$ defined by:

$$\gamma(z) := \left(\Gamma_0 \restriction \mathfrak{N}_z\right)^{-1} \qquad M(z) := \Gamma_1 \gamma(z), \quad z \in \rho(S_0), \tag{5}$$

are called the γ-field and the Weyl function, respectively, corresponding to the boundary triplet Π.

Clearly, the Weyl function can equivalently be defined by:

$$M(z)\Gamma_0 f_z = \Gamma_1 f_z, \qquad f_z \in \mathfrak{N}_z, \quad z \in \rho(S_0). \tag{6}$$

The γ-field $\gamma(\cdot)$ and the Weyl function $M(\cdot)$ in (5) are well defined. Moreover, both $\gamma(\cdot)$ and $M(\cdot)$ are holomorphic on $\rho(S_0)$ and the following relations:

$$\gamma(z) = \big(I + (z-\zeta)(S_0 - z)^{-1}\big)\gamma(\zeta),\ z,\zeta \in \rho(S_0), \tag{7}$$

and

$$M(z) - M(\zeta)^* = (z-\overline{\zeta})\gamma(\zeta)^*\gamma(z),\ z,\zeta \in \rho(S_0), \tag{8}$$

hold. Identity (8) yields that $M(\cdot)$ is $[\mathcal{H}]$-valued Nevanlinna function ($M(\cdot) \in R[\mathcal{H}]$), i.e. $M(\cdot)$ is $[\mathcal{H}]$-valued holomorphic function on $\mathbb{C}_\pm$ satisfying:

$$M(z) = M(\overline{z})^* \qquad \text{and} \qquad \frac{\mathrm{Im}(M(z))}{\mathrm{Im}(z)} \geqslant 0,\ z \in \mathbb{C}_+ \cup \mathbb{C}_-. \tag{9}$$

It also follows from (8) that $0 \in \rho(\mathrm{Im}(M(z)))$ for all $z \in \mathbb{C}_\pm$.

2.4. Krein-type formula for resolvents

Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for S^*, $M(\cdot)$ and $\gamma(\cdot)$ the corresponding Weyl function and γ-field, respectively. For any proper (not necessarily self-adjoint) extension $\widetilde{S}_\Theta \in \mathrm{Ext}_\mathrm{S}$ with non-empty resolvent set $\rho(\widetilde{S}_\Theta)$ the following Krein-type formula holds (cf. [11, 12]):

$$(S_\Theta - z)^{-1} - (S_0 - z)^{-1} = \gamma(z)(\Theta - M(z))^{-1}\gamma^*(\overline{z}),\ z \in \rho(S_0) \cap \rho(S_\Theta). \tag{10}$$

Formula (10) extends the known Krein formula for canonical resolvents to the case of any $S_\Theta \in \mathrm{Ext}_\mathrm{S}$ with $\rho(S_\Theta) \neq \emptyset$. Moreover, due to relations (3), (4) and (5) formula (10) is related to the boundary triplet Π. We emphasize, that this relation makes it possible to apply the Krein-type formula (10) to boundary value problems (see, e.g., [13, 14]).

2.5. Scattering

Let S be a densely defined closed symmetric operator with finite equal deficiency indices $n_\pm(S)$ and $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is a boundary triplet for S^*, Let $S_0 = S^* \upharpoonright \ker \Gamma_0$ and S_Θ is a self-adjoint extension corresponding to $\Theta \in \tilde{C}(\mathcal{H})$. As $\dim \mathcal{H}$ is finite, by 10

$$(S_\Theta - z)^{-1} - (S_0 - z)^{-1}, \tag{11}$$

is a finite rank operator and the system $\{S_\Theta, S_0\}$ is a so-called complete scattering system, i.e. the wave operators:

$$W_\pm(S_\Theta, S_0) = s - \lim_{t\to\pm\infty} e^{itS_\Theta} e^{-itS_0} P^{ac}(S_0) \tag{12}$$

exists and they are complete, i.e. their ranges coincide with the absolutely continuous subspace $\mathfrak{H}^{ac}(S_\Theta)$ of S_Θ (see, e.g. [17], [15], [16]). By $P^{ac}(S_0)$ we denote the orthogonal projection on absolutely continuous subspace $\mathfrak{H}^{ac}(S_0)$ of S_0. The scattering operator $S(S_\Theta, S_0)$ of a scattering system $\{S_\Theta, S_0\}$ is defined as:

$$S(S_\Theta, S_0) = W_+(S_\Theta, S_0)^* W_-(S_\Theta, S_0). \tag{13}$$

If we regard the scattering operator as an operator in $\mathfrak{H}^{ac}(S_0)$ then it becomes unitary and commutes with absolutely continuous part:

$$S_0^{ac} = S_0 \upharpoonright \mathfrak{H}^{ac}(S_0) \cap \mathrm{dom}\,(S_0). \tag{14}$$

of S_0 and thus it is unitarily equivalent to a multiplication operator induced by a family $\{S_\Theta(z)\}$ of unitary operators in a spectral representation of S_0^{ac} ([17], Proposition 9.57). Tis family is called a scattering matrix of a scattering system $S(S_\Theta, S_0)$.

Since the dimension $\dim \mathcal{H}$ is finite then the Weyl function $M(\cdot)$ corresponding to boundary triplet $\Pi = \{\mathfrak{H}, \Gamma_0, \Gamma_1\}$ is a matrix-valued Nevanlinna function. By Fatous theorem ([18]), the limit:

$$M(\lambda + i0) = \lim_{\varepsilon\to 0+0} M(\lambda + i\varepsilon) \tag{15}$$

exists for almost all $\lambda \in \mathbb{R}$. We denote the set of real point where the limit exists by Σ^M. We will use the notation:

$$\mathcal{H}_{M(\lambda)} = \mathrm{ran}\,(M(\lambda)), \quad \lambda \in \Sigma^M. \tag{16}$$

By $P_{M(\lambda)}$ we will denote the orthogonal projection on $\mathcal{H}_{M(\lambda)}$.

We will also use the notation:

$$N_\Theta(z) = (\Theta - M(z))^{-1}, \quad z \in \mathbb{C} \setminus \mathbb{R}, \tag{17}$$

where $\Theta \in \tilde{C}(\mathcal{H})$ is a self-adjoint relation corresponding to S_Θ. This function is well defined and the limit:

$$N_\Theta(\lambda + i0) = (\Theta - M(\lambda + i0))^{-1}, \tag{18}$$

exists almost for every $\lambda \in \mathbb{R}$. This set we will denote as Σ^N.

Theorem 2.5. *([14]) Let S be a densely defined symmetric operator with finite deficiency indices in separable Hilbert space $\mathfrak{H}$, let Π be a boundary triplet corresponding to S^* with corresponding Weyl function $M(\cdot)$, S_Θ is a self-adjoint extension of S, $S_0 = S^* \upharpoonright \ker \Gamma_0$, $\Theta \in \tilde{C}(\mathcal{H})$, then in $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{M(\lambda)})$ the scattering matrix of the complete scattering system $\{S_\Theta, S_0\}$ is given by:*

$$\mathfrak{S}_\Theta(\lambda) = I_{\mathcal{H}_{M(\lambda)}} + 2i\sqrt{\Im(M(\lambda+i0))}N_\theta(\lambda+i0)\sqrt{\Im(M(\lambda+i0))}, \tag{19}$$

for $\lambda \in \Sigma^M \cap \Sigma^N$.

3. Model construction

3.1. An electron in quantum graph

Let us consider a Hilbert space $\mathfrak{H}_1 = L^2(C_r \cup [-1, 0])$, $r > 0$, where:

$$C_r := \{x \in \mathbb{R}^2 : \ \rho(x, -1 - r) = r\}, \tag{20}$$

so that our Hilbert space is a union of a line segment $[-1, 1]$ and a ring with center at the point $(-1 - r) \in \mathbb{R}$ of radius r. In a ring we consider an operator (x stands for the angle φ in polar coordinates):

$$A_R f := -\left(\frac{1}{r}\frac{d}{dx} + i\Phi\right)^2 f \tag{21}$$

with domain $\operatorname{dom} A_R = \{f \in W^{2,2}[0, 2\pi] : f(0) = f(2\pi) = 0\}$. Let us show that the operator is self-adjoint. Integrating by parts, we have:

$$(A_R f, g) = -\int_0^{2\pi}\left(\frac{1}{r^2}f'' - \frac{2i}{r}\Phi f' - \Phi^2 f\right)\overline{g}dx = -\frac{1}{r^2}\int_0^{2\pi} f''\overline{g}dx + \frac{2i}{r}\Phi\int_0^{2\pi} f'\overline{g}dx - \Phi^2\int_0^{2\pi} f\overline{g}dx =$$

$$-\frac{1}{r^2}\left(f'(2\pi)\overline{g}(2\pi) - f'(0)\overline{g}(0) + f(0)\overline{g}'(0) - f(2\pi)\overline{g}'(2\pi) + \int_0^{2\pi} f\overline{g}''dx\right) +$$

$$\frac{2\Phi}{r}\left(i\left(f(2\pi)\overline{g}(2\pi) - f(0)\overline{g}(0)\right) + \int_0^{2\pi} f\overline{ig}dx\right) + \Phi^2\int_0^{2\pi} f\overline{g}dx =$$

$$-\frac{1}{r^2}\left(f'(2\pi)\overline{g}(2\pi) - f'(0)\overline{g}(0) + f(0)\overline{g}'(0) - f(2\pi)\overline{g}'(2\pi)\right) + \frac{2\Phi}{r}i\left(f(2\pi)\overline{g}(2\pi) - f(0)\overline{g}(0)\right) +$$

$$\int_0^{2\pi} f\overline{\left(-\frac{1}{r^2}g'' + \frac{2\Phi}{r}ig' + \Phi^2 g\right)}dx.$$

This proves the statement.

Now we introduce a self-adjoint operator $A_S := -\dfrac{d^2}{dx^2}$ in $L^2[-1, 0]$ with domain $\operatorname{dom} A_S = \{f \in W^{2,2}[-1, 0] : f(-1) = f(0) = 0\}$.

In compound system we consider an operator A_1 acting in $\mathfrak{H}_1$ as an operator A_R on a circle and A_S on a line segment. To make it symmetric, we restrict it on a set of functions with the conditions:

$$\begin{array}{c} f_2(-1) = f_1(0) = f_1(2\pi) \\ f_2'(-1) + \left(\dfrac{d}{dx} + i\Phi\right) f_1(0) - \left(\dfrac{d}{dx} + i\Phi\right) f_1(2\pi) = 0 \end{array}, \tag{22}$$

where $f_1 \in \operatorname{dom} A_R$, $f_2 \in \operatorname{dom} A_S$. To find the deficiency elements of A_1 we firstly solve the equation $A_R f = zf$ and come to an algebraic equation:

$$-\left(\frac{1}{r}\lambda - i\Phi\right)^2 = z \Leftrightarrow \frac{1}{r}\lambda - i\Phi = \pm\sqrt{z} \tag{23}$$

or $\lambda = i\left(r\Phi \pm r\sqrt{z}\right)$. The deficiency elements (if we choose the branch $\Im\sqrt{z} > 0$) are $e^{irx(\Phi\pm\sqrt{z})}$. For the operator A_S deficiency elements are $e^{\pm i\sqrt{z}}$. To find the deficiency elements of the considered operator A_1, we solve the system of algebraic equations. We start by introducing:

$$f_1 := c_3 e^{irx(\Phi+\sqrt{z})} + c_4 e^{irx(\Phi-\sqrt{z})}, \quad f_2 := c_1 e^{i\sqrt{z}} + c_2 e^{-i\sqrt{z}}, \quad c_i \in \mathbb{C} \tag{24}$$

and for simplicity introduce the notation $a := e^{-i\sqrt{z}}$, $b := e^{i\sqrt{z}}$, $f := e^{2\pi ir(\Phi+\sqrt{z})}$, $d := e^{2\pi ir(\Phi-\sqrt{z})}$. Then, from the boundary conditions, we obtain:

$$\begin{cases} c_1 a + c_2 b = c_3 + c_4, \\ c_3 + c_4 = c_3 f + c_4 d, \\ c_1\sqrt{z}a - c_2\sqrt{z}b + c_3\left(r(\Phi+\sqrt{z})(1-f) + \Phi(1-f)\right) + c_4\left(r(\Phi-\sqrt{z})(1-d) + \Phi(1-d)\right) = 0. \end{cases}$$

Solving the system above, we obtain:

$$f_1 = c_4 \frac{d-1}{1-f} e^{irx(\Phi+\sqrt{z})} + c_4 e^{irx(\Phi-\sqrt{z})}, \tag{25}$$

$$\begin{aligned} f_2 = \frac{c_4}{2a}\left(\frac{d - f - 2rd + 2rdf + 2r - 2rf}{1-f}\right) e^{i\sqrt{z}x} + \\ \frac{c_4}{2b}\left(\frac{d - f + 2rd - 2rdf - 2r + 2rf}{1-f}\right) e^{-i\sqrt{z}x}. \end{aligned} \tag{26}$$

So, the deficiency indices of the operator A_1 are equal to 1, i.e. $n_\pm(A_1) = 1$.

The boundary triplet for the operator A_1 is as follows:

$$\mathcal{H}^{A_1} := \mathbb{C}, \quad \Gamma_0^{A_1} := f(0), \quad \Gamma_1^{A_1} := -f'(0).$$

One immediately checks that the equation (2.2) is satisfied. For simplicity we put $c_4 = 2(1-f)$ in (25) and (26). Then,

$$\Gamma_0^{A_1} f_2 = \frac{1}{a}\left(d - f - 2rd + 2rdf + 2r - 2rf\right) + \frac{1}{b}\left(d - f + 2rd - 2rdf - 2r + 2rf\right). \tag{27}$$

Putting:

$$u := \frac{1}{a}\left(d - f - 2rd + 2rdf + 2r - 2rf\right), \tag{28}$$

$$v := \frac{1}{b}\left(d - f + 2rd - 2rdf - 2r + 2rf\right), \tag{29}$$

the γ-field $\gamma^{A_1}(z)$ has the form (in accordance with definition 2.4):

$$\gamma^{A_1}(z) := \frac{1}{u+v}\left(ue^{i\sqrt{z}x} + ve^{-i\sqrt{z}x}\right). \tag{30}$$

Then the Weyl function (in accordance with definition 2.4) is:

$$M^{A_1}(z) := \Gamma_1^{A_1}\gamma^{A_1}(z) = -\frac{i\sqrt{z}(u-v)}{u+v}. \tag{31}$$

To obtain the scattering matrix (19), we have to calculate the limit of the Weyl function (2.4) to the real axis from the upper half-plane. All the calculations with the final expressions are obtained in Appendix A.

3.2. Operator on a half-line

Let us consider an operator:

$$A_2 := -\frac{d^2}{dx^2}, \tag{32}$$

with the domain $\operatorname{dom} A_2 = W_{00}^{2,2} = \{f \in W^{2,2}(0,\infty) : f(0) = f'(0) = 0\}$ in $\mathfrak{H}_2 = L^2(0,\infty)$. It is symmetric and its deficiency indices are $n_\pm(A_3) = 1$. In accordance with [9], the Weyl function for this operator has the following form:

$$M^{A_3}(z) := i\sqrt{z}.$$

It is clear that:

$$\Im M^{A_3}(\lambda) = \Im\left(i\sqrt{\lambda}\right) = \sqrt{\lambda}, \quad \lambda \geqslant 0$$

and 0 otherwise.

3.3. The direct sum of the operators

We consider the Hilbert space $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2$ where $\mathfrak{H}_1$ and $\mathfrak{H}_2$ are defined above. We define an operator A as the operator:

$$A := A_1 \oplus A_2. \tag{33}$$

The operator A is symmetric and has deficiency indices $n_\pm(A) = 2$. It's Weyl function is obviously given by the expression:

$$M^A(z) = \begin{pmatrix} M^{A_1}(z) & 0 \\ 0 & M^{A_2}(z) \end{pmatrix} = \begin{pmatrix} -\dfrac{i\sqrt{z}(u-v)}{u+v} & 0 \\ 0 & i\sqrt{z} \end{pmatrix}. \tag{34}$$

3.4. Coupling to the two-level system

Now let us couple the considered operator to an operator:

$$T := \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \tag{35}$$

acting on the Hilbert space $\mathfrak{T} = \mathbb{C}^2$. For this purpose we consider an operator

$$S = A_{\mathfrak{H}} \otimes I_{\mathfrak{T}} + I_{\mathfrak{H}} \otimes T_{\mathfrak{T}}. \tag{36}$$

In accordance with [9], we have:

$$M^S(z) = M^A(z-1) \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + M^A(z-2) \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \tag{37}$$

$$\begin{pmatrix} M^{A_1}(z-1) & 0 & 0 & 0 \\ 0 & M^{A_1}(z-2) & 0 & 0 \\ 0 & 0 & M^{A_2}(z-1) & 0 \\ 0 & 0 & 0 & M^{A_2}(z-2) \end{pmatrix}. \tag{38}$$

To find the scattering matrix, we need to calculate the limit of the Weyl function to the real axis which is, obviously:

$$M^S(\lambda) = M^S(\lambda + i0) = \begin{pmatrix} M^{A_1}(\lambda-1) & 0 & 0 & 0 \\ 0 & M^{A_1}(\lambda-2) & 0 & 0 \\ 0 & 0 & M^{A_2}(\lambda-1) & 0 \\ 0 & 0 & 0 & M^{A_2}(\lambda-2) \end{pmatrix}. \tag{39}$$

Now we need to calculate the imaginary part of the obtained limit. This gives us

$$\sqrt{\Im M^S(\lambda)} = \begin{pmatrix} \sqrt{\Im M^{A_1}(\lambda-1)} & 0 & 0 & 0 \\ 0 & \sqrt{\Im M^{A_1}(\lambda-2)} & 0 & 0 \\ 0 & 0 & \sqrt{\Im M^{A_2}(\lambda-1)} & 0 \\ 0 & 0 & 0 & \sqrt{\Im M^{A_2}(\lambda-2)} \end{pmatrix}. \tag{40}$$

3.5. Scattering matrix

Let us take the matrix of parameters Θ in the form ($\alpha, \beta \in \mathbb{C}$):

$$\Theta = \begin{pmatrix} 0 & \alpha & 0 & 0 \\ \overline{\alpha} & 0 & \beta & 0 \\ 0 & \overline{\beta} & 0 & \alpha \\ 0 & 0 & \overline{\alpha} & 0 \end{pmatrix}. \tag{41}$$

Then:

$$N_\Theta(\lambda) = (\Theta - M^S(\lambda))^{-1} = \begin{pmatrix} -M^{A_1}(\lambda-1) & \alpha & 0 & 0 \\ \overline{\alpha} & -M^{A_1}(\lambda-2) & \beta & 0 \\ 0 & \overline{\beta} & -M^{A_2}(\lambda-1) & \alpha \\ 0 & 0 & \overline{\alpha} & -M^{A_2}(\lambda-2) \end{pmatrix}^{-1}. \tag{42}$$

We denote:

$$a_{11} = M^{A_1}(\lambda - 1), \quad a_{22} = M^{A_1}(\lambda - 2), \quad a_{33} = M^{A_2}(\lambda - 1), \quad a_{44} = M^{A_2}(\lambda - 2).$$

Then, one has:

$$N_\Theta = \frac{1}{a_{11}a_{22}a_{33}a_{44} - a_{11}a_{44}|\beta|^2 - a_{11}a_{22}|\alpha|^2 - a_{33}a_{44}|\alpha|^2 + |\alpha|^4} \cdot$$

$$\left(\begin{pmatrix} a_{44}(-a_{22}a_{33} + |\beta|^2) + |\alpha|^2 a_{22} & |\alpha|^2\alpha - \alpha a_{33}a_{44} & 0 & 0 \\ |\alpha|^2\overline{\alpha} - \overline{\alpha}a_{33}a_{44} & -a_{11}a_{33}a_{44} + |\alpha|^2 a_{11} & 0 & 0 \\ -\overline{\alpha}\overline{\beta}a_{44} & -\overline{\beta}a_{11}a_{44} & 0 & 0 \\ -\overline{\alpha}^2\overline{\beta} & -a_{11}\overline{\alpha}\overline{\beta} & 0 & 0 \end{pmatrix} + \right.$$

$$\left. \begin{pmatrix} 0 & 0 & -\alpha\beta a_{44} & -\alpha^2\beta \\ 0 & 0 & -\beta a_{11}a_{44} & -\alpha\beta a_{11} \\ 0 & 0 & -a_{11}a_{22}a_{44} + |\alpha|^2 a_{44} & |\alpha|^2\alpha - a_{11}a_{22}\alpha \\ 0 & 0 & |\alpha|^2\overline{\alpha} - a_{11}a_{22}\overline{\alpha} & -a_{33}(a_{11}a_{22} - |\alpha|^2) + a_{11}|\beta|^2 \end{pmatrix} \right).$$

Assuming:

$$\Delta := \frac{2i}{a_{11}a_{22}a_{33}a_{44} - a_{11}a_{44}|\beta|^2 - a_{11}a_{22}|\alpha|^2 - a_{33}a_{44}|\alpha|^2 + |\alpha|^4},$$

we, finally, obtain:

$$\mathfrak{S}_\Theta(\lambda) = I + \Delta \cdot$$

$$\left(\begin{pmatrix} \Im a_{11}\left(a_{44}(-a_{22}a_{33} + |\beta|^2) + |\alpha|^2 a_{22}\right) & \sqrt{\Im a_{11}\Im a_{22}}\left(|\alpha|^2\alpha - \alpha a_{33}a_{44}\right) & 0 & 0 \\ \sqrt{\Im a_{11}\Im a_{22}}\left(|\alpha|^2\overline{\alpha} - \overline{\alpha}a_{33}a_{44}\right) & \Im a_{22}\left(-a_{11}a_{33}a_{44} + |\alpha|^2 a_{11}\right) & 0 & 0 \\ -\sqrt{\Im a_{11}\Im a_{33}}\overline{\alpha}\overline{\beta}a_{44} & -\sqrt{\Im a_{22}\Im a_{33}}\overline{\beta}a_{11}a_{44} & 0 & 0 \\ -\sqrt{\Im a_{11}\Im a_{44}}\overline{\alpha}^2\overline{\beta} & -\sqrt{\Im a_{22}\Im a_{44}}a_{11}\overline{\alpha}\overline{\beta} & 0 & 0 \end{pmatrix} + \right.$$

$$\left. \begin{pmatrix} 0 & 0 & -\sqrt{\Im a_{11}\Im a_{33}}\alpha\beta a_{44} & -\sqrt{\Im a_{11}\Im a_{44}}\alpha^2\beta \\ 0 & 0 & -\sqrt{\Im a_{22}\Im a_{33}}\beta a_{11}a_{44} & -\sqrt{\Im a_{22}\Im a_{44}}\alpha\beta a_{11} \\ 0 & 0 & \Im a_{33}\left(-a_{11}a_{22}a_{44} + |\alpha|^2 a_{44}\right) & \sqrt{\Im a_{33}\Im a_{44}}\left(|\alpha|^2\alpha - a_{11}a_{22}\alpha\right) \\ 0 & 0 & \sqrt{\Im a_{33}\Im a_{44}}\left(|\alpha|^2\overline{\alpha} - a_{11}a_{22}\overline{\alpha}\right) & \Im a_{44}\left(-a_{33}(a_{11}a_{22} - |\alpha|^2) + a_{11}|\beta|^2\right) \end{pmatrix} \right).$$

Now, we have to take the projection onto the absolutely continuous part, we calculate:

$$\left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \end{pmatrix} \right) \mathfrak{S}_\Theta(\lambda) \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right) +$$

$$\left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \end{pmatrix} \right) \mathfrak{S}_\Theta(\lambda) \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right),$$

and obtain:

$$\begin{pmatrix} 2 + \Delta\Im a_{11}\left(a_{44}(-a_{22}a_{33} + |\beta|^2) + |\alpha|^2 a_{22}\right) + \Delta\Im a_{22}\left(-a_{11}a_{33}a_{44} + |\alpha|^2 a_{11}\right) & 0 \\ -\Delta\sqrt{\Im a_{11}\Im a_{33}}\overline{\alpha}\overline{\beta}a_{44} - \Delta\sqrt{\Im a_{22}\Im a_{44}}a_{11}\overline{\alpha}\overline{\beta} & 0 \end{pmatrix} +$$

$$\begin{pmatrix} 0 & -\Delta\sqrt{\Im a_{11}\Im a_{33}}\alpha\beta a_{44} - \Delta\sqrt{\Im a_{22}\Im a_{44}}\alpha\beta a_{11} \\ 0 & 2 + \Delta\Im a_{33}\left(-a_{11}a_{22}a_{44} + |\alpha|^2 a_{44}\right) + \Delta\Im a_{44}\left(-a_{33}(a_{11}a_{22} - |\alpha|^2) + a_{11}|\beta|^2\right) \end{pmatrix}.$$

We are interested in the argument of the coefficient:

$$r := 2 + \Delta\Im a_{33}\left(-a_{11}a_{22}a_{44} + |\alpha|^2 a_{44}\right) + \Delta\Im a_{44}\left(-a_{33}(a_{11}a_{22} - |\alpha|^2) + a_{11}|\beta|^2\right). \tag{43}$$

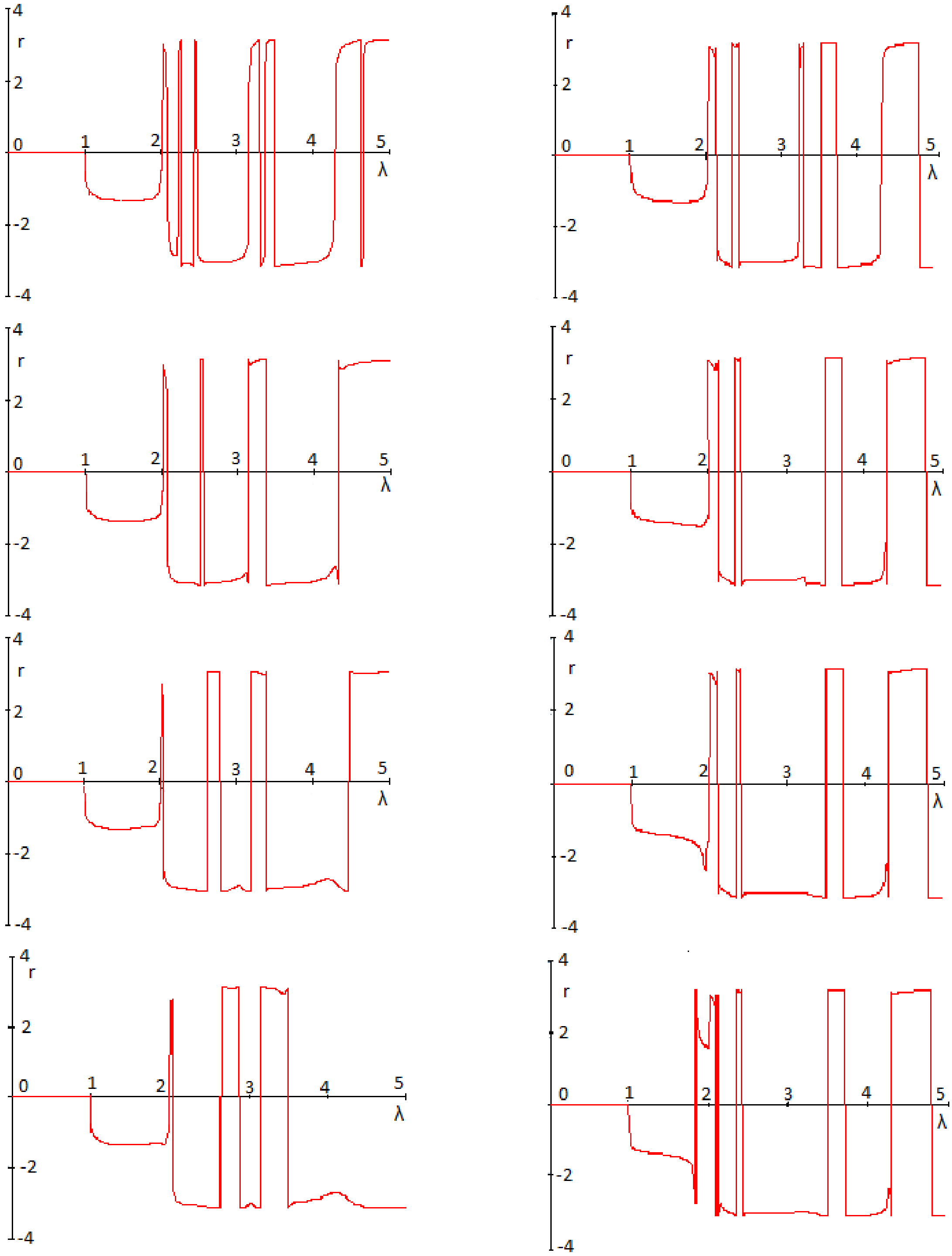

FIG. 1. Argument of the reflection coefficient $\arg r$ as a function of energy λ. Left column: $\alpha = \beta = 1/3$, values of Φ vary from top to bottom through, consequently, $1/4, 1/5, 1/8, 1/10$; right column: $\Phi = \beta = 1/3$, α vary from top to bottom through, consequently, $1/3, 1/5, 1/8, 1/12$ (arbitrary units)

3.6. Results and discussion

The dependence of the scattering phase $\arg r$ on the energy is shown in Fig. 1. Jumps of the phase correspond to resonances which positions depend on the magnetic field. One can observe this dependence looking through the left column of pictures. Naturally, for a weaker magnetic field, one has resonances closer to the corresponding eigenvalues of the operator for the ring without the magnetic field. As for influence of parameter α, it is shown in the left column of pictures in Fig. 1. Parameter α is responsible for the connection between the ring and the segment. Note that the coupling condition between the ring and the segment (22) depends on the magnetic field Φ (due to the "magnetic" derivatives the scattering phase changes). This explains the influence of α on the resonance position. As for β, which is responsible for the connection between the segment and the half-line, it does not influences on the resonance position essentially due to the absence of Φ in the coupling condition. Correspondingly, we did not present the pictures for different values of β (their variations are not essential).

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Appendix A: Limit of the Weyl function M^{A_1}

Let us investigate $M^{A_1}(\lambda)$, $\lambda \in \mathbb{R}$ and calculate it's imaginary part. We put $l = 2\pi r$ and calculate

$$u = -2\sin(l\sqrt{\lambda})\sin(l\Phi + \sqrt{\lambda}) - 4r\cos(l\sqrt{\lambda})\cos(\sqrt{\lambda} + l\Phi) + 2r\cos(2l\Phi + \sqrt{\lambda}) + 2r\cos\sqrt{\lambda} +$$
$$i\left(2\sin(l\sqrt{\lambda})\cos(l\Phi + \sqrt{\lambda}) - 4r\cos(l\sqrt{\lambda})\sin(\sqrt{\lambda} + l\Phi) + 2r\sin(2l\Phi + \sqrt{\lambda}) + 2r\sin\sqrt{\lambda}\right)$$

and

$$v = -2\sin(l\sqrt{\lambda})\sin(l\Phi - \sqrt{\lambda}) + 4r\cos(l\sqrt{\lambda})\cos(\sqrt{\lambda} - l\Phi) - 2r\cos(2l\Phi - \sqrt{\lambda}) - 2r\cos\sqrt{\lambda} +$$
$$i\left(2\sin(l\sqrt{\lambda})\cos(l\Phi - \sqrt{\lambda}) + 4r\cos(l\sqrt{\lambda})\sin(l\Phi - \sqrt{\lambda}) - 2r\sin(2l\Phi - \sqrt{\lambda}) + 2r\sin\sqrt{\lambda}\right).$$

Then,

$$u+v=-4\sin(l\sqrt{\lambda})\sin(l\Phi)\cos\sqrt{\lambda}+8r\cos(l\sqrt{\lambda})\sin\sqrt{\lambda}\sin(l\Phi)-4r\sin(2l\Phi)\sin\sqrt{\lambda}+$$
$$i\left(4\sin(l\sqrt{\lambda})\cos(l\Phi)\cos\sqrt{\lambda}-8r\cos(l\sqrt{\lambda})\sin\sqrt{\lambda}\cos(l\Phi)+4r\cos(2l\Phi)\sin\sqrt{\lambda}+4r\sin\sqrt{\lambda}\right).$$

If $\lambda<0$, then $\sqrt{\lambda}$ is purely complex, $\cos\sqrt{\lambda}\in\mathbb{R}$ and $\sin\sqrt{\lambda}$ are purely complex. Then for $\lambda\geqslant 0$ the lines above give real and imaginary part of $u+v$, i.e.

$$\Re(u+v)=$$
$$-4\sin(l\sqrt{\lambda})\sin(l\Phi)\cos\sqrt{\lambda}+8r\cos(l\sqrt{\lambda})\sin\sqrt{\lambda}\sin(l\Phi)-4r\sin(2l\Phi)\sin\sqrt{\lambda}$$
$$\Im(u+v)=$$
$$4\sin(l\sqrt{\lambda})\cos(l\Phi)\cos\sqrt{\lambda}-8r\cos(l\sqrt{\lambda})\sin\sqrt{\lambda}\cos(l\Phi)+4r\cos(2l\Phi)\sin\sqrt{\lambda}+4r\sin\sqrt{\lambda}$$

and for $\lambda<0$

$$\Re(u+v)=$$
$$i\left(4\sin(l\sqrt{\lambda})\cos(l\Phi)\cos\sqrt{\lambda}-8r\cos(l\sqrt{\lambda})\sin\sqrt{\lambda}\cos(l\Phi)+4r\cos(2l\Phi)\sin\sqrt{\lambda}+4r\sin\sqrt{\lambda}\right)$$
$$\Im(u+v)=$$
$$\frac{1}{i}\left(-4\sin(l\sqrt{\lambda})\sin(l\Phi)\cos\sqrt{\lambda}+8r\cos(l\sqrt{\lambda})\sin\sqrt{\lambda}\sin(l\Phi)-4r\sin(2l\Phi)\sin\sqrt{\lambda}\right)$$

In the same way we consider

$$u-v=$$
$$-4\sin(l\sqrt{\lambda})\cos(l\Phi)\sin\sqrt{\lambda}-8r\cos(l\sqrt{\lambda})\cos\sqrt{\lambda}\cos(l\Phi)+4r\cos(2l\Phi)\cos\sqrt{\lambda}+4r\cos\sqrt{\lambda}+$$
$$i\left(4\sin(l\sqrt{\lambda})\sin(l\Phi)\sin\sqrt{\lambda}-8r\cos(l\sqrt{\lambda})\cos\sqrt{\lambda}\sin(l\Phi)+4r\sin(2l\Phi)\cos\sqrt{\lambda}\right).$$

In this case for any $\lambda\in\mathbb{R}$ we have

$$\Re(u-v)=$$
$$-4\sin(l\sqrt{\lambda})\cos(l\Phi)\sin\sqrt{\lambda}-8r\cos(l\sqrt{\lambda})\cos\sqrt{\lambda}\cos(l\Phi)+4r\cos(2l\Phi)\cos\sqrt{\lambda}+4r\cos\sqrt{\lambda}$$
$$\Im(u-v)=$$
$$4\sin(l\sqrt{\lambda})\sin(l\Phi)\sin\sqrt{\lambda}-8r\cos(l\sqrt{\lambda})\cos\sqrt{\lambda}\sin(l\Phi)+4r\sin(2l\Phi)\cos\sqrt{\lambda}.$$

Then

$$M^A(\lambda)=-i\sqrt{\lambda}\frac{(\Re(u-v)+i\Im(u-v))\,(\Re(u+v)-i\Im(u+v))}{\Re^2(u+v)+\Im^2(u+v)}.$$

If $\lambda\geqslant 0$, then

$$\Im M^A(\lambda)=-\sqrt{\lambda}\frac{\Re(u+v)\Re(u-v)+\Im(u+v)\Im(u-v)}{\Re^2(u+v)+\Im^2(u+v)},$$

and if $\lambda<0$, then

$$\Im M^A(\lambda)=\sqrt{|\lambda|}\frac{\Im(u-v)\Re(u+v)-\Re(u-v)\Im(u+v)}{\Re^2(u+v)+\Im^2(u+v)}.$$