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1999 J. Phys. A: Math. Gen. 32 595

(http://iopscience.iop.org/0305-4470/32/4/006)

J. Phys. A: Math. Gen. **32** (1999) 595–630. Printed in the UK PII: S0305-4470(99)95197-1

Kirchhoff's rule for quantum wires*

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Received 15 June 1998, in final form 12 October 1998

Abstract. We formulate and discuss one-particle quantum scattering theory on an arbitrary finite graph with n open ends and where we define the Hamiltonian to be (minus) the Laplace operator with general boundary conditions at the vertices. This results in a scattering theory with n channels. The corresponding on-shell S-matrix formed by the reflection and transmission amplitudes for incoming plane waves of energy $E > 0$ is given explicitly in terms of the boundary conditions and the lengths of the internal lines. It is shown to be unitary, which may be viewed as the quantum version of Kirchhoff's law. We exhibit covariance and symmetry properties. It is symmetric if the boundary conditions are real. Also there is a duality transformation on the set of boundary conditions and the lengths of the internal lines such that the low-energy behaviour of one theory gives the high-energy behaviour of the transformed theory. Finally, we provide a composition rule by which the on-shell S-matrix of a graph is factorizable in terms of the S-matrices of its subgraphs. All proofs use only known facts from the theory of self-adjoint extensions, standard linear algebra, complex function theory and elementary arguments from the theory of Hermitian symplectic forms.

1. Introduction

At present mesoscopic quasi-one-dimensional structures like quantum [1, 2], atomic [3] and molecular [4] wires have become the subject of intensive experimental and theoretical studies. This kind of electronics is still far from being commercially useful. However, the enormous progress that has been made in the past years suggests that it will not be too long before the first molecule-sized electronic components become a reality (see, e.g., [5–7]).

According to already traditional physical terminology a quantum wire is a graph-like structure on the surface of a semiconductor, which confines an electron to potential grooves of width of about a few nanometres. An accurate theory for these nanostructures must include confinement, coupling between closely spaced wires, rough boundaries, impurities, etc. The simplest model describing conduction in quantum wires is a Hamiltonian on a planar graph. A similar model can be applied to a molecular wire—a quasi-one-dimensional molecule that can transport charge carriers (electrons or holes) between its ends [8]. Atomic wires, i.e. lines of metal atoms on the surface of a semiconductor provide another example of such quasi-one-dimensional structures. Also Hamiltonians on planar graphs arise naturally in the modelling of high-temperature granular superconductors [9–11].

* Dedicated to S P Novikov on the occasion of his 60th birthday.

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Although such models were proposed long ago (see, e.g., [12, 13]), probably it was Pavlov and Gerasimenko [14, 15] who initiated a rigorous mathematical analysis of such models, which later acquired the name of quantum wires. A more general approach to the problem of the corresponding mathematical structure was formulated in [16] several decades earlier. Here we do not intend to give a complete overview of the whole subject. We only mention some related studies. In [17, 18] networks with leads were used to study adiabatic transport and Chern numbers. Two-particle scattering theory on graphs was studied in [19]. Quantum waveguides [20–26], where the influence of confining potentials walls is modelled by the Dirichlet boundary condition, give a more realistic description of quasi-one-dimensional conductors. The wavefunction is allowed to have several mutually interacting transverse modes. In real quantum wires the number of these modes can be rather large (up to 10^2–10^3). For another more realistic model of a two-dimensional quantum wire see [27].

In this paper we consider idealized quantum wires, where the configuration space is a graph, i.e. a strictly one-dimensional object and the Hamiltonian is minus the Laplacian with arbitrary boundary conditions at the vertices of the graph and which makes it a self-adjoint operator. The graph need not to be planar and may be bent when realized as a subset of the three-dimensional Euclidean space $\mathbb{R}^3$. By now many explicit examples have been considered (see, e.g., [14, 28–37]) also including the Dirac operator with suitable boundary conditions [38]. Our approach gives a systematic discussion and covers, in particular, all these cases for the Laplace operator. We will, however, not be concerned with the question of which of these boundary conditions could be physically reasonable. The physical relevance of different boundary conditions is discussed, for example, in [31, 39].

The scattering theory for these operators exhibits a very rich structure (see, e.g., [40–42]) and by Landauer's theory [43] provides the background for understanding conductivity in mesoscopic systems. The on-shell S-matrix at energy E is an $n \times n$ matrix if the graph has n open ends, which we will show to be given in a closed matrix form in terms of the boundary conditions and the lengths of the internal lines of the graph. We exhibit covariance and invariance properties and show, in particular, that the on-shell S-matrix is symmetric for all energies if the boundary conditions are real in a sense which we will make precise. The main result of this paper is that this on-shell S-matrix is unitary, continuous in the energy and even real analytic except for an at most denumerable set of energies without finite accumulation points. This set is given in terms of the boundary conditions and the lengths of the internal lines. This result may be viewed as the quantum version of Kirchhoff's rule. For explicit examples this has been known (see, e.g., [39, 44]), but again our approach provides a unified treatment. Physically this unitarity is to be expected since there is a local Kirchhoff rule. In fact, the boundary conditions imply that the quantum probability currents of the components of any wavepacket associated to the different lines entering any vertex add up to zero. Our discussion of the boundary conditions will be based on Green's theorem and will just reflect this observation. We will actually give three different proofs, each of which will be of interest in its own right.

Finally, there is a general duality transformation on the boundary conditions (turning Dirichlet into Neumann boundary conditions and vice versa) which combined with an energy-dependent scale transformation on the lengths of the internal lines relates the high-energy behaviour of one theory to the low-energy behaviour of the transformed theory.

This paper is organized as follows. In section 2 we discuss the simple case with one vertex only but with an arbitrary number of open lines ending there. This will allow us to present the main elements of our strategy, which is the general theory of self-adjoint extensions of symmetric operators and its relation to boundary conditions in the context of Laplace operators. This discussion uses some elementary facts about Hermitian symplectic forms. Although some results will be proven again for the general set-up in section 3, for pedagogical reasons and because they are easier and more transparent in this simple case, we will also give proofs. In section 3 we discuss the general case with the techniques and mostly with proofs, which extend those of section 2. We start with a general algebraic formulation of boundary conditions involving a finite set of half lines and finite intervals but without any reference to local boundary conditions on a particular graph. Finally, we show that any of these boundary conditions may be viewed as local boundary conditions on a suitable (maximal) graph.

The connection between the theory of self-adjoint extensions of symmetric operators and Hermitian symplectic forms was brought to the attention of one of the authors (RS) by Segal in 1987. In a recent paper [45] Novikov stated that he learned this from Gelfand back in 1971. Unfortunately we were unable to trace back the precise history of this connection. It seems that it was made by several researchers at different times (see, e.g., [46–49]) but still was not analysed systematically. In sections 2 and 3 and in appendix A we will try to fill this gap.

In section 4 we consider the question of what happens if one decomposes a graph into two or more components by cutting some of its internal lines and replacing them by semi-infinite lines. One would like to compare the on-shell S-matrices obtained in this way with the original one. If the graph has two open ends and its subgraphs are connected by exactly one line, the Aktosun factorization formula [50] (see also [51–60]) for potential scattering on the line easily carries over to this case. Such rules are reminiscent of the Cutkosky cutting rules [61] for one-particle reducible Feynman diagrams. Also such relations are well known in network theories and then the composition law for the S-matrices figures under the name star product [51] (pp 285–6; we would like to thank Baake (Tübingen) for pointing out this reference), [52]. If the cutting involves more than one line, the situation becomes more complicated and leads to interesting phenomena related to the semiclassical Gutzwiller formula and the Selberg trace formula [42] (see also [17, 18, 53]). We provide a general composition rule for unitary matrices, which we will call a generalized star product and by which the on-shell S-matrix of an arbitrary graph (with local boundary conditions) can be factorized in terms of the S-matrices of its subgraphs. We expect that this general, highly nonlinear composition rule could also be of relevance in other contexts. Note that there is some similarity between our results and the recursive approach of [62]. Section 5 contains a summary and an outlook for possible applications and further investigations.

When this paper was already submitted for publication we learned about the work [45] (some results of which were announced in a short note [63]) by Novikov, where a programme similar to ours was carried out for discrete (combinatorial) Laplacians on tree graphs.

2. The quantum wire with a single vertex

In this section we will consider a quantum wire with n open ends and joined at a single vertex. This toy model will already exhibit most of the essential features of the general case and is also of interest in its own right. In particular, the general strategy and the main techniques of our approach will be formulated in this section. Let the Hilbert space be given as

$$\mathcal{H} = \bigoplus_{i=1}^{n} \mathcal{H}_i = \bigoplus_{i=1}^{n} L^2([0,\infty)).$$

Elements $\psi \in \mathcal{H}$ will be written as $(\psi_1, \psi_2, \ldots, \psi_n)$ and we will call ψ_j the component of ψ in channel j. The scalar product in $\mathcal{H}$ is

$$\langle \phi, \psi \rangle = \sum_{i=1}^{n} \langle \phi_i, \psi_i \rangle_{\mathcal{H}_i}$$

with the standard scalar product on $L^2([0,\infty))$ on the right-hand side. We consider the symmetric operator Δ^0 on $\mathcal{H}$, such that

$$\Delta^0\psi = \left(\frac{\mathrm{d}^2\psi_1}{\mathrm{d}x^2}, \ldots, \frac{\mathrm{d}^2\psi_n}{\mathrm{d}x^2}\right)$$

with the domain of definition $\mathcal{D}(\Delta^0)$ being the set of all ψ where each ψ_i, $1 \leqslant i \leqslant n$ together with their first and second generalized derivatives belong to $L^2(0,\infty)$ (i.e. $\psi_i \in W^{2,2}(0,\infty)$, a Sobolev space) and which vanish at $x = 0$ together with their first derivatives. It is clear that Δ^0 has defect indices (n, n), such that the set of all self-adjoint extensions can be parametrized (in a non-canonical way) by the unitary group $\mathsf{U}(n)$, which has real dimension n^2 (see, e.g., [64, 65]).

There is an alternative and equivalent description of all self-adjoint extensions in terms of symplectic theory which goes as follows. Let $\mathcal{D} \subset \mathcal{H}$ be the set of all ψ such that each ψ_i, $1 \leqslant i \leqslant n$ belongs to $W^{2,2}(0,\infty)$, and we will then say that $\psi \in W^{2,2}$. On $\mathcal{D}$ consider the following skew-Hermitian quadratic form given as

$$\Omega(\phi,\psi) = \langle\Delta\phi,\psi\rangle - \langle\phi,\Delta\psi\rangle = -\overline{\Omega(\psi,\phi)}$$

with the Laplace operator $\Delta = \mathrm{d}^2/\mathrm{d}x^2$ considered as a differential expression. Obviously Ω vanishes identically on $\mathcal{D}(\Delta^0)$. Any self-adjoint extension of Δ^0 is now given in terms of a maximal isotropic subspace of $\mathcal{D}$, i.e. a maximal (linear) subspace on which Ω vanishes identically. This notion corresponds to that of Lagrangian subspaces in the context of Euclidean symplectic forms (see, e.g., [66]). To find these maximal isotropic subspaces we perform an integration by parts (Green's theorem) and obtain with $'$ denoting the derivative and $\bar{}$ complex conjugation

$$\Omega(\phi,\psi) = \sum_{i=1}^{n}(\bar{\phi}_i(0)\,\psi_i'(0) - \bar{\phi}_i'(0)\,\psi_i(0)).$$

We rewrite this in the following form. Let $[\,]$: $\mathcal{D} \to \mathbb{C}^{2n}$ be the surjective linear map which associates to ψ and ψ' their boundary values at the origin:

$$[\psi] = (\psi_1(0), \ldots \psi_n(0), \psi_1'(0), \ldots \psi_n'(0))^T = \begin{pmatrix}\psi(0)\\ \psi'(0)\end{pmatrix}.$$

Here T denotes the transpose, so $[\psi]$, $\psi(0)$ and $\psi'(0)$ are considered to be column vectors of length $2n$ and n, respectively. The kernel of the map $[\,]$ is obviously equal to $\mathcal{D}(\Delta^0)$. Then we have

$$\Omega(\phi,\psi) = \omega([\phi],[\psi]) := \langle[\phi], J[\psi]\rangle_{\mathbb{C}^{2n}}$$

where $\langle\,,\,\rangle_{\mathbb{C}^{2n}}$ now denotes the scalar product on $\mathbb{C}^{2n}$ and where the $2n \times 2n$ matrix J is the canonical symplectic matrix on $\mathbb{C}^{2n}$:

$$J = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}. \tag{1}$$

Here and in what follows $\mathbb{I}$ is the unit matrix for the given context. Note that the Hermitian symplectic form ω differs from the Euclidean symplectic form on $\mathbb{C}^{2n}$ [66].

To find all maximal isotropic subspaces in $\mathcal{D}$ with respect to Ω it therefore suffices to find all maximal isotropic subspaces in $\mathbb{C}^{2n}$ with respect to ω and to take their preimage under the map $[\,]$. The set of all maximal isotropic subspaces corresponds to the Lagrangian Grassmann manifold in the context of Euclidean symplectic forms [66]. Since J is non-degenerate, such spaces all have complex dimension equal to n. This description is the local Kirchhoff rule referred to in the introduction. Moreover, with $\mathcal{M}^\perp$ denoting the orthogonal complement (with respect to $\langle\cdot,\cdot\rangle_{\mathbb{C}^{2n}}$) of a space $\mathcal{M}$ we have

Lemma 2.1. *A linear subspace $\mathcal{M}$ of $\mathbb{C}^{2n}$ is maximal isotropic iff $\mathcal{M}^\perp = J\mathcal{M}$ and iff $\mathcal{M}^\perp$ is maximal isotropic.*

The proof is standard and follows easily from the definition and the fact that $J^2 = -\mathbb{I}$ and $J^\dagger = -J$. We use this result in the following form. Let the linear subspace $\mathcal{M} = \mathcal{M}(A, B)$ of $\mathbb{C}^{2n}$ be given as the set of all $[\psi]$ in $\mathbb{C}^{2n}$ satisfying

$$A\psi(0) + B\psi'(0) = 0 \tag{2}$$

where A and B are two $n \times n$ matrices. If the $n \times 2n$ matrix (A, B) has maximal rank equal to n then obviously $\mathcal{M}$ has dimension equal to n and in this way we may describe all subspaces of dimension equal to n. Also the image of $\mathbb{C}^{2n}$ under the map (A, B) is then all of $\mathbb{C}^n$ because of the general result that for any linear map T from $\mathbb{C}^{2n}$ into $\mathbb{C}^n$ one always has $\dim \mathrm{Ker}(T) + \dim \mathrm{Ran}(T) = 2n$. Writing the adjoint of any (not necessarily square) matrix X as $X^\dagger = \bar{X}^T$ we claim

Lemma 2.2. *Let A and B be two $n \times n$ matrices such that (A, B) has maximal rank. Then $\mathcal{M}(A, B)$ is maximal isotropic iff $AB^\dagger$ is self-adjoint.*

The proof is easily obtained by writing the condition (2) in the form $\langle \Phi^k, [\psi] \rangle_{\mathbb{C}^{2n}} = 0$, $1 \leqslant k \leqslant n$, where Φ^k is given as the kth column vector of the $2n \times n$ matrix $(\bar{A}, \bar{B})^T = (A, B)^\dagger$. Obviously they are linearly independent. Then by the previous lemma $\mathcal{M}(A, B)$ is maximal isotropic iff the space spanned by the Φ^k is maximal isotropic. This condition in turn amounts to the condition that $(A, B)J(A, B)^\dagger = 0$, which means that $AB^\dagger$ has to be self-adjoint. The converse is also obviously true.

Example 2.1 ($n \geqslant 3$, n odd). *Consider*

$$\psi_j(0) + c_j(\psi'_{j-1}(0) + \psi'_{j+1}(0)) = 0 \qquad \textit{for} \quad 1 \leqslant j \leqslant n$$

with a $\mathrm{mod}\, n$ *convention. The resulting A is the identity matrix and $AB^\dagger$ is self-adjoint iff all c_j are equal ($= c$) and real. Then B is of the form $B_{jk} = c(\delta_{j+2\,k} + \delta_{j\,k+2})$. (If n is even the condition is that $c_j = \bar{c}_{j+1}$ and $c_j = c_{j+2}$ for all j.)*

Example 2.2 ($n \geqslant 3$). *Consider*

$$\psi_j(0) + \psi_{j+1}(0) + c_j(\psi'_j(0) - \psi'_{j+1}(0)) = 0 \qquad \textit{for} \quad 1 \leqslant j \leqslant n$$

again with a $\mathrm{mod}\, n$ *convention. The resulting A has maximal rank and $AB^\dagger$ is self-adjoint iff now all c_j are equal and purely imaginary.*

Example 2.3 ($n = 2$ (see, e.g., [35, 67, 68])). *To relate this case to familiar examples we realize $\mathcal{H}$ as $L^2(\mathbb{R}) = L^2((-\infty, 0]) \oplus L^2([0, \infty))$ and write the boundary conditions as*

$$\begin{pmatrix} \psi(0+) \\ \psi'(0+) \end{pmatrix} = \mathrm{e}^{\mathrm{i}\mu} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi(0-) \\ \psi'(0-) \end{pmatrix}.$$

Then $AB^\dagger$ is self-adjoint iff the matrix

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

belongs to $\mathsf{SL}(2, \mathbb{R})$ *and μ is real. Up to a set of measure zero in* $\mathsf{U}(2)$ *this gives all self-adjoint extensions. The interpretation of the parameters entering the boundary conditions can be found in [68]. The case $a - 1 = d - 1 = b = 0$,* $\exp(2\mathrm{i}\mu) = 1$ *gives the familiar δ-potential of strength c at the origin. The case $a - 1 = d - 1 = c = 0$,* $\exp(2\mathrm{i}\mu) = 1$ *gives the so-called δ'-interaction of strength b (see, e.g., [67, 69, 70] and references therein). The case $a = d^{-1}$,*

$b = c = 0$, $\exp(2\mathrm{i}\mu) = 1$ *gives the* δ'*-potential of strength* $-2(1-a)/(1+a)$ *[68, 71]. In particular, for the choice* $a - 1 = d - 1 = b = c = 0$, $\exp(2\mathrm{i}\mu) = 1$, *the corresponding free* S*-matrix (see below) is given by*

$$S_2^{\mathrm{free}}(E) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

More generally for n *lines* ($\simeq \mathbb{R}$) *with free propagation and with the appropriate labelling of the* $2n$ *ends the* $2n \times 2n$ *on-shell* S*-matrix takes the form*

$$S_{2n}^{\mathrm{free}}(E) = \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}. \tag{3}$$

We will make use of this observation in section 4, where we will exploit the fact that this $S_{2n}^{\mathrm{free}}(E)$ *serves as a unit matrix with respect to the generalized star product.*

In what follows we will always assume that A and B define a maximal isotropic subspace $\mathcal{M}(A, B)$, such that the resulting operator, which we denote by $\Delta(A, B)$, is self-adjoint. The core of this operator $\mathcal{D}(\Delta(A, B))$ is given as the preimage of $\mathcal{M}(\Delta(A, B))$ under the map [ ]. Note that $\mathcal{D}\big(\Delta^0\big)$ has codimension equal to n in any of these cores. Thus the quantum mechanical one-particle Hamiltonians we will consider are of the form $-\Delta(A, B)$ for any boundary condition (A, B) defining a maximal isotropic subspace.

The self-adjointness of $AB^\dagger$, i.e. the relation $AB^\dagger - BA^\dagger = 0$, will be the main *Leitmotiv* throughout this paper, since combined with the maximal rank condition it encodes the self-adjointness of the operator $\Delta(A, B)$ and is the algebraic formulation of the local Kirchhoff rule. The proof of lemma 2.2 combined with the previous lemma also shows that $\mathcal{M}(A, B)^\perp = J\mathcal{M}(A, B) = \mathcal{M}(-B, A)$. Note that $\big(A^\dagger, B^\dagger\big)$ does not necessarily define a maximal subspace if (A, B) does. As an example let H be self-adjoint and A invertible and set $B = H\big(A^{-1}\big)^\dagger$. Then (A, B) defines a maximal isotropic subspace since $AB^\dagger = H$, but $A^\dagger B = A^\dagger H\big(A^{-1}\big)^\dagger$, $B^\dagger A = A^{-1}HA$ and these two expressions differ if $AA^\dagger$ and H do not commute. If $A = 0$ such that B is invertible we have Neumann boundary conditions and if $B = 0$ such that A is invertible we have Dirichlet boundary conditions.

We will now calculate the on-shell S-matrix $S(E) = S_{A,B}(E)$ for all energies $E > 0$. This will be an $n \times n$ matrix whose matrix elements are defined by the following relations. We look for plane-wave solutions $\psi^k(\cdot, E)$, $1 \leqslant k \leqslant n$ of the Schrödinger equation for $-\Delta(A, B)$ in the form

$$\psi_j^k(x, E) = \begin{cases} S_{jk}(E)\,\mathrm{e}^{\mathrm{i}\sqrt{E}\,x} & \text{for} \quad j \neq k \\ \mathrm{e}^{-\mathrm{i}\sqrt{E}\,x} + S_{kk}(E)\,\mathrm{e}^{\mathrm{i}\sqrt{E}\,x} & \text{for} \quad j = k \end{cases} \tag{4}$$

and which satisfy the boundary conditions. Thus $S_{kk}(E)$ has the interpretation of being the reflection amplitude in channel k, while $S_{jk}(E)$ with $j \neq k$ is the transmission amplitude from channel k into channel j, both for an incoming plane wave $\exp\big(-\mathrm{i}\sqrt{E}\,x\big)$ in channel k. This definition of the S-matrix differs from the standard one used in potential scattering theory [72, 73], where the equal transmission amplitudes build up the diagonal. In particular, for $n = 2$ and general boundary conditions at the origin as described in example 2.3 we have

$$\begin{aligned} S(E) &= \begin{pmatrix} R(E) & T_1(E) \\ T_2(E) & L(E) \end{pmatrix} \\ &= \left(a - \mathrm{i}\sqrt{E}\,b + \frac{\mathrm{i}c}{\sqrt{E}} + d\right)^{-1} \begin{pmatrix} a - \mathrm{i}\sqrt{E}\,b - \dfrac{\mathrm{i}c}{\sqrt{E}} - d & 2\mathrm{e}^{\mathrm{i}\mu} \\ 2\mathrm{e}^{-\mathrm{i}\mu} & -a - \mathrm{i}\sqrt{E}\,b - \dfrac{\mathrm{i}c}{\sqrt{E}} + d \end{pmatrix} \end{aligned}$$

whereas

$$S_{\text{standard}}(E) = S(E)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} T_1(E) & R(E) \\ L(E) & T_2(E) \end{pmatrix}.$$

These S-matrices are unitarily equivalent iff $\Delta(A, B)$ is real (i.e. $\mathrm{e}^{2\mathrm{i}\mu} = 1$ such that $\Delta(A, B)$ commutes with complex conjugation, see also below for a general discussion) and is invariant with respect to reflection at the origin. In the latter case $T_1(E) = T_2(E)$ and $R(E) = L(E)$.

We return to the ansatz (4). After a short calculation the boundary conditions for the ψ^k take the form of a matrix equation for $S(E)$

$$\left(A + \mathrm{i}\sqrt{E}\, B\right) S(E) = -\left(A - \mathrm{i}\sqrt{E}\, B\right). \tag{5}$$

To solve for $S(E)$ we will establish the following

Lemma 2.3. *For all $E > 0$ both matrices $\left(A + \mathrm{i}\sqrt{E}\, B\right)$ and $\left(A - \mathrm{i}\sqrt{E}\, B\right)$ are invertible.*

Proof. Assume $\det\left(A + \mathrm{i}\sqrt{E}\, B\right) = 0$. But then also

$$\det\left(A^\dagger - \mathrm{i}\sqrt{E}\, B^\dagger\right) = \overline{\det\left(A + \mathrm{i}\sqrt{E}\, B\right)} = 0$$

so there is $\chi \neq 0$ such that $\left(A^\dagger - \mathrm{i}\sqrt{E}\, B^\dagger\right)\chi = 0$. In particular,

$$0 = \left\langle \chi, \left(A + \mathrm{i}\sqrt{E}\, B\right)\left(A^\dagger - \mathrm{i}\sqrt{E}\, B^\dagger\right)\chi \right\rangle = \left\langle A^\dagger\chi, A^\dagger\chi \right\rangle + E\left\langle B^\dagger\chi, B^\dagger\chi \right\rangle$$

where we have used the fact that $AB^\dagger$ is self-adjoint. But this implies that $A^\dagger\chi = B^\dagger\chi = 0$. Hence $\langle A\phi + B\phi', \chi\rangle = 0$ for all $\phi, \phi' \in \mathbb{C}^n$. But as already remarked the range of the map $(A, B)\colon \mathbb{C}^{2n} \to \mathbb{C}^n$ is all of $\mathbb{C}^n$. Hence $\chi = 0$ and we have arrived at a contradiction. This proves the lemma since the invertibility of $A - \mathrm{i}\sqrt{E}\, B$ is proved in the same way. Also we have shown that $AA^\dagger + EBB^\dagger$ is a strictly positive operator and hence an invertible operator on $\mathbb{C}^n$ for all $E > 0$. If A (or B) is invertible there is an easier proof of the lemma. Indeed, assume there is $\chi \neq 0$ such that $\left(A + \mathrm{i}\sqrt{E}\, B\right)\chi = 0$. Then we have $A^{-1}B\chi = \mathrm{i}/\sqrt{E}\,\chi$. But $A^{-1}B$ is self-adjoint since $AB^\dagger$ is and therefore has only real eigenvalues giving a contradiction. □

To sum up we have proved the first part of

Theorem 2.1. *For the above quantum wire with one vertex and boundary conditions given by the pair (A, B) the on-shell S-matrix is given as*

$$\begin{aligned} S_{A,B}(E) &= -\left(A + \mathrm{i}\sqrt{E}\, B\right)^{-1}\left(A - \mathrm{i}\sqrt{E}\, B\right) \\ &= -\left(A^\dagger - \mathrm{i}\sqrt{E}\, B^\dagger\right)\left(AA^\dagger + EBB^\dagger\right)^{-1}\left(A - \mathrm{i}\sqrt{E}\, B\right) \end{aligned} \tag{6}$$

and is unitary and real analytic in $E > 0$.

To prove unitarity, we observe that $S^\dagger(E) = -\left(A^\dagger + \mathrm{i}\sqrt{E}\, B^\dagger\right)\left(A^\dagger - \mathrm{i}\sqrt{E}\, B^\dagger\right)^{-1}$ and $S(E)^{-1} = -\left(A - \mathrm{i}\sqrt{E}\, B\right)^{-1}\left(A + \mathrm{i}\sqrt{E}\, B\right)$. Now it is easy to see that these expressions are equal using again the fact that $AB^\dagger$ is self-adjoint. Note that unitarity follows from abstract reasoning. In fact, the difference of the resolvents of the operators $\Delta(A = 0, B = \mathbb{I})$ (Neumann boundary conditions and with S-matrix equal to $\mathbb{I}$) and $\Delta(A, B)$ by Krein's formula (see, e.g., [64]) is a finite rank operator since we are dealing with finite defect indices, so in particular this difference is trace class. Therefore by the Birman–Kato theory the entire S-matrix exists and is unitary. Also the S-matrix for Dirichlet boundary conditions ($A = \mathbb{I}$, $B = 0$) is $-\mathbb{I}$. The second relation in (6) can be used to discuss the bound state problem for $-\Delta(A, B)$, which, however, we will not do in this paper.

Relation (6) is a remarkable matrix analogue of the representation in potential scattering theory of the on-shell S-matrix at given angular momentum l as a quotient of Jost functions, i.e. $S_l\bigl(k = \sqrt{E}\bigr) = f_l(k)/f_l(-k)$ (see [74, 75]). As in potential scattering theory the scattering matrix $S_{A,B}(E)$ as a function of $\sqrt{E}$ can be analytically continued to a meromorphic function in the whole complex plane. In fact, by the self-adjointness of $\Delta(A, B)$ it is analytic in the physical energy sheet $\operatorname{Im}\sqrt{E} > 0$ except for poles on the positive imaginary axis corresponding to bound states and may have additional poles (i.e. resonances) in the unphysical energy sheet $\operatorname{Im}\sqrt{E} < 0$.

If C is any invertible $n \times n$ matrix then obviously (CA, CB) defines the same boundary conditions as (A, B) such that $\mathcal{M}(CA, CB) = \mathcal{M}(A, B)$ and $\Delta(CA, CB) = \Delta(A, B)$ and this is reflected by the fact that $S_{CA,CB}(E) = S_{A,B}(E)$. Conversely, if $\mathcal{M}(A, B) = \mathcal{M}(A', B')$ then there is an invertible C such that $A = CA'$, $B = CB'$. This follows easily from the defining relation (2). We want to use this observation to show that the on-shell S-matrix uniquely fixes the boundary conditions. In fact, assume that $S_{A,B}(E) = S_{A',B'}(E)$ or equivalently $S_{A,B}(E)S_{A',B'}(E)^\dagger = \mathbb{I}$ holds for some $E > 0$. By a short calculation this holds iff $A'B^\dagger - B'A^\dagger = 0$, i.e. $(A', B')J(A, B)^\dagger = 0$. But by the proof of lemma 2.2 this means that $\mathcal{M}(A, B)^\perp = \mathcal{M}(A', B')^\perp$ so the two maximal isotropic subspaces $\mathcal{M}(A, B)$ and $\mathcal{M}(A', B')$ are equal as was the claim.

To fix the freedom in parametrizing a maximal isotropic subspace by the pair (A, B), consider the Lie group $\mathcal{G}(2n)$, consisting of all $2n \times 2n$ matrices g which preserve the Hermitian symplectic structure, i.e. $g^\dagger J g = J$. We claim that this group is isomorphic to the classical group $\mathsf{U}(n, n)$ (see, e.g., [76]). Indeed $\mathrm{i}J$ is Hermitian, $(\mathrm{i}J)^2 = \mathbb{I}$ and $\operatorname{Tr} J = 0$ such that the only eigenvalues ± 1 are of equal multiplicity. Therefore there is a unitary W such that

$$W \mathrm{i} J W^{-1} = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}.$$

Thus elements g in the group $W\mathcal{G}(2n)W^{-1}$ satisfy

$$g^\dagger \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix} g = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}$$

such that $W\mathcal{G}(2n)W^{-1} = \mathsf{U}(n, n)$. The group $\mathsf{U}(n, n)$ and hence $\mathcal{G}(2n)$ has real dimension $4n^2$ and the latter acts transitively on the set of all maximal isotropic subspaces. In particular, $\mathcal{M}(A, B)$ is the image of $\mathcal{M}(A = 0, B = \mathbb{I})$ under the map given by the group element

$$\begin{pmatrix} B^\dagger\bigl(AA^\dagger + BB^\dagger\bigr)^{-1/2} & A^\dagger\bigl(AA^\dagger + BB^\dagger\bigr)^{-1/2} \\ -A^\dagger\bigl(AA^\dagger + BB^\dagger\bigr)^{-1/2} & B^\dagger\bigl(AA^\dagger + BB^\dagger\bigr)^{-1/2} \end{pmatrix}.$$

Let $\mathcal{K}(2n)$ be the isotropy group of $\mathcal{M}(A = 0, B = \mathbb{I})$, i.e. the subgroup which leaves $\mathcal{M}(A = 0, B = \mathbb{I})$ fixed. It is of real dimension $3n^2$. The set of all maximal isotropic subspaces is in one-to-one correspondence with the right coset space $\mathcal{G}(2n)/\mathcal{K}(2n)$ which has dimension n^2 as it should. Also this space may be shown to be compact. In appendix A we will relate the present discussion of self-adjoint extensions of Δ^0 with von Neumann's theory of self-adjoint extensions. In this context it is worthwhile to note that the parametrization of self-adjoint extensions in terms of maximal isotropic spaces is much more convenient for the description of these graph Hamiltonians, rather than the standard von Neumann parametrization. In particular, the content of appendix A is not needed for an understanding of the main material presented in this paper.

Now we establish some properties of these on-shell S-matrices. Although we shall prove corresponding results in the general case they are more transparent and easier to prove in this simple situation. In particular, if the boundary condition (A, B) is such that A is invertible one may choose $C = A^{-1}$ and similarly $C = B^{-1}$ if B is invertible. To determine $S_{A,B}(E)$ for all E in these cases it therefore suffices to diagonalize the self-adjoint matrices $A^{-1}B$ and $B^{-1}A$, respectively. Thus if $A^{-1}B = VHV^{-1}$ with a unitary V and diagonal, self-adjoint H, then $S_{A,B}(E) = -V\big(\mathbb{I} + \mathrm{i}\sqrt{E}\,H\big)^{-1}\big(\mathbb{I} - \mathrm{i}\sqrt{E}\,H\big)V^{-1}$.

Thus in example 2.1 H and V are given as $H_{kl} = \delta_{kl} 2c \cos 2\pi(l-1)/n$ and

$$V_{kl} = \frac{1}{\sqrt{n}} \mathrm{e}^{(2\mathrm{i}\pi/n)(k-1)(l-1)}$$

resulting in an on-shell S-matrix of the form

$$S_{jk}(E) = -\frac{1}{n}\sum_{l=1}^{n} \mathrm{e}^{(2\mathrm{i}\pi/n)(k-j)(l-1)} \frac{1 - 2\mathrm{i}c\sqrt{E}\cos[(2\pi/n)(l-1)]}{1 + 2\mathrm{i}c\sqrt{E}\cos[(2\pi/n)(l-1)]}. \tag{7}$$

With the equivalence $(A, B) \sim (CA, CB)$ for invertible C in mind, it follows easily that $S_{A,B}(E)$ is diagonal for all E iff A and B are both diagonal (Robin boundary conditions).

Let U be a unitary operator on $\mathbb{C}^n$. Then U defines a unitary operator $\mathcal{U}$ on $\mathcal{H}$ in a natural way via $(\mathcal{U}\psi)_i = \sum_{j=1}^{n} U_{ij}\psi_j$. As a special case this covers the situation where U is a gauge transformation of the form $\psi_j \to \exp(\mathrm{i}\chi_j)\psi_j$ with constant χ_j. Also (AU, BU) defines a maximal isotropic subspace and we have $\Delta(AU, BU) = \mathcal{U}^{-1}\Delta(A, B)\mathcal{U}$. Correspondingly we have $S_{AU,BU}(E) = U^{-1}S_{A,B}(E)U$. Assume, in particular, that there is a unitary U and an invertible C such that $CA = AU$ and $CB = BU$. Then the relations $\Delta(AU, BU) = \mathcal{U}^{-1}\Delta(A, B)\mathcal{U} = \Delta(A, B)$ and $S_{A,B}(E) = U^{-1}S_{A,B}(E)U$ are valid. This has a special application. There is a natural unitary representation $\pi \to U(\pi)$ of the permutation group of n elements into the unitaries of $\mathbb{C}^n$ and analogously a representation $\pi \to \mathcal{U}(\pi)$ into the unitaries of $\mathcal{H}$. For any permutation π such that $AU(\pi) = CA$ and $BU(\pi) = CB$ holds for an invertible $C = C(\pi)$ one has $S_{A,B}(E) = U(\pi)^{-1}S_{A,B}(E)U(\pi)$. In examples 2.1 and 2.2 one may take π to be the cyclic permutation and $C(\pi) = U(\pi)$. Consequently the on-shell S-matrix for example 2.1 given by (7) satisfies $S_{j+l\,k+l}(E) = S_{jk}(E) \bmod n$ for all l (see also, e.g., [36] for other examples).

Next we claim that if A and B are both real such that $A^\dagger = A^T$ and $B^\dagger = B^T$ then $S_{A,B}(E)$ equals its transpose. In particular, the on-shell S-matrix (7) for example 2.1 is symmetric. This is in analogy to potential scattering on the line, where the Hamiltonian is also real (i.e. commutes with complex conjugation). There the transmission amplitude for the incoming plane wave from the left equals the transmission amplitude for the incoming plane wave from the right (see, e.g., [72, 73]). In fact, one has a general result. For given (A, B) defining the self-adjoint operator $\Delta(A, B)$, $(\bar{A}, \bar{B})$ also defines a self-adjoint operator $\Delta(\bar{A}, \bar{B})$, since $(\bar{A}, \bar{B})$ has maximal rank and $\bar{A}\bar{B}^\dagger$ is also self-adjoint. It is easy to see that $\Delta(\bar{A}, \bar{B})$ has domain $\mathcal{D}(\Delta(\bar{A}, \bar{B})) = \{\psi \mid \bar{\psi} \in \mathcal{D}(\Delta(A, B))\}$ and $\Delta(\bar{A}, \bar{B})\psi = \overline{\Delta(A, B)\bar{\psi}}$. In particular, $\Delta(A, B)$ is a real operator if the matrices A and B are real. Thus the Laplace operators obtained from example 2.1 are real, while those obtained from example 2.2 are not real. In example 2.3 (A, B) is real iff $\exp(2\mathrm{i}\mu) = 1$. More generally we will say that the boundary conditions (A, B) are real if there is an invertible map C such that CA and CB are real. Thus Robin boundary conditions are real. For invertible A (or B) a necessary and sufficient condition is that the self-adjoint matrix $A^{-1}B$ (or $B^{-1}A$) is real. We have

Corollary 2.1. *The on-shell S-matrices satisfy the following relation:*

$$S_{\bar{A},\bar{B}}(E)^T = S_{A,B}(E). \tag{8}$$

For the proof observe that $S_{\bar{A},\bar{B}}(E)^T = -\big(A^\dagger - \mathrm{i}\sqrt{E}\,B^\dagger\big)\big(A^\dagger + \mathrm{i}\sqrt{E}\,B^\dagger\big)^{-1}$ and the claim again easily follows from the fact that $AB^\dagger$ is self-adjoint.

As a next observation we want to exploit the fact that A and B play an almost symmetric role. First we recall that if (A, B) defines a maximal isotropic subspace then $(-B, A)$ also defines a maximal isotropic subspace, which is just the orthogonal complement. In particular, Dirichlet boundary conditions turn into Neumann boundary conditions and vice versa under this correspondence. Although the Laplace operators $\Delta(A, B)$ and $\Delta(-B, A)$ are not directly related, there is a relation for their on-shell S-matrices. In fact, from (6) we immediately obtain

Corollary 2.2. *The on-shell S-matrices for the operators $-\Delta(A, B)$ and $-\Delta(-B, A)$ are related by*

$$S_{-B,A}(E) = -S_{A,B}\big(E^{-1}\big) \tag{9}$$

for all $E > 0$.

Adapting the notation from string theory (see, e.g., [77]) we call the map θ: $(A, B) \mapsto (-B, A)$ a duality transformation and (9) a duality relation. On the level of Laplace operators and on-shell S-matrices θ is obviously an involution. Since $\mathcal{M}(-B, A) = \mathcal{M}(A, B)^{\perp}$ there are no self-dual boundary conditions.

We conclude this section by providing a necessary and sufficient condition for $S_{A,B}(E)$ to be independent of E, i.e. to be a constant matrix. In fact, this will occur if (A, B) is such that none of the linear conditions involve both $\psi(0)$ and $\psi'(0)$. This means that the boundary conditions are scale invariant, i.e. invariant under the variable transformation $x \to \lambda^{-1}x$, $x, \lambda \in \mathbb{R}^{+}$. The algebraic formulation is given by

Corollary 2.3. *Assume the boundary condition is such that to any $\lambda > 0$ there is an invertible $C(\lambda)$ with $C(\lambda)A = A$ and $C(\lambda)B = \lambda B$. Then both $S_{A,B}(E)$ and $S_{-B,A}(E)$ are independent of E. The only eigenvalues of $S_{A,B}(E)$ are* +1 *and* -1 *with multiplicities equal to* rank B *and* rank A. *Also $AB^{\dagger} = 0$ and both $S_{A,B}(E)$ and $S_{-B,A}(E)$ are Hermitian such that by unitarity they are also involutive maps. If in addition the boundary conditions are real, then $S_{A,B}(E)$ and $S_{-B,A}(E)$ are also real. Conversely if $S_{A,B}(E)$ is constant then there is $C(\lambda)$ with the above property.*

Proof. The first part is obvious. To prove the second part recall (5). Since $S_{A,B}(E)$ is constant this implies $S_{A,B}(E)^{\dagger}B^{\dagger} = B^{\dagger}$ and $S_{A,B}(E)^{\dagger}A^{\dagger} = -A^{\dagger}$. Thus the column vectors of $B^{\dagger}$ and $A^{\dagger}$ are eigenvectors of $S_{A,B}(E)^{\dagger} = S_{A,B}(E)^{-1}$ and therefore of $S_{A,B}(E)$ with eigenvalues +1 and -1, respectively. They span subspaces of dimensions equal to rank $B^{\dagger} =$ rank B and rank $A^{\dagger} =$ rank A. To see that these vectors combined span all of $\mathbb{C}^n$ assume there is a vector ψ orthogonal to both these spaces. But this means that $A\psi = B\psi = 0$ and this is possible only if $\psi = 0$ since $A - \mathrm{i}\sqrt{E}\,B$ is invertible. Also eigenvectors for different eigenvalues are orthogonal which means that $AB^{\dagger} = 0$. The Hermiticity of $S_{A,B}(E)$ and $S_{-B,A}(E)$ therefore follows easily from (6). The reality of $S_{A,B}(E)$ and $S_{-B,A}(E)$ if the boundary conditions are real follows from corollary 2.1. As for the converse we first observe that by the above arguments a constant $S_{A,B}(E)$ implies the previous properties concerning eigenvalues and eigenvectors. Let therefore U be a unitary map which diagonalizes $S_{A,B}(E)$, i.e.

$$US_{A,B}(E)U^{-1} = \begin{pmatrix} -\mathbb{I} & 0 \\ 0 & \mathbb{I} \end{pmatrix}$$

holds with an obvious block notation. Also trivially

$$US_{A,B}(E)U^{-1}UA^{\dagger} = -UA^{\dagger} \qquad US_{A,B}(E)U^{-1}UB^{\dagger} = UB^{\dagger}.$$

Therefore A and B are necessarily of the form

$$A = \begin{pmatrix} a'_{11} & 0 \\ a'_{21} & 0 \end{pmatrix} U \qquad B = \begin{pmatrix} 0 & b'_{12} \\ 0 & b'_{22} \end{pmatrix} U$$

again in the same block notation. Since (A, B) and hence (AU, BU) has maximal rank, the matrix

$$\begin{pmatrix} a'_{11} & b'_{12} \\ a'_{21} & b'_{22} \end{pmatrix}$$

is invertible. Let D denote its inverse, such that

$$DA = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & 0 \end{pmatrix} U \qquad DB = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{I} \end{pmatrix} U.$$

Then

$$C(\lambda) = D^{-1} \begin{pmatrix} \mathbb{I} & 0 \\ 0 & \lambda\mathbb{I} \end{pmatrix} D$$

does the job, concluding the proof of the corollary. □

The following example will be reconsidered in section 4.

Example 2.4 ($n = 3$). *Let the boundary conditions be given as*

$$\psi_1(0) = \psi_2(0) = \psi_3(0)$$
$$\psi'_1(0) + \psi'_2(0) + \psi'_3(0) = 0$$

i.e.

$$A = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix} \qquad C(\lambda) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \lambda \end{pmatrix}.$$

Thus A has rank 2, B rank 1 and $AB^\dagger = 0$. The resulting on-shell S-matrix is given as

$$S(E) = \begin{pmatrix} -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{pmatrix}$$

for all E. Since it is Hermitian and unitary the eigenvalues are indeed ± 1 with the desired multiplicities since $\mathrm{Tr}\, S(E) = -1$.

3. Arbitrary finite quantum wires

In this section we will discuss the general case employing the methods used in the previous section. Let $\mathcal{E}$ and $\mathcal{I}$ be finite sets with n and m elements, respectively, and ordered in an arbitrary but fixed way. $\mathcal{E}$ labels the external lines and $\mathcal{I}$ labels the internal lines, i.e. we consider a graph with m internal (of finite length) and n external lines. Unless stated otherwise $n \neq 0$, since we will mainly focus on scattering theory. The discussion in the previous section already covered the case $m = 0$ so we will also assume $m \neq 0$. To each $e \in \mathcal{E}$ we associate the infinite interval $[0, \infty)$ and to each $i \in \mathcal{I}$ the finite interval $[0, a_i]$ where $a_i > 0$. The Hilbert space is now defined as

$$\mathcal{H} = \bigoplus_{e\in\mathcal{E}} \mathcal{H}_e \bigoplus_{i\in\mathcal{I}} \mathcal{H}_i = \mathcal{H}_\mathcal{E} \oplus \mathcal{H}_\mathcal{I}$$

where $\mathcal{H}_e = L^2([0, \infty))$ for $e \in \mathcal{E}$ and $\mathcal{H}_i = L^2([0, a_i])$ for $i \in \mathcal{I}$. $\mathcal{H}_\mathcal{E}$ is called the exterior and $\mathcal{H}_\mathcal{I}$ is called the interior component of $\mathcal{H}$. Elements in $\mathcal{H}$ are written as

$$\psi = (\{\psi_e\}_{e\in\mathcal{E}}, \{\psi_i\}_{i\in\mathcal{I}})^T = (\psi_\mathcal{E}, \psi_\mathcal{I})^T.$$

Thus the previous case is the special case when $\mathcal{I}$ is empty. Now let Δ^0 be the Laplace operator with the domain of definition $\mathcal{D}(\Delta^0)$ being given as the set of all ψ with ψ_e, $e \in \mathcal{E}$ belonging to $W^{2,2}(0,\infty)$ and vanishing at $x = 0$ together with their first derivatives while ψ_i belong to $W^{2,2}(0, a_i)$ for all $i \in \mathcal{I}$ and vanish at the ends of the interval together their first derivatives. Obviously Δ^0 has defect indices $(n+2m, n+2m)$. To find all self-adjoint extensions let now $\mathcal{D}$ be the set of all ψ with ψ_e, $e \in \mathcal{E}$ belonging to $W^{2,2}(0,\infty)$, while $\psi_i \in W^{2,2}(0, a_i)$, $i \in \mathcal{I}$. Also the skew-Hermitian quadratic form Ω on $\mathcal{D}$ is now defined as

$$\Omega(\phi, \psi) = \langle \Delta\phi, \psi\rangle - \langle \phi, \Delta\psi\rangle = -\overline{\Omega(\psi, \phi)}.$$

Let $[\,]\colon \mathcal{D} \to \mathbb{C}^{2(n+2m)}$ be the surjective linear map which associates to each ψ the element $[\psi]$ given as

$$[\psi] = \begin{pmatrix} (\psi_e(0)_{e\in\mathcal{E}}, \psi_i(0)_{i\in\mathcal{I}}, \psi_i(a_i)_{i\in\mathcal{I}})^T \\ (\psi_e'(0)_{e\in\mathcal{E}}, \psi_i'(0)_{i\in\mathcal{I}}, -\psi_i'(a_i)_{i\in\mathcal{I}})^T \end{pmatrix} = \begin{pmatrix} \underline{\psi} \\ \underline{\psi}' \end{pmatrix} \tag{10}$$

again viewed as a column vector with the ordering given by the ordering of $\mathcal{E}$ and $\mathcal{I}$. Obviously $\mathcal{D}(\Delta^0)$ is the kernel of the map $[\,]$. By partial integration we again obtain

$$\Omega(\phi, \psi) = \omega([\phi], [\psi]) = \langle [\phi], J[\psi]\rangle_{\mathbb{C}^{2(n+2m)}}$$

where now J is the canonical symplectic form on $\mathbb{C}^{2(n+2m)}$ of the same form as in (1) and $\langle\,,\rangle_{\mathbb{C}^{2(n+2m)}}$ is now the canonical scalar product on $\mathbb{C}^{2(n+2m)}$. The formulation of the boundary condition is as in the previous section. Let now A and B be $(n+2m)\times(n+2m)$ matrices and let $\mathcal{M}(A, B)$ be the linear space of all $[\psi]$ in $\mathbb{C}^{2(n+2m)}$ such that

$$A\underline{\psi} + B\underline{\psi}' = 0. \tag{11}$$

Then $\mathcal{M}(A, B)$ has dimension $n+2m$ iff the $(n+2m)\times 2(n+2m)$ matrix (A, B) has maximal rank equal to $n+2m$. If, in addition, $AB^\dagger$ is self-adjoint then $\mathcal{M}(A, B)$ is maximal isotropic. The resulting self-adjoint operator will again be denoted by $\Delta(A, B)$. Again in what follows we will always assume that the boundary conditions (A, B) have these properties.

Similarly to the discussion in the case of single vertex graph (see appendix A) we can relate von Neumann's parametrization of self-adjoint extensions of Δ^0 to the matrices A and B. Corresponding details can easily be worked out and therefore we omit them.

To determine the resulting on-shell S-matrix, we now look for plane-wave solutions $\psi^k(\cdot, E)$, $k \in \mathcal{E}$ of the stationary Schrödinger equation for $-\Delta(A, B)$ at energy $E > 0$ which satisfy the boundary conditions (A, B) and which are of the following form and which generalize (4)

$$\psi_j^k(x, E) = \begin{cases} S_{jk}(E)\,\mathrm{e}^{\mathrm{i}\sqrt{E}\,x} & \text{for} \quad j \in \mathcal{E},\ j \neq k \\ \mathrm{e}^{-\mathrm{i}\sqrt{E}\,x} + S_{kk}(E)\,\mathrm{e}^{\mathrm{i}\sqrt{E}\,x} & \text{for} \quad j \in \mathcal{E},\ j = k \\ \alpha_{jk}(E)\,\mathrm{e}^{\mathrm{i}\sqrt{E}\,x} + \beta_{jk}(E)\,\mathrm{e}^{-\mathrm{i}\sqrt{E}\,x} & \text{for} \quad j \in \mathcal{I}. \end{cases} \tag{12}$$

The aim is thus to determine the $n \times n$ matrix $S(E) = S_{A,B}(E)$ and the $m \times n$ matrices $\alpha(E) = \alpha_{A,B}(E)$ and $\beta(E) = \beta_{A,B}(E)$. The physical interpretation of the matrix elements $S_{jk}(E)$ is as before and the matrix elements of $\alpha(E)$ and $\beta(E)$ are 'interior' amplitudes. It is advisable to write matrices like A and B in a 3×3 block form, i.e.

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}$$

where A_{11} is an $n \times n$ matrix, A_{12} and A_{13} are $n \times m$ matrices, etc. Thus, for example, the matrices A_{1i}, A_{i1}, B_{1i}, B_{i1}, $i = 2, 3$ describe the coupling of the exterior to the interior.

Correspondingly $\underline{\psi}$ and $\underline{\psi}'$ are written as (cf equation (10))

$$\underline{\psi} = \begin{pmatrix} \psi_{\mathcal{E}}(0) \\ \psi_{\mathcal{I}}(0) \\ \psi_{\mathcal{I}}(\underline{a}) \end{pmatrix} \qquad \underline{\psi}' = \begin{pmatrix} \psi'_{\mathcal{E}}(0) \\ \psi'_{\mathcal{I}}(0) \\ -\psi'_{\mathcal{I}}(\underline{a}) \end{pmatrix}$$

where $\underline{a} = (a_1, \ldots, a_m)$. Also we introduce the diagonal $m \times m$ matrices $\exp(\pm \mathrm{i}\sqrt{E}\,\underline{a})$ by

$$\exp\left(\pm \mathrm{i}\sqrt{E}\,\underline{a}\right)_{jk} = \delta_{jk} \mathrm{e}^{\pm \mathrm{i}\sqrt{E}\,a_j} \qquad \text{for} \quad j, k \in \mathcal{I}.$$

The equations for the matrices $S(E)$, $\alpha(E)$ and $\beta(E)$ now take the following form:

$$A \begin{pmatrix} S(E) + \mathbb{I} \\ \alpha(E) + \beta(E) \\ \mathrm{e}^{\mathrm{i}\sqrt{E}\,\underline{a}}\alpha(E) + \mathrm{e}^{-\mathrm{i}\sqrt{E}\,\underline{a}}\beta(E) \end{pmatrix} + \mathrm{i}\sqrt{E}\,B \begin{pmatrix} S(E) - \mathbb{I} \\ \alpha(E) - \beta(E) \\ -\mathrm{e}^{\mathrm{i}\sqrt{E}\,\underline{a}}\alpha(E) + \mathrm{e}^{-\mathrm{i}\sqrt{E}\,\underline{a}}\beta(E) \end{pmatrix} = 0$$

which is a $(n+2m) \times n$ matrix equation with matrix multiplication between $(n+2m) \times (n+2m)$ and $(n+2m) \times n$ matrices. We rewrite this equation as an inhomogeneous equation generalizing equation (5),

$$Z_{A,B}(E) \begin{pmatrix} S(E) \\ \alpha(E) \\ \beta(E) \end{pmatrix} = -\left(A - \mathrm{i}\sqrt{E}\,B\right) \begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} \tag{13}$$

where

$$Z_{A,B}(E) = AX(E) + \mathrm{i}\sqrt{E}\,BY(E)$$

with

$$X(E) = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & \mathbb{I} \\ 0 & \mathrm{e}^{\mathrm{i}\sqrt{E}\,\underline{a}} & \mathrm{e}^{-\mathrm{i}\sqrt{E}\,\underline{a}} \end{pmatrix}$$

and

$$Y(E) = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & -\mathbb{I} \\ 0 & -\mathrm{e}^{\mathrm{i}\sqrt{E}\,\underline{a}} & \mathrm{e}^{-\mathrm{i}\sqrt{E}\,\underline{a}} \end{pmatrix}.$$

If $\det Z_{A,B}(E) \neq 0$ the scattering matrix $S(E) = S_{A,B}(E)$ as well as the $m \times n$ matrices $\alpha(E)$ and $\beta(E)$ can be uniquely determined by solving equation (13),

$$\begin{pmatrix} S(E) \\ \alpha(E) \\ \beta(E) \end{pmatrix} = -Z_{A,B}(E)^{-1}\left(A - \mathrm{i}\sqrt{E}\,B\right) \begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix}. \tag{14}$$

We recall that by the Birman–Kato theory $S_{A,B}(E)$ is defined and unitary for almost all $E > 0$ because $\Delta(A, B)$ is a finite rank perturbation of $\Delta(A = 0, B = \mathbb{I})$. We denote by $\Sigma_{A,B} = \{E > 0 | \ \det Z_{A,B}(E) = 0\}$ the set of exceptional points for which $Z_{A,B}(E)$ is not invertible. Now we prove

Theorem 3.1. *For any boundary condition* (A, B) *the set* $\Sigma_{A,B}$ *equals the set* $\sigma_{A,B}$ *of all positive eigenvalues of* $-\Delta(A, B)$*. This set is discrete and has no finite accumulation points in* $\mathbb{R}_+$.

Proof. First we prove that for every $E \in \Sigma_{A,B}$ all elements of Ker $Z_{A,B}(E)$ have the form $\left(0, \hat{\alpha}^T, \hat{\beta}^T\right)^T$ with $\hat{\alpha}$ and $\hat{\beta}$ being (column) vectors in $\mathbb{C}^m$. Let us suppose the converse, i.e. that there is a column vector $\left(\hat{s}^T, \hat{\alpha}^T, \hat{\beta}^T\right)^T \in \mathbb{C}^{n+2m}$ such that

$$Z_{A,B}(E) \begin{pmatrix} \hat{s} \\ \hat{\alpha} \\ \hat{\beta} \end{pmatrix} = 0 \tag{15}$$

or equivalently

$$\left(A + \mathrm{i}\sqrt{E}\, B\right) \begin{pmatrix} \hat{s} \\ \hat{\alpha} \\ \mathrm{e}^{-\mathrm{i}\sqrt{E}\,\underline{a}} \hat{\beta} \end{pmatrix} + \left(A - \mathrm{i}\sqrt{E}\, B\right) \begin{pmatrix} 0 \\ \hat{\beta} \\ \mathrm{e}^{\mathrm{i}\sqrt{E}\,\underline{a}} \hat{\alpha} \end{pmatrix} = 0.$$

As in the proofs of lemma 2.3 and theorem 2.1 $A + \mathrm{i}\sqrt{E}\, B$ and $A - \mathrm{i}\sqrt{E}\, B$ are invertible and $\left(A + \mathrm{i}\sqrt{E}\, B\right)^{-1}\left(A - \mathrm{i}\sqrt{E}\, B\right)$ is unitary such that

$$\begin{pmatrix} \hat{s} \\ \hat{\alpha} \\ \mathrm{e}^{-\mathrm{i}\sqrt{E}\,\underline{a}} \hat{\beta} \end{pmatrix} = -\left(A + \mathrm{i}\sqrt{E}\, B\right)^{-1}\left(A - \mathrm{i}\sqrt{E}\, B\right) \begin{pmatrix} 0 \\ \hat{\beta} \\ \mathrm{e}^{\mathrm{i}\sqrt{E}\,\underline{a}} \hat{\alpha} \end{pmatrix}.$$

Since unitary transformations preserve the Euclidean norm we find

$$\|\hat{s}\|^2_{\mathbb{C}^n} + \|\hat{\alpha}\|^2_{\mathbb{C}^m} + \|\hat{\beta}\|^2_{\mathbb{C}^m} = \|\hat{\alpha}\|^2_{\mathbb{C}^m} + \|\hat{\beta}\|^2_{\mathbb{C}^m}$$

such that $\hat{s} = 0$.

Now for arbitrary $\left(0, \hat{\alpha}^T, \hat{\beta}^T\right)^T \in \operatorname{Ker} Z_{A,B}(E)$ we consider

$$\psi_j(x) = \begin{cases} 0 & \text{for} \quad j \in \mathcal{E} \\ \hat{\alpha}_j \, \mathrm{e}^{\mathrm{i}\sqrt{E}\,x} + \hat{\beta}_j \, \mathrm{e}^{-\mathrm{i}\sqrt{E}\,x} & \text{for} \quad j \in \mathcal{I}. \end{cases}$$

Obviously $\psi(x)$ is an eigenfunction of $-\Delta(A, B)$. Thus we have proved that $\Sigma_{A,B} \subseteq \sigma_{A,B}$. We note that this inclusion is non-trivial, since *a priori* we cannot exclude real energy resonances.

Conversely, let $E \in \sigma_{A,B}$. Observing that positive energy eigenfunctions must have support on the internal lines of the graph and repeating the arguments, which led to equation (13), we see that there exists a non-zero vector $\left(0, \hat{\alpha}^T, \hat{\beta}^T\right)^T \in \mathbb{C}^{n+2m}$ such that (15) is satisfied, and hence $\sigma_{A,B} \subseteq \Sigma_{A,B}$. We notice that det $Z_{A,B}(E)$ is an entire function of $\sqrt{E}$ in the complex plane $\mathbb{C}$. Also det $Z_{A,B}(E)$ does not vanish identically since by the preceding arguments det $Z_{A,B}(E) = 0$ for $E \in \mathbb{C} \setminus \mathbb{R}$ implies that E is an eigenvalue of $-\Delta(A, B)$, which in turn contradicts the self-adjointness. Thus all real zeros of det $Z_{A,B}(E)$ are isolated. This concludes the proof of the theorem. □

Remark 3.1. *The case $n = 0$ with no associated S-matrix is of interest in its own right. Then (13) takes the form of a homogeneous equation*

$$Z_{A,B}(E) \begin{pmatrix} \hat{\alpha}(E) \\ \hat{\beta}(E) \end{pmatrix} = 0 \tag{16}$$

with $\hat{\alpha}(E)$ and $\hat{\beta}(E)$ being column vectors in $\mathbb{C}^m$. It has solutions iff $E \in \mathbb{R}$ is such that det $Z_{A,B}(E) = 0$*. By what has been said so far it is clear that the solutions of (16) give the eigenvalues and the eigenfunctions of a quantum wire without open ends. As a possible example one might consider the graph associated to the semiclassical description of the fullerene and choose appropriate boundary conditions at the vertices (see, e.g., [78]).*

Before we proceed further with the study of equation (13) we consider several examples. Starting with the case, where everything works well without any singularities, we consider the following

Example 3.1 ($n = m = 1$). *We choose the following realization of the Hilbert space $\mathcal{H}$:*

$$\mathcal{H} = L^2([0,\infty)) = L^2([1,\infty)) \oplus L^2([0,1]).$$

We take Robin boundary conditions at the origin and a δ potential of strength c at $x = 1$, i.e.

$$\begin{aligned}
&\sin\varphi\psi(0) + \cos\varphi\psi'(0) = 0\\
&\psi(1+) - \psi(1-) = 0\\
&\psi'(1+) - \psi'(1-) - c\psi(1) = 0.
\end{aligned}$$

$S(E)$, $\alpha(E)$ and $\beta(E)$ are now functions and a straightforward calculation gives the following result. Let $S_R(E)$ denote the on-shell S-matrix for the Robin boundary condition alone, i.e.

$$S_R(E) = \mathrm{e}^{2\mathrm{i}\delta_R(E)} = -\frac{\sin\varphi - \mathrm{i}\sqrt{E}\cos\varphi}{\sin\varphi + \mathrm{i}\sqrt{E}\cos\varphi}.$$

Then

$$\begin{aligned}
S(E) &= \frac{\left(2\mathrm{i}\sqrt{E} + c\right)\mathrm{e}^{\mathrm{i}(\sqrt{E}+2\delta_R(E))} + c\mathrm{e}^{-\mathrm{i}\sqrt{E}}}{\left(2\mathrm{i}\sqrt{E} - c\right)\mathrm{e}^{-\mathrm{i}\sqrt{E}} - c\mathrm{e}^{\mathrm{i}(\sqrt{E}+2\delta_R(E))}}\mathrm{e}^{-2\mathrm{i}\sqrt{E}}\\
\alpha(E) &= \frac{2\mathrm{i}\sqrt{E}\,\mathrm{e}^{-\mathrm{i}(\sqrt{E}-2\delta_R(E))}}{\left(2\mathrm{i}\sqrt{E} - c\right)\mathrm{e}^{-\mathrm{i}\sqrt{E}} + c\mathrm{e}^{\mathrm{i}(\sqrt{E}+2\delta_R(E))}}\\
\beta(E) &= \frac{2\mathrm{i}\sqrt{E}\mathrm{e}^{-\mathrm{i}\sqrt{E}}}{\left(2\mathrm{i}\sqrt{E} - c\right)\mathrm{e}^{-\mathrm{i}\sqrt{E}} + c\mathrm{e}^{\mathrm{i}(\sqrt{E}+2\delta_R(E))}}.
\end{aligned}$$

In particular, these quantities are finite for all $E > 0$.

Example 3.2. *Consider the graph depicted in figure 1 with $\mathcal{E} = \{1, 2\}$, $\mathcal{I} = \{3, 4\}$, and with $a_3 = a_4 = a$, i.e. the internal lines have equal length. The arrows on the graph segments show*

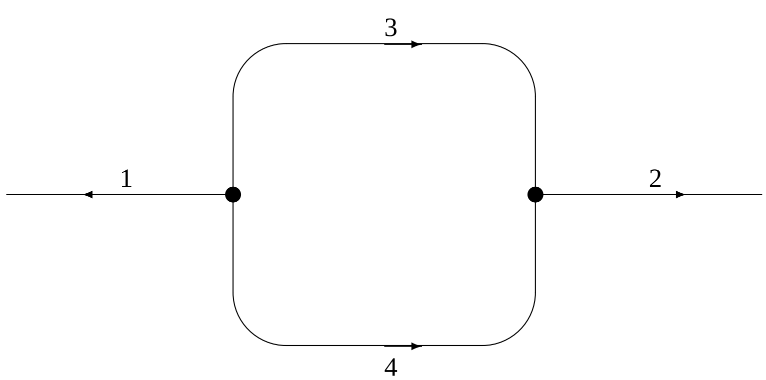

Figure 1. The graph from example 3.2. The arrows show the positive direction for every segment.

the positive directions. We pose the following real boundary conditions, obviously defining a self-adjoint operator:

$$\begin{aligned}
&\psi_1(0) = \psi_3(0) = \psi_4(0)\\
&\psi_2(0) = \psi_3(a) = \psi_4(a)\\
&\psi_1'(0) + \psi_3'(0) + \psi_4'(0) = 0\\
&\psi_2'(0) - \psi_3'(a) - \psi_4'(a) = 0.
\end{aligned}$$

Straightforward calculations yield

$$\det Z(E) = \left(10 - \mathrm{e}^{2\mathrm{i}\sqrt{E}\,a} - 9\mathrm{e}^{-2\mathrm{i}\sqrt{E}\,a}\right)E$$

such that $\Sigma_{A,B} = \{n^2\pi^2/a^2,\ n \in \mathbb{N}\}$. *The corresponding wavefunctions have the form* $\psi_1 = \psi_2 \equiv 0$, $\psi_3(x) = -\psi_4(x) = \sin(n\pi x/a)$. *Note that these eigenfunctions for the embedded eigenvalues have compact support. This is in contrast to standard Schrödinger operators of the form* $-\Delta + V$*, where bound state eigenfunctions cannot have compact support due to the ellipticity of* $-\Delta$*. The on-shell* S*-matrix can also be easily calculated, giving*

$$S(E) = -\frac{1}{\mathrm{e}^{2\mathrm{i}\sqrt{E}\,a} - 9}\begin{pmatrix} 3\left(\mathrm{e}^{2\mathrm{i}\sqrt{E}\,a} - 1\right) & 8\mathrm{e}^{\mathrm{i}\sqrt{E}\,a} \\ 8\mathrm{e}^{\mathrm{i}\sqrt{E}\,a} & 3\left(\mathrm{e}^{2\mathrm{i}\sqrt{E}\,a} - 1\right) \end{pmatrix}. \tag{17}$$

Equation (13) is solvable for all $E \in \Sigma_{A,B}$ *and defines* $S(E)$ *uniquely.* $S(E)$ *is well behaved for all* $E > 0$ *and there is no influence of the bound states, except that the (equal) reflection amplitudes vanish for* $E \in \Sigma_{A,B}$*. This is in contrast to Schrödinger operators of the form* $-\Delta + \lambda P$ *with appropriate real* λ *and with* P *being the orthogonal projector onto any given one-dimensional linear subspace of the Hilbert space [79], or to Schrödinger operators with Wigner–von Neumann-type potentials [80]. The scattering matrix (17) has poles only in the unphysical sheet (resonances),*

$$\sqrt{E_n} = \frac{\pi n}{a} - \mathrm{i}\frac{\log 9}{2a} \qquad n \in \mathbb{Z}.$$

The relation

$$\lim_{a\downarrow 0} S(E) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = S_2^{\mathrm{free}}(E)$$

holds as is to be expected from the boundary conditions.

Let us observe that

$$\det X(E) = \det Y(E) = \prod_{j\in\mathcal{I}} \left(-2\mathrm{i}\sin\sqrt{E}\,a_j\right).$$

Therefore if $E \in \Sigma_{\underline{a}} = \bigcup_{j\in\mathcal{I}} \Sigma_{\underline{a}}(j) = \bigcup_{j\in\mathcal{I}}\{E > 0 |\ \sin\sqrt{E}\,a_j = 0\}$ then $Z_{A,B}(E)$ will not be invertible for (A, B) defining Dirichlet or Neumann boundary conditions, since then $\det Z_{A,B}(E) = \det X(E)$. In particular, in these two cases the exterior and the interior decouple such that then we have

$$\Delta(A, B) = \Delta_{\mathcal{E}}(A, B) \oplus \Delta_{\mathcal{I}}(A, B).$$

Here $\Delta_{\mathcal{E}}(A, B)$ for both $(A = \mathbb{I}, B = 0)$ and $(A = 0, B = \mathbb{I})$ have an absolutely continuous spectrum and $\Delta_{\mathcal{I}}(A, B)$ has a purely discrete spectrum which on the set $E > 0$ equals $\Sigma_{\underline{a}}$. This means that we have eigenvalues embedded in the continuum. Now equation (13) for Dirichlet or Neumann boundary conditions has a unique solution $S(E) = -\mathbb{I}$ and $S(E) = \mathbb{I}$, respectively, and $\alpha(E) = \beta(E) = 0$ whenever E is not in $\Sigma_{\underline{a}}$. If E is in $\Sigma_{\underline{a}}$, then $S(E)$ is still of this form but $\alpha(E)$ and $\beta(E)$ are non-unique and of the form $\alpha(E) = \beta(E)$ and $\alpha(E) = -\beta(E)$ for Dirichlet and Neumann boundary conditions, respectively, with α_{jk} being arbitrary whenever $E \in \Sigma_{\underline{a}}(j)$ and zero otherwise.

A similar result is valid for arbitrary boundary conditions:

Theorem 3.2. *For any boundary condition (A, B) and all $E \in \Sigma_{A,B}$ equation (13) is solvable and determines $S_{A,B}(E)$ uniquely.*

Proof. Let ψ be an arbitrary element of Ker $Z(E)^{\dagger}$, i.e. ψ solves the adjoint homogeneous equation corresponding to (13),

$$\big(X(E)^{\dagger}A^{\dagger} - \mathrm{i}\sqrt{E}\, Y(E)^{\dagger}B^{\dagger}\big)\psi = 0. \tag{18}$$

Suppose first that $B = 0$, such that A has full rank (Dirichlet boundary conditions). Moreover, $\Sigma_{A,B} = \Sigma_{\underline{a}}$. Any solution of (18) may be written as $\psi = A^{\dagger\,-1}\chi$ with χ being a solution of $X(E)^{\dagger}\chi = 0$. χ is necessarily of the form $\chi = \big(0, \hat{\alpha}^T, \hat{\beta}^T\big)^T$ for some $\hat{\alpha}, \hat{\beta} \in \mathbb{C}^m$. Let $\phi_i \in \mathbb{C}^{n+2m}$, $i = 1, \ldots, n$ be such that $(\phi_i)_k = \delta_{ik}$. Then

$$(\psi, A\phi_i) = \big(A^{\dagger}\psi, \phi_i\big) = (\chi, \phi_i) = 0$$

for all $i = 1, \ldots, n$. We now apply the Fredholm alternative as follows. First we note that Ker $Z(E)^{\dagger} = (\mathrm{Ran}\, Z(E))^{\perp}$, the orthogonal complement of the range of $Z(E)$. Therefore the last relation states that all column vectors of

$$\big(A - \mathrm{i}\sqrt{E}\, B\big)\begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} = A\begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix}$$

are in the range of $Z(E)$. Thus (13) has a solution and since all elements of Ker $Z(E)$ are of the form $\big(0, \hat{\alpha}^T, \hat{\beta}^T\big)^T$, the on-shell S-matrix $S_{A,B}(E)$ is determined uniquely. □

Now we suppose that $B \neq 0$. First we consider the case $E \in \Sigma_{A,B}$ and $E \notin \Sigma_{\underline{a}}$. From (18) it follows that

$$A^{\dagger}\psi = \mathrm{i}\sqrt{E}\, X(E)^{\dagger\,-1}Y(E)^{\dagger}B^{\dagger}\psi$$

and thus

$$\big(\psi, BA^{\dagger}\psi\big) = \mathrm{i}\sqrt{E}\big(B^{\dagger}\psi, X(E)^{\dagger\,-1}Y(E)^{\dagger}B^{\dagger}\psi\big). \tag{19}$$

Since $BA^{\dagger}$ is self-adjoint the left-hand side of (19) is real. To analyse the right-hand side we note that

$$X(E)^{\dagger\,-1}Y(E)^{\dagger} = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \mathrm{i}\begin{pmatrix} 0 & 0 & 0 \\ 0 & \operatorname{cotan}\big(\sqrt{E}\,\underline{a}\big) & -\dfrac{1}{\sin\big(\sqrt{E}\,\underline{a}\big)} \\ 0 & -\dfrac{1}{\sin\big(\sqrt{E}\,\underline{a}\big)} & \operatorname{cotan}\big(\sqrt{E}\,\underline{a}\big) \end{pmatrix} \tag{20}$$

where the first term is self-adjoint and the second skew-self-adjoint. Therefore

$$\mathrm{Re}\,\big(B^{\dagger}\psi, X(E)^{\dagger\,-1}Y(E)^{\dagger}B^{\dagger}\psi\big) = \left(B^{\dagger}\psi, \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} B^{\dagger}\psi\right).$$

Since the left-hand side of (19) is real, it follows that

$$\left(B^{\dagger}\psi, \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} B^{\dagger}\psi\right) = 0 \tag{21}$$

and thus

$$\left(\phi_i, B^\dagger\psi\right) = 0 \tag{22}$$

for all $i = 1, \ldots, n$. Multiplying the equation (18) by ϕ_i from the left we obtain

$$\left(\phi_i, A^\dagger\psi\right) - \mathrm{i}\sqrt{E}\left(\phi_i, B^\dagger\psi\right) = 0.$$

Thus from (22) it follows that $\left(\phi_i, A^\dagger\psi\right) = 0$. Therefore

$$\left(\psi, \left(A - \mathrm{i}\sqrt{E}\, B\right)\phi_i\right) = 0$$

for all $i = 1, \ldots, n$. Therefore we may again invoke the Fredholm alternative and obtain a unique on-shell S-matrix. Finally we turn to the case $E \in \Sigma_{A,B} \cap \Sigma_{\underline{a}}$. An important ingredient of the proof in this case is the Moore–Penrose generalized inverse (or pseudoinverse) (see, e.g., [81]). Recall that for any (not necessary square) matrix M its generalized inverse $M^\star$ is uniquely defined by the Penrose equations

$$\begin{aligned} &MM^\star M = M && M^\star MM^\star = M^\star \\ &(M^\star M)^\dagger = M^\star M && (MM^\star)^\dagger = MM^\star. \end{aligned}$$

One also has

$$\begin{aligned} &(M^\star)^\dagger = \left(M^\dagger\right)^\star \\ &\mathrm{Ran}\, M^\star = \mathrm{Ran}\, M^\dagger \\ &\mathrm{Ker}\, M^\star = \mathrm{Ker}\, M^\dagger \end{aligned}$$

and $MM^\star = P_{\mathrm{Ran}\, M}$, $M^\star M = P_{\mathrm{Ran}\, M^\dagger}$, where $P_{\mathcal{H}}$ denotes the orthogonal projector onto the subspace $\mathcal{H}$. Moreover, $0^\star = 0$. If M is a square matrix of full rank $M^\star = M^{-1}$. However, the product formula for inverse matrices $(M_1M_2)^\star = M_2^\star M_1^\star$ does not hold in general. The pseudoinverse of any diagonal matrix Λ with $\det\Lambda = 0$ is given by

$$\Lambda^\star = \begin{pmatrix} \lambda_1 & & & & & \\ & \ddots & & & & \\ & & \lambda_r & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix}^\star = \begin{pmatrix} \lambda_1^{-1} & & & & & \\ & \ddots & & & & \\ & & \lambda_r^{-1} & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix}.$$

Using the fact that $\left(Q^\dagger MQ\right)^\star = Q^\dagger M^\star Q$ for any unitary Q one can easily calculate the generalized inverse by means of the formulae

$$M^\star = \left(M^\dagger M\right)^\star M^\dagger = M^\dagger\left(MM^\dagger\right)^\star.$$

With these preparatory remarks we return to the proof. We will say that $\chi \in \mathrm{Ker}\, X(E)^\dagger$ is a basis element of $\mathrm{Ker}\, X(E)^\dagger$ if $\chi = \left(0, \hat{\alpha}^T, \hat{\beta}^T\right)^T$ with $\hat{\alpha}_i = \hat{\beta}_i = 0$ for all $i = 1, \ldots, m$ except for some $k = 1, \ldots, m$ and $\hat{\alpha}_k \neq 0$, $\hat{\beta}_k \neq 0$. For any basis element χ either

$$X(E)\chi = 0 \qquad \text{and} \qquad Y(E)\chi = c_Y\chi \tag{23}$$

or

$$Y(E)\chi = 0 \qquad \text{and} \qquad X(E)\chi = c_X\chi \tag{24}$$

with some $c_X, c_Y \neq 0$. The proof is elementary and is left to the reader. Taking the scalar product of (18) with χ we obtain

$$\big(X(E)\chi, A^\dagger\psi\big) = \mathrm{i}\sqrt{E}\big(Y(E)\chi, B^\dagger\psi\big).$$

In the case (23) we have $\big(\chi, B^\dagger\psi\big)$=0, and in the case (24) $\big(\chi, A^\dagger\psi\big) = 0$.

Multiplying equation (18) by $X(E)^{\star\dagger}$ we obtain

$$P_{\mathrm{Ran}\, X(E)} A^\dagger\psi = \mathrm{i}\sqrt{E}\, X(E)^{\star\dagger} Y(E)^\dagger B^\dagger\psi$$

and thus

$$\big(\psi, B P_{\mathrm{Ran}\, X(E)} A^\dagger\psi\big) = \mathrm{i}\sqrt{E}\big(B^\dagger\psi, X(E)^{\star\dagger} Y(E)^\dagger B^\dagger\psi\big). \tag{25}$$

The matrix $X(E)^{\star\dagger} Y(E)^\dagger$ has the form of the right-hand side of (20), where the singular entries must be replaced by zeros. Thus

$$\mathrm{Re}\,\big(B^\dagger\psi, X(E)^{\star\dagger} Y(E)^\dagger B^\dagger\psi\big) = \left(B^\dagger\psi, \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} B^\dagger\psi\right).$$

Using the relation $P_{\mathrm{Ran}\, X(E)} = \mathbb{I} - P_{\mathrm{Ran}\, X(E)^\perp} = \mathbb{I} - P_{\mathrm{Ker}\, X(E)^\dagger}$ we may rewrite the left-hand side of (25) as

$$\big(\psi, B P_{\mathrm{Ran}\, X(E)} A^\dagger\psi\big) = \big(\psi, B A^\dagger\psi\big) - \big(B^\dagger\psi, P_{\mathrm{Ker}\, X(E)^\dagger} A^\dagger\psi\big).$$

With χ_i ($1 \leqslant i \leqslant \dim\, \mathrm{Ker}\, X(E)^\dagger$) being the basis elements of $\mathrm{Ker}\, X(E)^\dagger$ we have

$$\big(B^\dagger\psi, P_{\mathrm{Ker}\, X(E)^\dagger} A^\dagger\psi\big) = \sum_{i=1}^{\dim \mathrm{Ker}\, X(E)^\dagger} \overline{\big(\chi_i, B^\dagger\psi\big)}\big(\chi_i, A^\dagger\psi\big).$$

By the discussion above all terms in this sum are zero. Thus we again obtain (21). The rest of the proof is as in the preceding cases. Theorem 3.2 in particular says that the presence of bound states does not spoil the existence and uniqueness of the on-shell S-matrix. This is to be expected since bound states do not participate in the scattering. The same is true for resonances due to their finite lifetime.

We are now prepared to formulate the main result of this paper.

Theorem 3.3. *For any boundary condition (A, B) defining the self-adjoint operator $-\Delta(A, B)$ the resulting on-shell S-matrix $S_{A,B}(E)$ is unitary for all $E \in \mathbb{R}_+$.*

Proof. The proof is quite elementary. By arguments used in the proof of theorem 3.1 we obtain that any solution of (13) satisfies

$$\begin{pmatrix} S(E) \\ \alpha(E) \\ \mathrm{e}^{-\mathrm{i}\sqrt{E}\,\underline{a}}\beta(E) \end{pmatrix} = -\big(A + \mathrm{i}\sqrt{E}\, B\big)^{-1}\big(A - \mathrm{i}\sqrt{E}\, B\big) \begin{pmatrix} \mathbb{I} \\ \beta(E) \\ \mathrm{e}^{\mathrm{i}\sqrt{E}\,\underline{a}}\alpha(E) \end{pmatrix}.$$

Now $\big(A + \mathrm{i}\sqrt{E}\, B\big)^{-1}\big(A - \mathrm{i}\sqrt{E}\, B\big)$ is unitary. Multiplying each side with its adjoint from the left we therefore obtain

$$S(E)^\dagger S(E) + \alpha(E)^\dagger\alpha(E) + \beta(E)^\dagger\beta(E) = \mathbb{I} + \beta(E)^\dagger\beta(E) + \alpha(E)^\dagger\alpha(E)$$

which gives $S(E)^\dagger S(E) = \mathbb{I}$ and which is unitarity. A second 'analytic' proof is given in appendix B (see also section 4 for a third proof based on the generalized star product). □

We now discuss some properties of $S_{A,B}(E)$. Obviously $Z_{A,B}(E)$ can be analytically continued to the complex $\sqrt{E}$-plane. By the self-adjointness of $\Delta(A, B)$ the determinant

$\det Z_{A,B}(E)$ cannot have zeros for E with $\operatorname{Im}\sqrt{E} > 0$ except for those on the positive imaginary semi-axis corresponding to the bound states. It may have additional zeros (resonances) in the unphysical energy sheet $\operatorname{Im}\sqrt{E} < 0$. By means of (14) the scattering matrix $S_{A,B}(E)$ can be analytically continued to the whole complex plane as a meromorphic function of $\sqrt{E}$. In fact, it is a rational function in $\sqrt{E}$, $\exp\left(\mathrm{i}\sqrt{E}\, a_j\right)$, and $\exp\left(-\mathrm{i}\sqrt{E}\, a_j\right)$. Therefore it is real analytic for all $E \in \mathbb{R}_+ \setminus \Sigma_{A,B}$. Since $S_{A,B}(E)$ for $E \in \Sigma_{A,B}$ is well defined and unitary, it is also continuous for all $E \in \mathbb{R}$.

As for the low- and high-energy behaviour we have the following obvious property. If A is invertible then $\lim_{E\downarrow 0} S_{A,B}(E) = -\mathbb{I}$ and if B is invertible then $\lim_{E\uparrow\infty} S_{A,B}(E) = \mathbb{I}$. For arbitrary (A, B) the corresponding relations do not hold in general as may be seen from looking at the Dirichlet ($A = \mathbb{I}$, $B = 0$) and Neumann ($A = 0$, $B = \mathbb{I}$) boundary conditions.

Let C be an invertible map on $\mathbb{C}^{n+2m}$ such that $\Delta(CA, CB) = \Delta(A, B)$. Correspondingly we have $S_{CA,CB}(E) = S_{A,B}(E)$ as it should be, since $Z_{CA,CB}(E) = CZ_{A,B}(E)$. Furthermore, let U be a unitary map on $\mathbb{C}^n$. Then U induces a unitary map $\hat{U}$ on $\mathbb{C}^{n+2m}$ by

$$\hat{U} = \begin{pmatrix} U & 0 & 0 \\ 0 & \mathbb{I} & 0 \\ 0 & 0 & \mathbb{I} \end{pmatrix}$$

and a unitary $\mathcal{U}$ on $\mathcal{H}$ via

$$(\mathcal{U}\psi)_j = \begin{cases} \sum_{k\in\mathcal{E}} U_{jk}\psi_k & \text{for} \quad j \in \mathcal{E} \\ \psi_j & \text{otherwise} \end{cases}$$

such that $\Delta(A\hat{U}, B\hat{U}) = \mathcal{U}^{-1}\Delta(A, B)\mathcal{U}$. We recall that all spaces $\mathcal{H}_e$ ($e \in \mathcal{E}$) are the L^2 space $L^2([0,\infty))$, so the definition of $\mathcal{U}$ makes sense. Also $Z_{A\hat{U},B\hat{U}}(E) = Z_{A,B}(E)\hat{U}$ since $\hat{U}$ commutes with $X(E)$ and $Y(E)$, such that $\Sigma_{A,B} = \Sigma_{A\hat{U},B\hat{U}}$. Next we observe that

$$\hat{U}\begin{pmatrix} S_{A\hat{U},B\hat{U}}(E) \\ \alpha_{A\hat{U},B\hat{U}}(E) \\ \beta_{A\hat{U},B\hat{U}}(E) \end{pmatrix} = \begin{pmatrix} US_{A\hat{U},B\hat{U}}(E) \\ \alpha_{A\hat{U},B\hat{U}}(E) \\ \beta_{A\hat{U},B\hat{U}}(E) \end{pmatrix}$$

and

$$\left(A\hat{U} - \mathrm{i}\sqrt{E}\, B\hat{U}\right)\begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} = \left(A - \mathrm{i}\sqrt{E}\, B\right)\begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} U.$$

From this we immediately obtain first for E outside $\Sigma_{A,B}$ and then by continuity for all $E > 0$

Corollary 3.1. *The following covariance properties hold for all $E > 0$:*

$$\begin{aligned} S_{A\hat{U},B\hat{U}}(E) &= U^{-1}S_{A,B}(E)U \\ \alpha_{A\hat{U},B\hat{U}}(E) &= \alpha_{A,B}(E)U \\ \beta_{A\hat{U},B\hat{U}}(E) &= \beta_{A,B}(E)U. \end{aligned} \tag{26}$$

In particular, if U is such that there exists an invertible $C = C(U)$ with $CA = A\hat{U}$ and $CB = B\hat{U}$ then $S_{A,B}(E) = U^{-1}S_{A,B}(E)U$ for all $E > 0$.

We have the following special application. There is a canonical representation $\pi \to U(\pi)$ of the permutation group of n elements into the unitaries of $\mathbb{C}^n$. If there is a π and an invertible $C = C(\pi)$ such that $CA = A\hat{U}(\pi)$ and $CB = B\hat{U}(\pi)$ then $S_{A,B}(E) = U^{-1}(\pi)S_{A,B}(E)U(\pi)$ for all $E > 0$. The on-shell S-matrix in example 3.2 is obviously invariant under the permutation $1 \leftrightarrow 2$ of the two external legs.

Remark 3.2. *This discussion may be extended to the case that some of the interval lengths a_i are equal resulting in more general covariance and possibly invariance properties described by some $U, \mathcal{U}$ and $\hat{U}$ such that $\hat{U}_{11} = U$ and $\hat{U}_{i1} = \hat{U}_{1i} = 0$ for $i = 2, 3$. We leave out the details, which may be worked out easily.*

Corollary 2.1 has the following generalization

Corollary 3.2. *For all boundary conditions (A, B) and all $E > 0$ the following relation holds:*

$$S_{\bar{A},\bar{B}}(E)^T = S_{A,B}(E). \tag{27}$$

In particular, for real boundary conditions the transmission coefficient from channel j to channel k, $k \neq j$ ($j, k \in \mathcal{E}$) equals the transmission coefficient from channel k to channel j for all $E > 0$.

Proof. We start with two remarks. First the relation

$$\big(A - \mathrm{i}\sqrt{E}\, B\big) \begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} = \big(AX' - \mathrm{i}\sqrt{E}\, BY'\big) \begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix}$$

holds for any X' of the form

$$X' = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & X'_{22} & X'_{23} \\ 0 & X'_{32} & X'_{33} \end{pmatrix}$$

and similarly for Y'. Secondly, the matrix

$$\begin{pmatrix} S_{A,B}(E) \\ \alpha_{A,B}(E) \\ \beta_{A,B}(E) \end{pmatrix}$$

constitutes the first n columns of the matrix $-Z_{A,B}(E)^{-1}\big(AX' - \mathrm{i}\sqrt{E}\, BY'B\big)$ with X' and Y' arbitrary as above. Assume for a moment that E is not in $\Sigma_{\underline{a}}$. To prove the corollary for such E it therefore suffices to show that

$$\big(Z_{\bar{A},\bar{B}}(E)^{-1}\big(\bar{A}Y(E)^{-1^T} - \mathrm{i}\sqrt{E}\bar{B}X(E)^{-1^T}\big)\big)^T = Z_{A,B}(E)^{-1}\big(AY(E)^{-1^T} - \mathrm{i}\sqrt{E}\, BX(E)^{-1^T}\big)$$

which is equivalent to

$$\begin{aligned}\big(AX(E) + \mathrm{i}\sqrt{E}\, BY(E)\big)&\big(Y(E)^{-1}A^\dagger - \mathrm{i}\sqrt{E}\, X(E)^{-1}B^\dagger\big) \\ &= \big(AY(E)^{-1^T} - \mathrm{i}\sqrt{E}\, BX(E)^{-1^T}\big)\big(X(E)^T A^\dagger + \mathrm{i}\sqrt{E}\, Y(E)^T B^\dagger\big).\end{aligned}$$

But this relation follows from the self-adjointness of $AB^\dagger$ and the observation that $X(E)\, Y(E)^{-1}$ is symmetric, such that the relations $X(E)\, Y(E)^{-1} = Y(E)^{-1^T} X(E)^T$ and $Y(E)\, X(E)^{-1} = X(E)^{-1^T} Y(E)^T$ hold. Finally, by continuity we may drop the condition that E is not in $\Sigma_{\underline{a}}$, thus completing the proof. The on-shell S-matrix of example 3.2 is obviously symmetric. □

To generalize the duality map of the previous section, we have to take the $\underline{a}$ dependence into account, so we write $S_{A,B,\underline{a}}$, etc. The reason is that the length scales a_j induce corresponding energy scales. Also the Hilbert spaces depend on $\underline{a}$, $\mathcal{H} = \mathcal{H}_{\underline{a}}$, so we will compare on-shell S-matrices related to theories in different Hilbert spaces.

For given $\underline{a}$ let $\underline{a}(E)$ be given by $a_i(E) = Ea_i$, $i \in \mathcal{I}$ such that $X_{\underline{a}(E)}\big(E^{-1}\big) = X_{\underline{a}}(E)$ and $Y_{\underline{a}(E)}\big(E^{-1}\big) = Y_{\underline{a}}(E)$ for all $E > 0$. Also set

$$T = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & 0 \\ 0 & 0 & -\mathbb{I} \end{pmatrix}$$

such that $T^\dagger = T$, $T^2 = \mathbb{I}$ and $TX_{\underline{a}}(E)T = Y_{\underline{a}}(E)$. We now define $\theta(A, B) = (-BT, AT)$. It is easy to see that $\theta(A, B)$ defines a maximal subspace. Also E^{-1} is not in $\Sigma_{\theta(A,B),\underline{a}(E)}$ if E is not in $\Sigma_{A,B,\underline{a}}$ and vice versa.

This leads to the following generalization of corollary 2.2

Corollary 3.3. *For all boundary conditions (A, B) and all $E > 0$ the following identities hold:*

$$\begin{aligned} S_{\theta(A,B),\underline{a}(E)}\big(E^{-1}\big) &= -S_{A,B,\underline{a}}(E) \\ \alpha_{\theta(A,B),\underline{a}(E)}\big(E^{-1}\big) &= -\alpha_{A,B,\underline{a}}(E) \\ \beta_{\theta(A,B),\underline{a}(E)}\big(E^{-1}\big) &= \beta_{A,B,\underline{a}}(E). \end{aligned} \tag{28}$$

The proof is easy by observing that

$$Z_{\theta(A,B),\underline{a}(E)}\big(E^{-1}\big) = \frac{\mathrm{i}}{\sqrt{E}} Z_{A,B,\underline{a}}(E)T$$

and

$$-BT - \frac{\mathrm{i}}{\sqrt{E}} AT = -\frac{\mathrm{i}}{\sqrt{E}}\big(A - \mathrm{i}\sqrt{E}\, B\big)T.$$

We conclude this section by giving a geometrical description of an arbitrary boundary condition as a local boundary condition at the vertices of a suitable graph.

For given sets $\mathcal{E}$ and $\mathcal{I}$ and $\underline{a}$, we label the halfline $[0, \infty)$ associated to $e \in \mathcal{E}$ by $I_e = [0_e, \infty_e)$ and the closed interval $[0, a_i]$ associated to $i \in \mathcal{I}$ by $I_i = [0_i, a_i]$ (considering a_i as a generic variable there should be no confusion between the number a_i and the label a_i). By $I = \bigcup_{e\in\mathcal{E}} I_e \bigcup_{i\in\mathcal{I}} I_i$ we denote the disjoint union. Let $\mathcal{V} = \bigcup_{e\in\mathcal{E}}\{0_e\} \bigcup_{i\in\mathcal{I}}\{0_i, a_i\} \subset I$ be the set of 'endpoints' in I. Clearly the number of points in $\mathcal{V}$ equals $|\mathcal{E}| + 2|\mathcal{I}| = n + 2m$. Consider a decomposition

$$\mathcal{V} = \bigcup_{\xi\in\Xi} \mathcal{V}_\xi \tag{29}$$

of $\mathcal{V}$ into non-empty disjoint subsets $\mathcal{V}_\xi$ with Ξ being just an index set. We say that the points in $\mathcal{V} \subset I$ are equivalent ($\sim$) when they lie in the same $\mathcal{V}_\xi$. By identifying equivalent points in $\mathcal{V} \subset I$ we obtain a graph Γ, $\Gamma = I/\sim$. In mathematical language Γ is a one-dimensional simplicial complex, which in particular is a topological space and non-compact if $\mathcal{E}$ is non-empty. Obviously the vertices in Γ are in one-to-one correspondence with the elements $\xi \in \Xi$. Note that Γ need not be connected. Also there may be 'tadpoles', i.e. we allow that 0_i and a_i for some $i \in \mathcal{I}$ belong to a same set $\mathcal{V}_\xi$. There is no restriction on the number of lines entering a vertex. In particular this number may equal 1 (so-called dead end side branches [10]), see example 3.1. The graph need not be planar.

Let $\{A, B\}$ be the equivalence class of the boundary condition (A, B) with respect to the equivalence relation given as $(A', B') \sim (A, B)$ iff there exists an invertible C such that $A' = CA$, $B' = CB$. By our previous discussion $\Delta(A, B)$ only depends on $\{A, B\}$. We say that $\{A, B\}$ has a description as a local boundary condition on the graph Γ if the following holds. First observe that we may label the columns of A and B by the elements v in $\mathcal{V}$ (see equation (10)). With this convention there is supposed to exist $(A', B') \in \{A, B\}$ with the following properties. To each k labelling the rows of A' and B' there is $\xi = \xi(k)$, such that $A'_{kv} = B'_{kv} = 0$ for all v not in $\mathcal{V}_\xi$. In other words the boundary condition labelled by k only involves the value of ψ and its derivative at those points in $\mathcal{V}$ which belong to $\mathcal{V}_\xi$ and this set is in one-to-one correspondence with a vertex in Γ. Of course if Γ is the unique graph consisting of one vertex only then this Γ does the job for any boundary condition $\{A, B\}$. However, one may convince oneself that for any given boundary condition $\{A, B\}$ there is a unique maximal graph $\Gamma = \Gamma(\{A, B\})$ describing $\{A, B\}$ as a local boundary condition, where maximal means that the number of vertices is maximal.

Let us briefly indicate the proof. Arrange the $2(n+2m)$ columns of the $(n+2m)\times 2(n+2m)$ matrix (A, B) in such a way that the first $n + 2m$ columns are linearly independent. Call this matrix X. Then there is an invertible matrix C such that the $(n+2m)\times(n+2m)$ matrix made of the first $n+2m$ columns of CX is the unit matrix. Now rearrange CX by undoing the previous arrangement giving (CA, CB).The decomposition (29) and hence $\Gamma(\{A, B\})$ may be read off the 'connectivity' of (CA, CB). The self-adjointness of $AB^\dagger$ may now be verified locally at each vertex (the local Kirchhoff rule), see examples 3.1 and 3.2. Of course different boundary conditions may still give the same Γ in this way. Also in this sense the graphs associated with the discussion in section 2 may actually consist of several disconnected parts, each with one vertex but without tadpoles.

In particular, this discussion shows that the results of this section cover all local boundary conditions on all graphs with arbitrary lengths in the interior and which describe Hamiltonians with free propagation away from the vertices.

4. The generalized star product and factorization of the S-matrix

In this section we will define a new composition rule for unitary matrices not necessarily of equal rank. This composition rule will generalize the star product for unitary 2×2 matrices so we will call it a generalized star product. It will be associative and the resulting matrix will again be unitary. We will apply this new composition rule to obtain the on-shell S-matrix for a graph from the on-shell S-matrices at the same energy of two subgraphs obtained by cutting the graph along an arbitrary numbers of lines. By iteration this will, in particular, allow us to obtain the on-shell S-matrix for an arbitrary graph from the on-shell S-matrices associated to its vertices (see section 2), thus leading to a third proof of unitarity.

Let V be any unitary $p \times p$ matrix $(p > 0)$. The composition rule will depend on V and will be denoted by $*_V$, such that for any unitary $n' \times n'$ matrix U' with $n' \geqslant p$ and any unitary $n'' \times n''$ matrix U'' with $n'' \geqslant p$, $2p < n' + n''$ and subject to a certain condition (see below) there will be a resulting unitary $n \times n$ matrix $U = U' *_V U''$ with $n = n' + n'' - 2p$. This generalized star product may be viewed as an amalgamation of U' and U'' and with V acting as an amalgam. To construct $*_V$ we write U' and U'' in a 2×2-block form

$$U' = \begin{pmatrix} U'_{11} & U'_{12} \\ U'_{21} & U'_{22} \end{pmatrix}, \qquad U'' = \begin{pmatrix} U''_{11} & U''_{12} \\ U''_{21} & U''_{22} \end{pmatrix} \tag{30}$$

where U'_{22} and U''_{11} are $p \times p$ matrices, U'_{11} is an $(n' - p) \times (n' - p)$ matrix, U''_{22} is an $(n'' - p) \times (n'' - p)$ matrix, etc. The unitarity condition for U' then reads

$$\begin{aligned}
&U'^\dagger_{11}U'_{11} + U'^\dagger_{21}U'_{21} = \mathbb{I}\\
&U'^\dagger_{12}U'_{12} + U'^\dagger_{22}U'_{22} = \mathbb{I}\\
&U'^\dagger_{11}U'_{12} + U'^\dagger_{21}U'_{22} = 0\\
&U'^\dagger_{12}U'_{11} + U'^\dagger_{22}U'_{21} = 0
\end{aligned}$$

and similarly for U''.

Condition A. The $p \times p$ matrix $VU'_{22}V^{-1}U''_{11}$ does not have 1 as an eigenvalue.

Note that by unitarity of U', U'' and V one has $\|VU'_{22}V^{-1}U''_{11}\| \leqslant 1$. Strict inequality holds whenever $\|U'_{22}\| < 1$ or $\|U''_{11}\| < 1$ and then condition A is satisfied. In general, if condition A is satisfied it is easy to see that the following $p \times p$ matrices exist:

$$
\begin{aligned}
K_1 &= (\mathbb{I} - VU'_{22}V^{-1}U''_{11})^{-1}V = V(1 - U'_{22}V^{-1}U''_{11}V)^{-1} \\
K_2 &= (\mathbb{I} - V^{-1}U''_{11}VU'_{22})^{-1}V^{-1} = V^{-1}\big(1 - U''_{11}VU'_{22}V^{-1}\big)^{-1}.
\end{aligned}
$$

An easy calculation establishes the following relations:

$$
\begin{aligned}
K_1 &= V + VU'_{22}V^{-1}U''_{11}K_1 = V + VU'_{22}K_2U''_{11}V \\
&= V + K_1U'_{22}V^{-1}U''_{11}V \\
K_2 &= V^{-1} + V^{-1}U''_{11}VU'_{22}K_2 = V^{-1} + V^{-1}U''_{11}K_1U'_{22}V^{-1} \\
&= V^{-1} + K_2U''_{11}VU'_{22}V^{-1}.
\end{aligned}
\tag{31}
$$

Note that formally one has

$$
\begin{aligned}
K_1 &= \sum_{m=0}^{\infty} \big(VU'_{22}V^{-1}U''_{11}\big)^m V \\
K_2 &= \sum_{m=0}^{\infty} \big(V^{-1}U''_{11}VU'_{22}\big)^m V^{-1}.
\end{aligned}
\tag{32}
$$

With these preparations the matrix $U = U' *_V U''$ is now defined as follows. Write U in a 2×2 block form as

$$
U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}
$$

where U_{11} is an $(n' - p) \times (n' - p)$ matrix, U_{22} is an $(n'' - p) \times (n'' - p)$ matrix, etc. These matrices are now defined as

$$
\begin{aligned}
U_{11} &= U'_{11} + U'_{12}K_2U''_{11}VU'_{21} \\
U_{22} &= U''_{22} + U''_{21}K_1U'_{22}V^{-1}U''_{12} \\
U_{12} &= U'_{12}K_2U''_{12} \\
U_{21} &= U''_{21}K_1U'_{21}.
\end{aligned}
\tag{33}
$$

In particular, if $n' = 2p$ then

$$
\begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix} *_V U'' = \begin{pmatrix} V^{-1} & 0 \\ 0 & \mathbb{I} \end{pmatrix} U'' \begin{pmatrix} V & 0 \\ 0 & \mathbb{I} \end{pmatrix}.
$$

Similarly if $n'' = 2p$ then

$$
U' *_V \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix} = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & V \end{pmatrix} U' \begin{pmatrix} \mathbb{I} & 0 \\ 0 & V^{-1} \end{pmatrix}.
$$

In this sense the matrices $\left(\begin{smallmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{smallmatrix}\right)$ serve as units when $V = \mathbb{I}$.

A straightforward but somewhat lengthy calculation presented in appendix C gives

Theorem 4.1. *If condition A is satisfied then the matrix $U = U' *_V U''$ is unitary.*

Analogously one may prove associativity. More precisely let U''' be a unitary $n''' \times n'''$ and V' a unitary $p' \times p'$ matrix with $p' \leqslant n''$, $p' \leqslant n'''$. If $p + p' \leqslant n'$, then

$$
U' *_V (U'' *_{V'} U''') = (U' *_V U'') *_{V'} U'''
$$

holds whenever condition A is satisfied for the compositions involved.

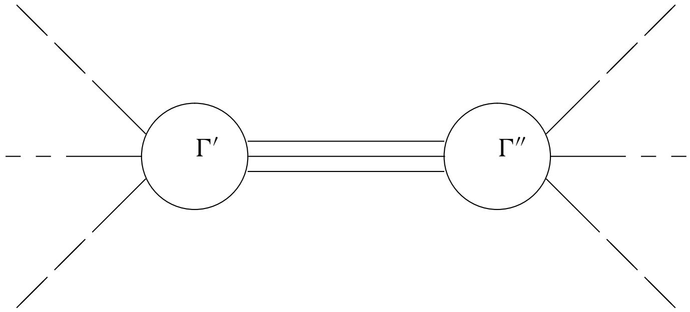

Figure 2. Decomposition of the graph.

We apply this to the on-shell S-matrices of quantum wires as follows. For the special case $V = \mathbb{I}$ we introduce the notation $*_p = *_{V=\mathbb{I}}$. Let Γ' and Γ'' be two graphs with n' and n'' external lines labelled by $\mathcal{E}'$ and $\mathcal{E}''$, i.e. $|\mathcal{E}'| = n'$, $|\mathcal{E}''| = n''$ and an arbitrary number of internal lines. Furthermore, at all vertices we have local boundary conditions giving Laplace operators $\Delta(\Gamma')$ on Γ' and $\Delta(\Gamma'')$ on Γ'' and on-shell S-matrices $S'(E)$ and $S''(E)$. Now let $\mathcal{E}_0'$ and $\mathcal{E}_0''$ be subsets of $\mathcal{E}'$ and $\mathcal{E}''$, respectively, having an equal number $(= p > 0)$ of elements. Also let φ_0: $\mathcal{E}_0' \to \mathcal{E}_0''$ be a one-to-one map. Finally, to each $k \in \mathcal{E}_0'$ we associate a number $a_k > 0$. With these data we can now form a graph Γ by connecting the external line $k \in \mathcal{E}_0'$ with the line $\varphi_0(k) \in \mathcal{E}_0''$ to form a line of length a_k. In other words, the intervals $[0_k, \infty_k)$ belonging to Γ' and the intervals $[0_{\varphi_0(k)}, \infty_{\varphi_0(k)})$ belonging to Γ'' are replaced by the finite interval $[0_k, a_k]$ with 0_k being associated to the same vertex in Γ' as previously and a_k being associated to the same vertex in Γ'' as $0_{\phi_0(k)}$ before in the sense of the discussion at the end of section 3. Recall that the graphs need not be planar. Thus Γ has $n = n' + n'' - 2p$ external lines indexed by elements in $(\mathcal{E}' \setminus \mathcal{E}_0') \cup (\mathcal{E}'' \setminus \mathcal{E}_0'')$ and p internal lines indexed by elements in $\mathcal{E}_0'$ in addition to those of Γ' and Γ''. There are no new vertices in addition to those of Γ' and Γ'' so the boundary conditions on Γ' and Γ'' define boundary conditions on Γ resulting in a Laplace operator $\Delta(\Gamma)$. The following formula relates the corresponding on-shell S-matrices $S'(E)$, $S''(E)$ and $S(E)$. First let the indices of $\mathcal{E}_0'$ in $\mathcal{E}'$ come after the indices in $\mathcal{E}' \setminus \mathcal{E}_0'$ (in an arbitrary but fixed order) (see equation (30)). Via the map φ_0 we may identify $\mathcal{E}_0''$ with $\mathcal{E}_0'$ so let these indices now come first in $\mathcal{E}''$, but again in the same order. Finally let the diagonal matrix $V(\underline{a})$ be given as

$$V(\underline{a}) = \begin{pmatrix} \exp \mathrm{i}\sqrt{E}\,\underline{a} & 0 \\ 0 & \mathbb{I} \end{pmatrix}$$

where $\exp\left(\mathrm{i}\sqrt{E}\,\underline{a}\right)$ again is the diagonal $p \times p$ matrix given by the p lengths a_k, $k \in \mathcal{E}_0'$. Then we claim that the relation

$$S(E) = S'(E) *_p V(\underline{a}) S''(E) V(\underline{a}) \tag{34}$$

holds. The operators K_1 and K_2 involved now depend on E and are singular for E in a denumerable set, namely when condition A is violated. This follows by arguments similar to those made after theorem 3.3. Thus these values have to be left out in (34). In the end one may then extend (34) to these singular values of E by arguments analogous to those after remark 3.1. If Γ is simply the disjoint union of Γ' and Γ'', i.e. if no connections are made (corresponding to $p = 0$ and $n = n' + n''$), then $S(E)$ is just the tensor product of $S'(E)$ and $S''(E)$. In this sense the generalized star product is a generalization of the tensor product. Also by a previous discussion (see equation (3)) $V^{-1}S(E)V = S_{2n}^{\mathrm{free}}(E) *_V S(E)$ for any on-shell S-matrix with n open ends and any unitary $n \times n$ matrix V. Similarly $S(E) *_V S_{2n}^{\mathrm{free}}(E) = VS(E)V^{-1}$. Using (34) the on-shell S-matrix associated to any graph and its boundary conditions is obtained from the on-shell S-matrices associated to its subgraphs each having one vertex only. In fact, pick one vertex and choose all the internal lines connecting to all other vertices. This leads to two graphs and the rule (34) may be applied. Iterating this procedure L times, where L is the number of vertices, gives the desired result.

We will not prove the claim (34) here but only give formal and intuitive arguments which also apply in the physical context of the usual star product or Aktosun formula for potential scattering on the line and which are based on a rearrangement of the Born series for the on-shell S-matrix. For partial results in potential scattering in higher dimensions when the separation of two (or more) potentials tends to infinity see [82, 83]. The complete proof of (34) will be given elsewhere [84].

For the sake of definiteness we consider the amplitudes $S(E)_{kl}$, $k, l \in \mathcal{E}' \setminus \mathcal{E}'_0$, which form U_{11} in this context, since we have $U' = S'(E)$, etc. The other amplitudes may be discussed analogously. The first non-trivial contribution is $S'(E)_{kl}$ corresponding to the first term in the first relation of (33). In next order the incoming plane wave in channel l may cross within Γ' into channel $k' \in \mathcal{E}'_0$ picking up a factor $S'(E)_{k'l}$. Then it propagates from Γ' to Γ'' picking up a phase factor $\exp\left(\mathrm{i}\sqrt{E}\, a_{k'}\right)$. To end up in channel k it then has to be transmitted within Γ'' into another channel k'' which is in $\mathcal{E}''_0$ and which we have identified with $\mathcal{E}'_0$. Therefore it picks up a factor $S''(E)_{k''k'}$ and then a factor $\exp\left(\mathrm{i}\sqrt{E}\, a_{k''}\right)$ when propagating back to Γ' and finally comes the factor $S'(E)_{k\,k''}$ from propagation within Γ' before ending up in channel k. By the superposition principle summation has to be carried over all such k' and k''. This contribution therefore corresponds to the term with $m = 0$ in the expression for K_2 in (32) when inserted into the second term in the first relation of (33). The higher-order contributions arise if the plane wave is reflected $m + 1 > 1$ times back and forth between Γ' and Γ''. Again by the superposition principle one finally has to sum over all m, giving the desired relation for $S(E)_{kl}$.

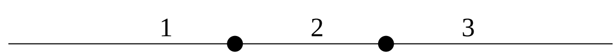

Figure 3. The graph from example 4.1.

Example 4.1. *Consider an arbitrary self-adjoint Laplacian $\Delta(A, B)$ with local boundary conditions on the graph depicted in figure 3, where the distance between the vertices is a. The composition rule (34) with*

$$V(a) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\sqrt{E}\,a} & 0 \\ 0 & 1 \end{pmatrix}$$

easily gives

$$S_{11} = S'_{11} + S'_{12}S''_{11}S'_{21}\left(1 - S'_{22}S''_{11}\mathrm{e}^{2\mathrm{i}a\sqrt{E}}\right)^{-1}$$
$$S_{22} = S''_{22} + S'_{22}S''_{21}S''_{12}\left(1 - S'_{22}S''_{11}\mathrm{e}^{2\mathrm{i}a\sqrt{E}}\right)^{-1}$$

$$S_{12} = S'_{12} S''_{12} \big(1 - S'_{22} S''_{11} \mathrm{e}^{2\mathrm{i}a\sqrt{E}}\big)^{-1}$$
$$S_{21} = S''_{21} S'_{21} \big(1 - S'_{22} S''_{11} \mathrm{e}^{2\mathrm{i}a\sqrt{E}}\big)^{-1}$$

where the S-matrices are written in the form analogous to (30)

$$S' = \begin{pmatrix} S'_{11} & S'_{12} \\ S'_{21} & S'_{22} \end{pmatrix} \qquad S'' = \begin{pmatrix} S''_{11} & S''_{12} \\ S''_{21} & S''_{22} \end{pmatrix}$$

leaving out the E dependence. These relations are equivalent to the Aktosun factorization formula applied to the Laplacian on a line with boundary conditions posed at $x = 0$ and $x = a$.

Example 4.2. *Consider the Laplacian on the graph from example 3.2 (figure 1). The relation (34) holds with*

$$V(a) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\sqrt{E}\,a} & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\sqrt{E}\,a} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and $S' = S''$ calculated in the example 2.4. It is easy to check that

$$K_1 = K_2 = \big(1 - \mathrm{e}^{2\mathrm{i}\sqrt{E}\,a}/9\big)^{-1} \big(1 - \mathrm{e}^{2\mathrm{i}\sqrt{E}\,a}\big)^{-1} \begin{pmatrix} 1 - \frac{5}{9}\mathrm{e}^{2\mathrm{i}\sqrt{E}\,a} & -\frac{4}{9}\mathrm{e}^{2\mathrm{i}\sqrt{E}\,a} \\ -\frac{4}{9}\mathrm{e}^{2\mathrm{i}\sqrt{E}\,a} & 1 - \frac{5}{9}\mathrm{e}^{2\mathrm{i}\sqrt{E}\,a} \end{pmatrix}.$$

Therefore from (33), equation (17) again follows. Note that $K_1 = K_2$ is singular at $\Sigma_{A,B}$, but these singularities disappear in the on-shell S-matrix.

As already remarked multiple application of (34) to an arbitrary graph allows one by complete induction on the number of vertices to calculate its S-matrix from the S-matrices corresponding to single-vertex graphs. If these single-vertex graphs contain no tadpoles, i.e. internal lines starting and ending at the vertex, then (6) and (34) give a complete explicit construction of the S-matrix in terms of the on-shell S-matrices discussed in section 2. In the case when a resulting single-vertex graph contains tadpoles we proceed as follows. Let the graph Γ have one vertex, n external lines and m tadpoles of lengths a_i. To calculate the S-matrix of Γ we insert an extra vertex on each of the internal lines (for definiteness, say, at $x = a_i/2$). At these new vertices we impose trivial boundary conditions given by the choice $a - 1 = d - 1 = b = c = 0$, $\exp(2\mathrm{i}\mu) = 1$ of example 3.2. With these new vertices we may now repeat our previous procedure. Thus in the end we arrive at graphs with one vertex only and no tadpoles. But the unitarity of the associated on-shell S-matrices was established in section 2, so this property in the general case follows from theorem 4.1. This is our third proof of unitarity. As an illustration we consider the following.

Example 4.3. *Consider the Laplacian on the graph Γ depicted in figure 4 with a circle of length a and the same boundary conditions at the 3-vertex as in example 2.4. Then*

$$S_{\mathrm{tadpole}}(E) = \mathrm{e}^{\mathrm{i}\sqrt{E}\,a} \frac{\mathrm{e}^{-\mathrm{i}\sqrt{E}\,a} - 3}{\mathrm{e}^{\mathrm{i}\sqrt{E}\,a} - 3}.$$

An easy calculation shows that

$$S_{\mathrm{tadpole}}(E) = S_2^{\mathrm{free}}(E) *_{p=2} V(a)\, S(E)\, V(a)$$

where $S(E)$ is the on-shell S-matrix of example 2.4 and

$$V(a) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\sqrt{E}\,a/2} & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\sqrt{E}\,a/2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

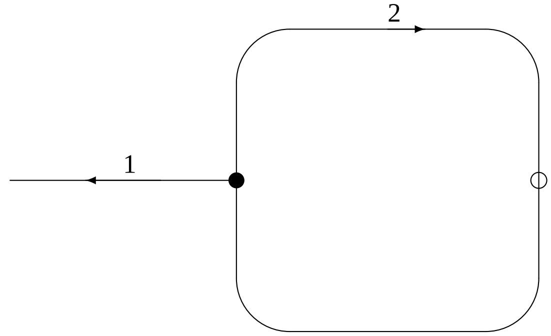

Figure 4. The graph Γ with $n = 1$ and $m = 1$: a closed loop (i.e. tadpole) of length a plus one external line. The open circle denotes the vertex added.

In this case K_1 *equals*

$$K_1 = \left(1 - \tfrac{1}{3}\mathrm{e}^{\mathrm{i}\sqrt{E}\,a}\right)^{-1}\left(1 - \mathrm{e}^{\mathrm{i}\sqrt{E}\,a}\right)^{-1} \begin{pmatrix} 1 - \frac{2}{3}\mathrm{e}^{\mathrm{i}\sqrt{E}\,a} & -\frac{1}{3}\mathrm{e}^{\mathrm{i}\sqrt{E}\,a} \\ -\frac{1}{3}\mathrm{e}^{\mathrm{i}\sqrt{E}\,a} & 1 - \frac{2}{3}\mathrm{e}^{\mathrm{i}\sqrt{E}\,a} \end{pmatrix}$$

which is singular for $E = (2\pi n)^2 / a^2$.

The feature exhibited in this example (see also example 3.2) may be generalized as follows. Let Γ be a graph with local boundary conditions at each vertex which are scale invariant in the sense of corollary 2.3. Then by (34) the E dependence of the on-shell S-matrix $S_\Gamma(E)$ for this graph only enters through the lengths $\underline{a}$ in the form $\exp\left(\mathrm{i}\sqrt{E}\,a_j\right)$. In particular, $\lim_{\underline{a}\to 0} S_\Gamma(E)$ is independent of the energy. This observation might be helpful in deciding which boundary conditions might be physically realized in a given experimental context.

5. Conclusions and outlook

In this paper we have established unitarity of the S-matrix for arbitrary finite quantum wires with a Hamiltonian given by an arbitrary self-adjoint extension of the Laplace operator. The explicit determination of the on-shell S-matrix has been reduced to a finite matrix problem, which thus is accessible to computer calculations. A quantum wire with two open ends but arbitrary interior and arbitrary boundary conditions may be viewed as a theory with point interaction and an internal structure (see, e.g., [48, 85]). Ultimately relativistic, local quantum field theories provide the appropriate set-up for considering point-like interactions and internal structures. Thus, for example, the Φ^4-theory is the quantum field-theoretic version of the δ-potential. The composition rule established in section 4 gives a generalization to arbitrary graphs of the Aktosun factorization formula [50] for potential scattering on the line.

Our approach offers several generalizations. First it is possible to introduce a potential V on the entire wire thus replacing $-\Delta(A, B)$ by $-\Delta(A, B) + V$ (see, e.g., [86, 87]). Although solutions for the on-shell S-matrix in closed form like above may not be obtainable in general, most structural properties should still hold, provided the potential is sufficiently strongly decaying at the infinities. Also one may construct lattice models in the following way. To each lattice site $j \in \mathbb{Z}^k$ in $\mathbb{R}^k$ one may associate an S-matrix with $2k$ open ends and connect neighbouring lattice sites accordingly (see, e.g., [33, 36, 88]). This would lead to the possibility of considering infinite quantum wires—obtained as 'thermodynamic' limits of finite quantum wires—and study their conductance properties in the spirit of, for example, the analysis in [33]. Thus if one takes the same S-matrices at each site the resulting theory will be translation invariant. The generalized star product also offers the possibility of introducing a transfer matrix theory (see again [33]). For the case $k = 1$ this will generalize the Kronig–Penney model [34, 89]. Finally, the S-matrices at the lattice sites could vary stochastically allowing the study of percolation effects.

The present discussion of Laplace operators on graphs could also be used to study Brownian motion and the associated diffusion process. More precisely we expect the heat kernel $\exp(t\Delta(A, B))(x, y)$ to be non-negative if the boundary conditions (A, B) are real. It would be interesting to obtain a representation in the spirit of the Selberg and Gutzwiller trace formula. If the boundary conditions are not real, reflecting the presence of a magnetic field say, we expect a corresponding Ito formula to be valid and Aharonov–Bohm-like effects to show up.

Acknowledgments

The authors are indebted to Y Avron, Th Bröcker, J M Combes, M Karowski, P Kurasov and L Sadun for valuable comments. We thank G Dell'Antonio for pointing out [45] and to S P Novikov for sending us the manuscript of [45] prior to its publication. Suggestions of anonymous referees are also acknowledged.

Appendix A

In this appendix we will describe $\Delta(A, B)$ defined on a graph with a single vertex from the viewpoint of von Neumann's extension theory (see, e.g., [65]). According to von Neumann's theorem any self-adjoint extension $\Delta(A, B)$ of Δ^0 can be uniquely parametrized by a linear isometric isomorphism $\mathcal{W}_{A,B}$: $\mathrm{Ker}\left(-\Delta^{0\dagger} - \mathrm{i}\right) \to \mathrm{Ker}\left(-\Delta^{0\dagger} + \mathrm{i}\right)$ according to the formula

$$\mathcal{D}(\Delta(A, B)) = \left\{\psi + \psi_+ + \mathcal{W}_{A,B}\psi_+ \,\middle|\, \psi \in \mathcal{D}\big(\Delta^0\big), \psi_+ \in \mathrm{Ker}\left(-\Delta^{0\dagger} - \mathrm{i}\right)\right\}$$
$$-\Delta(A, B)(\psi + \psi_+ + \mathcal{W}_{A,B}\psi_+) = -\Delta^0\psi + \mathrm{i}\psi_+ - \mathrm{i}\mathcal{W}_{A,B}\psi_+.$$

To express $\mathcal{W}_{A,B}$ in terms of the matrices A and B we compare $\Delta(A, B)$ with another self-adjoint extension $\Delta(A', B')$ of Δ^0. For definiteness we take $A' = \mathbb{I}$ and $B' = 0$, which corresponds to the Dirichlet boundary conditions (but another choice would also be possible).

Let $u_j \in \mathrm{Ker}\left(-\Delta^{0\dagger} - \mathrm{i}\right)$ and $v_j \in \mathrm{Ker}\left(-\Delta^{0\dagger} + \mathrm{i}\right)$, $j = 1, \ldots, n$ be given as

$$(u_j(x))_k = \delta_{jk} 2^{1/4} \mathrm{e}^{(1/\sqrt{2})(-1+\mathrm{i})x} \qquad (v_j(x))_k = \delta_{jk} 2^{1/4} \mathrm{e}^{(1/\sqrt{2})(-1-\mathrm{i})x} \qquad k = 1, \ldots, n. \tag{A1}$$

One can easily verify that $\{u\}_{j=1}^n$ and $\{v\}_{j=1}^n$ are orthonormal bases for $\mathrm{Ker}\left(-\Delta^{0\dagger} - \mathrm{i}\right)$ and $\mathrm{Ker}\left(-\Delta^{0\dagger} + \mathrm{i}\right)$, respectively. Denote by $W_{A,B}$ the unitary matrix representation of $\mathcal{W}_{A,B}$ with respect to the bases $\{u\}_{j=1}^n$ and $\{v\}_{j=1}^n$, i.e.

$$\mathcal{W}_{A,B} u_j = \sum_{k=1}^n (W_{A,B})_{kj} v_k.$$

It is easy to see that $W_{A'=\mathbb{I}, B'=0} = -\mathbb{I}$. Our strategy will be to apply Krein's formula (see, e.g., [64]) to obtain $W_{A,B}$ in terms of the matrices A and B. To construct $\Delta(A, B)$ in the sense of von Neumann we proceed in two steps. In the first step let $\tilde{\Delta}$ be the maximal common part of $\Delta(A, B)$ and $\Delta(A' = \mathbb{I}, B' = 0)$, i.e. $\tilde{\Delta}$ is the largest closed extension of Δ^0 with

$$\mathcal{D}(\tilde{\Delta}) = \mathcal{D}(\Delta(A, B)) \cap \mathcal{D}(\Delta(A' = \mathbb{I}, B' = 0)) = \{\psi \mid \psi(0) = 0, B\psi'(0) = 0\}.$$

Obviously, $\tilde{\Delta}$ is a symmetric operator with defect indices (r, r), $r = \operatorname{rank} B$ $(0 \leqslant r \leqslant n)$. Also one has $\operatorname{Ker}\left(-\tilde{\Delta}^\dagger \mp \mathrm{i}\right) \subseteq \operatorname{Ker}\left(-\Delta^{0\dagger} \mp \mathrm{i}\right)$ such that we may decompose

$$\operatorname{Ker}\left(-\Delta^{0\dagger} \mp \mathrm{i}\right) = \operatorname{Ker}\left(-\tilde{\Delta}^\dagger \mp \mathrm{i}\right) \oplus \mathcal{M}_\pm. \tag{A2}$$

Performing, if necessary, a renumeration of the basis elements we may assume that $\{u\}_{j=1}^r$ and $\{v\}_{j=1}^r$ are bases for $\operatorname{Ker}\left(-\tilde{\Delta}^\dagger - \mathrm{i}\right)$ and $\operatorname{Ker}\left(-\tilde{\Delta}^\dagger + \mathrm{i}\right)$, respectively.

Von Neumann's theorem describes $\tilde{\Delta}$ as a symmetric extension of Δ^0. All such extensions are parametrized by linear partial isometries $\mathcal{W}'$: $\operatorname{Ker}\left(-\Delta^{0\dagger} - \mathrm{i}\right) \to \operatorname{Ker}\left(-\Delta^{0\dagger} + \mathrm{i}\right)$. For the case at hand it is easy to see that the isometry corresponding to $\tilde{\Delta}$ defines an isometric isomorphism $\tilde{\mathcal{W}}$: $\mathcal{M}_+ \to \mathcal{M}_-$ and therefore

$$\mathcal{D}(\tilde{\Delta}) = \left\{\psi + \psi_+ + \tilde{\mathcal{W}}\psi_+ \,\middle|\, \psi \in \mathcal{D}\left(\Delta^0\right), \psi_+ \in \mathcal{M}_+\right\}$$
$$-\tilde{\Delta}(\psi + \psi_+ + \tilde{\mathcal{W}}\psi_+) = -\Delta^0\psi + \mathrm{i}\psi_+ - \mathrm{i}\tilde{\mathcal{W}}\psi_+.$$

Denoting by $\tilde{W}$ the matrix representation of $\tilde{\mathcal{W}}$ in the bases $\{u\}_{j=r+1}^n$ and $\{v\}_{j=r+1}^n$ we find that $\tilde{W} = -\mathbb{I}$.

In the second step let $\tilde{\mathcal{W}}_{A,B}$: $\operatorname{Ker}\left(-\tilde{\Delta}^\dagger - \mathrm{i}\right) \to \operatorname{Ker}\left(-\tilde{\Delta}^\dagger + \mathrm{i}\right)$ be the linear isometric isomorphism parametrizing $\Delta(A, B)$ as a self-adjoint extension of $\tilde{\Delta}$. Denote by $\tilde{W}_{A,B}$ its unitary matrix representation with respect to the bases $\{u\}_{j=1}^r$ and $\{v\}_{j=1}^r$. Again it is easy to see that $\tilde{W}_{A'=\mathbb{I},B'=0} = -\mathbb{I}$ ($r \times r$ matrix). Also from the discussion above it follows that

$$W_{A,B} = \tilde{W}_{A,B} \oplus (-\mathbb{I}) \tag{A3}$$

with respect to the decomposition (A2).

Krein's formula (see, e.g., [64]) now states that the difference of the resolvents of $-\Delta(A, B)$ and $-\Delta(A' = \mathbb{I}, B' = 0)$ at the point $z = \mathrm{i}$ is given by

$$R_{A,B}(\mathrm{i}) - R_{A'=\mathbb{I},B'=0}(\mathrm{i}) = \sum_{j,k=1}^{r} \tilde{P}_{jk}(v_k, \cdot)v_j \tag{A4}$$

with some $r \times r$ matrix $\tilde{P}$ of maximal rank. By corollary B.3 of [90] it follows that

$$\tilde{P} = \tfrac{1}{2}\mathrm{i}\left(\mathbb{I} + \tilde{W}_{A,B}^{-1}\right). \tag{A5}$$

Obviously, relation (A4) can be rewritten in the form

$$R_{A,B}(\mathrm{i}) - R_{A'=\mathbb{I},B'=0}(\mathrm{i}) = \sum_{j,k=1}^{n} P_{jk}(v_k, \cdot)v_j \tag{A6}$$

where P is an $n \times n$ matrix of rank r such that $P = \tilde{P} \oplus 0$ with respect to the decomposition (A2). Thus from (A5) and (A3) it follows that

$$P = \tfrac{1}{2}\mathrm{i}\left(\mathbb{I} + W_{A,B}^{-1}\right). \tag{A7}$$

The resolvent $R_{A'=\mathbb{I},B'=0}(\mathrm{i})$ of $\Delta(A' = \mathbb{I}, B' = 0)$ can be given explicitly. Its integral kernel (Green's function) for $x < y$ has the form

$$R_{A'=\mathbb{I},B'=0}(x, y; \mathrm{i}) = \mathbb{I}\frac{\sin\sqrt{\mathrm{i}}\,x}{\sqrt{\mathrm{i}}}\mathrm{e}^{(1/\sqrt{2})(-1+\mathrm{i})y}$$

such that

$$R_{A'=\mathbb{I},B'=0}(0,y;\mathrm{i}) = 0 \qquad \frac{\partial R_{A'=\mathbb{I},B'=0}}{\partial x}(0,y;\mathrm{i}) = \mathbb{I}\mathrm{e}^{(1/\sqrt{2})(-1+\mathrm{i})y}.$$

Since the boundary conditions take the form

$$AR_{A,B}(0,y;\mathrm{i}) + B\frac{\partial R_{A,B}}{\partial x}(0,y;\mathrm{i}) = 0$$

for all $y > 0$ in terms of the resolvents, from (A6) we obtain

$$\left(A + \frac{1}{\sqrt{2}}(-1+\mathrm{i})B\right)P = -\frac{1}{\sqrt{2}}B.$$

Comparing this with (A7) we obtain

$$W_{A,B}^{-1} = -\left(A + \frac{1}{\sqrt{2}}(-1+\mathrm{i})B\right)^{-1}\left(A - \frac{1}{\sqrt{2}}(1+\mathrm{i})B\right).$$

Note that $(\hat{A},\hat{B})$ given as

$$\hat{A} = A - \frac{1}{\sqrt{2}}B \qquad \hat{B} = \frac{1}{\sqrt{2}}B$$

also defines a maximal isotropic subspace and $W_{A,B}^{-1} = S_{\hat{A},\hat{B}}(E=1)$ (the S-matrix for the single-vertex theory) holds, such that in particular $W_{A,B}$ is unitary and satisfies $W_{A,B} = W_{CA,CB}$ for any invertible C, as it should be. As an example, for $A=0$ and $B=\mathbb{I}$ (Neumann boundary conditions) this gives $W_{A=0,B=\mathbb{I}} = \mathrm{i}\mathbb{I}$, again as it should be.

Appendix B

Here we give an alternative 'analytic' proof of theorem 3.3, i.e. of the unitarity of the on-shell S-matrix. We resort to an argument which is a modification of well known arguments used to prove orthogonality relations for improper eigenfunctions of Schrödinger Hamiltonians (see also the remark at the end of this appendix) and which is instructive in its own right. For this purpose we introduce Hilbert spaces $\mathcal{H}_R$ indexed by $R > 0$ and given as

$$\mathcal{H}_R = \bigoplus_{e\in\mathcal{E}}\mathcal{H}_{e,R}\bigoplus_{i\in\mathcal{I}}\mathcal{H}_i$$

where the spaces $\mathcal{H}_i$ are as before and where $\mathcal{H}_{e,R} = L^2([0,R])$ for all $e \in \mathcal{E}$. Then $\psi^k(\cdot,E) \in \mathcal{H}_R$ for all $e \in \mathcal{E}$ and all $0 < R < \infty$. Let $\langle\,,\rangle_R$ denote the canonical scalar product on $\mathcal{H}_R$. Also we have $\Delta\psi^k(\cdot,E) = -E\psi^k(\cdot,E)$ such that for all $E, E' \in \mathbb{R}\setminus\Sigma_{A,B}$ and all $k,l \in \mathcal{E}$

$$\langle\Delta\psi^k(\cdot,E),\psi^l(\cdot,E')\rangle_R - \langle\psi^k(\cdot,E),\Delta\psi^l(\cdot,E')\rangle_R = (E'-E)\langle\psi^k(\cdot,E),\psi^l(\cdot,E')\rangle_R. \quad \text{(B1)}$$

Now all terms in this equation are smooth in $E, E' \in \mathbb{R}\setminus\Sigma_{A,B}$ and R. We may therefore take the limit $E' \to E$. This gives for the right-hand side of (B1)

$$\lim_{E'\to E}(E'-E)\langle\psi^k(\cdot,E),\psi^l(\cdot,E')\rangle_R = 0.$$

On the other hand, we may evaluate the left-hand side of (B1) by performing a partial integration. Since both $\psi^k(\cdot,E)$ and $\psi^l(\cdot,E')$ satisfy the boundary conditions (A,B), the only contributions arise at the n 'new' boundaries $x = R$, i.e.

$$
\begin{aligned}
\big\langle \Delta\psi^k(\cdot, E), \psi^l(\cdot, E')\big\rangle_R - \big\langle \psi^k(\cdot, E), \Delta\psi^l(\cdot, E')\big\rangle_R
&= \sum_{e\in\mathcal{E}} \big(\bar{\psi}_e^{k\,\prime}(R, E)\,\psi_e^l(R, E') - \bar{\psi}_e^k(R, E)\,\psi_e^{l\,\prime}(R, E')\big) \\
&= -\,\mathrm{i}\big(\sqrt{E'} + \sqrt{E}\big)\mathrm{e}^{\mathrm{i}(\sqrt{E'}-\sqrt{E})R} \sum_{e\in\mathcal{E}} \overline{S_{ek}(E)} S_{el}(E') \\
&\quad + \mathrm{i}\big(\sqrt{E'} + \sqrt{E}\big)\mathrm{e}^{-\mathrm{i}(\sqrt{E'}-\sqrt{E})R}\delta_{kl} + \mathrm{i}\big(\sqrt{E'} - \sqrt{E}\big)\mathrm{e}^{\mathrm{i}(\sqrt{E'}+\sqrt{E})R}\overline{S_{lk}(E)} \\
&\quad - \mathrm{i}\big(\sqrt{E'} - \sqrt{E}\big)\mathrm{e}^{\mathrm{i}(\sqrt{E'}+\sqrt{E})R} S_{kl}(E').
\end{aligned}
$$

The limit of the right-hand side as $E' \to E$ equals

$$
-2\mathrm{i}\sqrt{E}\left(\sum_{e\in\mathcal{E}} \overline{S_{ek}(E)} S_{el}(E) - \delta_{kl}\right)
$$

which by the preceding arguments is zero, concluding this second proof of unitarity.

We could have chosen $E' = E$ from the very beginning. However, the present discussion may be applied to show general orthogonality properties for the improper eigenfunctions $\psi^k(\cdot, E)$. This is achieved by first dividing (B1) by $E' - E$ and then taking the limit $R \to \infty$ in the sense of distributions in E' and E.

Appendix C

This appendix is devoted to a proof of theorem 4.1. We start with the following observation. For U' written in block form as in (30) we define a map $U' \to U'^{\tau}$ with $\tau = \tau(n' - p, p)$ given as

$$
U'^{\tau} = \begin{pmatrix} U'_{22} & U'_{21} \\ U'_{12} & U'_{11} \end{pmatrix}
$$

which amounts to interchanging the first $n' - p$ indices with the last p indices while keeping the order of the indices otherwise fixed. U''^{τ} and U^{τ} are defined analogously with $\tau = \tau(p, n''-p)$ and $\tau = \tau(n' - p, n'' - p)$, respectively. From the definition of $*_V$ it follows immediately that the following 'transposition law' holds:

$$
U^{\tau} = U''^{\tau} *_{V^{-1}} U'^{\tau}
$$

whenever $U = U' *_V U''$. To prove theorem 4.1 we have to show that the following four relations hold:

$$
\begin{aligned}
&U_{11}^{\dagger} U_{11} + U_{21}^{\dagger} U_{21} = \mathbb{I} \\
&U_{11}^{\dagger} U_{12} + U_{21}^{\dagger} U_{22} = 0 \\
&U_{12}^{\dagger} U_{12} + U_{22}^{\dagger} U_{22} = \mathbb{I} \\
&U_{12}^{\dagger} U_{11} + U_{22}^{\dagger} U_{21} = 0.
\end{aligned}
$$

By our previous observation it suffices to prove only the first two relations. To prove the first one, we insert the definition of U and obtain

$$
\begin{aligned}
U_{11}^{\dagger} U_{11} + U_{21}^{\dagger} U_{21} &= U_{11}'^{\dagger} U'_{11} + U_{11}'^{\dagger} U'_{12} K_2 U''_{11} V U'_{21} + U_{21}'^{\dagger} V^{-1} U_{11}''^{\dagger} K_2 U_{12}'^{\dagger} U'_{11} \\
&\quad + U_{21}'^{\dagger} V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{12}'^{\dagger} U'_{12} K_2 U''_{11} V U'_{21} + U_{21}'^{\dagger} K_1^{\dagger} U_{21}''^{\dagger} U''_{21} K_1 U'_{21} \\
&= \sum_{i=1}^{5} a_i .
\end{aligned}
$$

We now use the unitarity relations for U' and U''. This gives

$$\begin{aligned}\sum_{i=2}^{5} a_i &= U_{21}'^{\dagger}\big\{ - U_{22}' K_2 U_{11}'' V - V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}' \\ &\quad + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{12}'^{\dagger} U_{12}' K_2 U_{11}'' V + K_1^{\dagger} U_{21}''^{\dagger} U_{21}'' K_1 \big\} U_{21}' \\ &= U_{21}'^{\dagger}\big\{ -U_{22}' K_2 U_{11}'' V - V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}' + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} K_2 U_{11}'' V \\ &\quad - V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} U_{22}' K_2 U_{11}'' V + K_1^{\dagger} K_1 - K_1^{\dagger} U_{11}''^{\dagger} U_{11}'' K_1 \big\} U_{21}'.\end{aligned}$$

To establish $\sum_{i=1}^{5} a_i = \mathbb{I}$ it therefore suffices to show that the expression in braces equals $\mathbb{I}$. Using one of the relations in (31) and its adjoint we have

$$K_1^{\dagger} K_1 = \mathbb{I} + U_{22}' K_2 U_{11}'' V + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} U_{22}' K_2 U_{11}'' V$$

and

$$K_1^{\dagger} U_{11}''^{\dagger} U_{11}'' K_1 = V^{-1}\big(\mathbb{I} + U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} V^{-1}\big) U_{11}''^{\dagger} U_{11}'' (\mathbb{I} + V U_{22}' K_2 U_{11}'') V.$$

Hence it suffices to show that

$$-\big(\mathbb{I} + U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} V^{-1}\big) U_{11}''^{\dagger} U_{11}'' (\mathbb{I} + V U_{22}' K_2 U_{11}'') + U_{11}''^{\dagger} K_2^{\dagger} K_2 U_{11}'' = 0.$$

To show this it suffices in turn to prove that

$$K_2^{\dagger} K_2 = \mathbb{I} + K_2^{\dagger} U_{22}'^{\dagger} V^{-1} U_{11}''^{\dagger} + U_{11}'' V U_{22}' K_2 + K_2^{\dagger} U_{22}'^{\dagger} V^{-1} U_{11}''^{\dagger} U_{11}'' V U_{22}' K_2.$$

But this relation follows by inserting the relation

$$K_2 = V^{-1} + V^{-1} U_{11}'' V U_{22}' K_2$$

and its adjoint into the left-hand side. To sum up we have proved the first of the unitarity relations for U. To prove the second relation we again insert the definition of U, use the unitarity relations for U' and U'' twice and obtain

$$\begin{aligned}U_{11}^{\dagger} U_{12} + U_{21}^{\dagger} U_{22} &= U_{21}'^{\dagger}\big\{ -U_{22}' K_2 + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} K_2 - V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} U_{22}' K_2 \\ &\quad -K_1^{\dagger} U_{11}''^{\dagger} + K_1^{\dagger} K_1 U_{22}' V^{-1} - K_1^{\dagger} U_{11}''^{\dagger} U_{11}'' K_1 U_{22}' V^{-1} \big\} U_{12}''.\end{aligned}$$

Hence it suffices to show that the expression in braces ($= a_6$) vanishes. But

$$\begin{aligned}-K_1^{\dagger} U_{11}''^{\dagger} - K_1^{\dagger} U_{11}''^{\dagger} U_{11}'' K_1 U_{22}' V^{-1} &= -K_1^{\dagger} U_{11}''^{\dagger} V K_2 \\ &= -V^{-1}\big(\mathbb{I} + U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} V^{-1}\big) U_{11}''^{\dagger} V K_2 \\ &= -V^{-1} U_{11}''^{\dagger} V K_2 - V^{-1} U_{11}''^{\dagger}\big(K_2^{\dagger} - V\big) K_2 \\ &= -V^{-1} U_{11}''^{\dagger} K_2^{\dagger} K_2\end{aligned}$$

implies

$$a_6 = -U_{22}' K_2 - V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} U_{22}' K_2 + K_1^{\dagger} K_1 U_{22}' V^{-1}.$$

The chain of equalities

$$\begin{aligned}K_1^{\dagger} K_1 U_{22}' V^{-1} &= \big(\mathbb{I} + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger}\big)(\mathbb{I} + U_{22}' K_2 U_{11}'' V) U_{22}' V^{-1} \\ &= U_{22}' V^{-1} + U_{22}' K_2 U_{11}'' V U_{22}' V^{-1} \\ &\quad + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} U_{22}' K_2 U_{11}'' V U_{22}' V^{-1} \\ &\quad + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} U_{22}' V^{-1} \\ &= U_{22}' V^{-1} + U_{22}'\big(K_2 - V^{-1}\big) \\ &\quad + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} U_{22}'\big(K_2 - V^{-1}\big) \\ &\quad + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} U_{22}' V^{-1} \\ &= U_{22}' K_2 + V^{-1} U_{11}''^{\dagger} K_2^{\dagger} U_{22}'^{\dagger} U_{22}' K_2\end{aligned}$$

finally leads to $a_6 = 0$ as desired concluding the proof of theorem 4.1.

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