Kirchhoff’s Rule for Quantum Wires. II: The Inverse Problem with Possible Applications to Quantum Computers

V. Kostrykin*
Lehrstuhl für Lasertechnik
Rheinisch - Westfälische Technische Hochschule Aachen
Steinbachstraße 15, D-52074 Aachen, Germany

and

R. Schrader†
Institut für Theoretische Physik
Freie Universität Berlin, Arnimallee 14
D-14195 Berlin, Germany

August 22, 2018

Abstract

In this article we continue our investigations of one particle quantum scattering theory for Schrödinger operators on a set of connected (idealized one-dimensional) wires forming a graph with an arbitrary number of open ends. The Hamiltonian is given as minus the Laplace operator with suitable linear boundary conditions at the vertices (the local Kirchhoff law). In “Kirchhoff’s rule for quantum wires” [J. Phys. A: Math. Gen. 32, 595 – 630 (1999)] we provided an explicit algebraic expression for the resulting (on-shell) S-matrix in terms of the boundary conditions and the lengths of the internal lines and we also proved its unitarity. Here we address the inverse problem in the simplest context with one vertex only but with an arbitrary number of open ends. We provide an explicit formula for the boundary conditions in terms of the S-matrix at a fixed, prescribed energy. We show that any unitary $n \times n$ matrix may be realized as the S-matrix at a given energy by choosing appropriate (unique) boundary conditions. This might possibly be used for the design of elementary gates in quantum computing. As an illustration we calculate the boundary conditions associated to the unitary operators of some elementary gates for quantum computers and raise the issue whether in general the unitary operators associated to quantum gates should rather be viewed as scattering operators instead of time evolution operators for a given time associated to a quantum mechanical Hamiltonian. We also suggest an approach by which the S-matrix in our context may be obtained from “scattering experiments”, another aspect of the inverse problem. Finally we extend our previous discussion, how our approach is related to von Neumann’s theory of selfadjoint extensions.

*e-mail: kostrykin@t-online.de, kostrykin@ilt.fhg.de
†e-mail: schrader@physik.fu-berlin.de, Supported in part by DFG SFB 288 “Differentialgeometrie und Quantenphysik”
1 Introduction

In this article we continue our investigation of quantum mechanical scattering theory on a set of connected wires idealized to have zero diameter and with an arbitrary number of open ends [20]. The dynamics is given by the one-dimensional Laplacian with arbitrary boundary conditions at the vertices, which makes it a self-adjoint operator. We view this as an idealized version of a thin conducting wire with electrons in the conductance band, i.e. we have set $\hbar = 2m^* = 1$ with $m^*$ being the effective mass and we have neglected the spin. Also if the wires are sufficiently thin, transversal modes may be neglected and only longitudinal modes, i.e. motion in the direction of the graph, should play a role. Below we will comment briefly on the associated mathematical problem. A concrete example we have in mind are nanotubes, which are considered to be interesting candidates for the design of microscopic electronic devices (see e.g. [52, 35, 36] for recent, possibly relevant experiments). In fact, the possibility of connecting nanotubes of different diameter and chirality has created considerable interest recently (see e.g. [17, 42, 7, 8, 30, 47]). Alternatively such graphs could be realized in terms of grooves etched on suitable surfaces or in terms of strings of atoms forming a (planar) graph deposited again on a suitable surface [15, 54, 50], see also [31, 32].

For our graph model we provided an explicit algebraic expression for the S-matrix at a given energy in terms of the boundary conditions and the lengths of the internal wires. We proved unitarity so this provides an example for the Landauer-Büttiker formalism [24, 6], see also e.g. [10] for an extensive discussion. We note that the transmission rate for the connection of two nanotubes with different diameter has been calculated in [51]. The influence of disorder on the conductance characteristics of nanotubes was studied in [3].

In this article we will also address the inverse problem, namely the determination of the boundary conditions given the S-matrix at a fixed energy. We will only cover the case of one vertex only, since the general case with internal wires and several vertices is much more difficult. Note that another kind of inverse problems was considered previously in [16].

We will use this discussion of the one vertex case to indicate possible applications in the design of quantum computers (see e.g. [34, 46, 48] and the literature quoted there). Recall that in classical network theory one uses the theory of unitary matrices to describe (deterministic) input-output relations and one even speaks of scattering matrices (see e.g. [38, 39]). For quantum computers we advocate the idea that one should use the theory of quantum scattering and the associated notion of a unitary S-matrix to formulate (probabilistic) quantum input-output relations. This differs from standard discussions on this subject in which the unitary matrix is considered to be the unitary time evolution operator for a given, fixed time and with a Hamiltonian as infinitesimal generator, which describes the dynamics. Also we consider the rule by which the connection of gates is supposed to correspond to matrix multiplication of the associated unitary matrices not to be quite convincing. In fact, connecting two gates means that one has a coupled system for which the relevance of the Hamiltonians of the two subsystems remains unclear. So from the point of view of information transmission, we consider it at least natural to ask for the relevance of scattering matrices in the context of quantum computation. In fact, it is our understanding that most of the present experimental designs for quantum gates describe scattering experiments. In the present context of quantum wires the incoming signals would be plane waves at a fixed energy in each of the wires and which will be scattered at the vertex into outgoing plane waves again in each of the wires and of the same energy.
In this context it is worthwhile to mention the connection between the time dependent quantum mechanical description and scattering theory. The latter describes the long time behaviour of quantum evolution. Thus the use of scattering matrices instead of unitary time evolution operators can only be adequate provided the “tact frequency” of the quantum computer is not too high and this depends on its physical realization. However, a discussion of this issue as well as the question of how to incorporate this proposed realization of quantum gates into the general context of quantum computation with its notion of entanglement lies outside the scope of the present article.

The discussion below will be based on our result that in the situation of a single vertex quantum wire any unitary matrix may be uniquely realized as the S-matrix at a given energy by choosing appropriate boundary conditions. In spirit this is similar to the discussion in e.g. [37] by which any unitary matrix in principle can be realized with suitable beam splitters and phase shifters. As an illustration we will calculate these boundary conditions for some simple gates. We leave out the question of how to implement these boundary conditions at the vertices of concrete physical wires. However, in the present context we will discuss the general experimental difficulty associated with designing quantum gates with a prescribed unitary matrix. It has to do with the well known fact that usually only the absolute values of matrix elements of the S-matrix are observable (conventionally given in terms of cross sections). We will suggest an “experimental” prescription, how one may also determine the phases of the S-matrix elements by suitable experiments. This method may also be applied to potential scattering theory for Schrödinger operators [22].

We conclude this article by elaborating in more detail than in [20] on the relation of our discussion of selfadjoint extensions with the corresponding theory of von Neumann.

2 The inverse problem for a quantum wire with a single vertex

In this section we first discuss the inverse problem for \( n \) (infinite) wires ending at a single vertex, i.e. we will determine the boundary conditions given the S-matrix. We briefly recall the set-up for this situation. Let the Hilbert space be given as

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

Intuitively the \( n \) origins 0 are to be identified. This will be achieved in a moment by describing the quantum mechanical dynamics. Elements \( \psi \in \mathcal{H} \) will be written as \( \psi = (\psi_1, \psi_2, ..., \psi_n) \) and derivatives as \( \psi' = (\psi'_1, \psi'_2, ..., \psi'_n) \) We will call \( \psi_j \) the component of \( \psi \) 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. Now the dynamics will be given by the Laplace operator away from the origin supplemented by suitable boundary conditions at the origin. For this we proceed as follows. Consider the symmetric operator \( \Delta^0 \) on \( \mathcal{H} \), such that

\[
\Delta^0 \psi = \left( -\frac{d^2\psi_1}{dx^2}, \ldots, -\frac{d^2\psi_n}{dx^2} \right)
\]

with domain of definition \( \mathcal{D}(\Delta^0) \) being the set of all \( \psi \) with \( \psi, \psi', \psi'' \in \mathcal{H} \) and such that \( \psi_i(0) = \psi'_i(0) = 0 \) for all \( 1 \leq i \leq n \). All selfadjoint extensions are now given as
follows. Let $D \subset H$ be the set of all $\psi$ such that $\psi, \psi', \psi''$ are all in $H$. On $D$ 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 $\Delta = -d^2/dx^2$ considered as a differential operator. Obviously $\Omega$ vanishes identically on $D(\Delta^0)$. Any self-adjoint extension of $\Delta^0$ is now given in terms of a maximal isotropic subspace of $D$, i.e. a maximal (linear) subspace on which $\Omega$ vanishes identically. To find these maximal isotropic subspaces, let $[\cdot] : D \to \mathbb{C}^{2n}$ be the surjective linear map which associates to $\psi$ and $\psi'$ their boundary values at the origin:

$$[\psi] = (\psi(0), \ldots, \psi_n(0), \psi'_1(0), \ldots, \psi'_n(0))^T = \begin{pmatrix} \psi(0) \\ \psi'(0) \end{pmatrix}.$$ 

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 $[\cdot]$ is obviously equal to $D(\Delta^0)$. 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 $\mathbb{C}^{2n}$:

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

Here and in what follows $I$ is the unit matrix for the given context.

To find all maximal isotropic subspaces in $D$ with respect to $\Omega$ it therefore suffices to find all maximal isotropic subspaces in $\mathbb{C}^{2n}$ with respect to $\omega$ and to take their preimage under the map $[\cdot]$. Let the linear subspace $M = M(A, B)$ 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 $n$ and if $AB^\dagger$ is selfadjoint then $M(A, B)$ is maximal isotropic and in this way one obtains all maximal isotropic subspaces in $\mathbb{C}^{2n}$. Two maximal isotropic subspaces $M(A', B')$ and $M(A, B)$ are equal iff there is an invertible $n \times n$ matrix $C$ such that $(A', B') = (CA, CB)$. In this sense we will say that the $n \times 2n$ matrix $(A, B)$ is uniquely fixed by the boundary condition. Let $D(A, B)$ denote the inverse image of $M(A, B)$ under the map $[\cdot]$. Then $D(\Delta^0) \subset D(A, B) \subset D$ and $\Delta \upharpoonright D(A, B)$ is the core for a selfadjoint extension of $\Delta^0$ and which is denoted by $\Delta(A, B)$. This one-dimensional set-up could be a limiting case of a more realistic set-up with wires having non zero diameter. More precisely consider a graph to be a fixed subset of $\mathbb{R}^3$ such that in particular the angles between the edges ending at any vertex are fixed. Now form a tubular $\epsilon$-neighborhood of this graph, i.e. a real system of connected wires of diameter $\epsilon$. In mathematical terms this means that the graph is a deformation retract of any of these tubular neighborhoods. Consider the Laplace operator on this 3-dimensional set with Neumann boundary conditions its boundary, i.e. on its surface. Now the mathematical question arises whether for $\epsilon \downarrow 0$ the resolvent (i.e. the Green’s function) converges suitably to the resolvent of a Laplace operator on the graph and which is of the above type. If this is the case its boundary conditions must then be given in terms of geometrical data, i.e. on how this graph lies in $\mathbb{R}^3$. In other words
and as already mentioned in the introduction, when $\epsilon \downarrow 0$ the transversal modes (except 0) should tend to infinity while the “longitudinal” modes should converge to those of a suitable Laplace operator on the graph. For some simple cases this is indeed known to be true (see for example [15]). The S-matrix $S(E) = S_{A,B}(E)$ for any fixed energy $E > 0$ is now given as follows. It is an $n \times n$ matrix whose elements are defined by the following relations. Consider the plane wave solutions $\psi^k(\cdot, E)$, $1 \leq k \leq n$ of the form

$$\psi^k_j(x, E) = \delta_{jk} e^{-i \sqrt{E} x} + S_{jk}(E) e^{i \sqrt{E} x}$$

(3)

and which satisfy the boundary conditions. Then the S-matrix at energy $E$ for the boundary condition $(A, B)$ is given as

$$S_{A,B}(E) = -(A + i \sqrt{E} B)^{-1} (A - i \sqrt{E} B) = -(A^\dagger - i \sqrt{EB^\dagger})(AA^\dagger + EBB^\dagger)^{-1} (A - i \sqrt{E} B)$$

(4)

and is unitary and real analytic in $E > 0$. Note that $S_{A,B}(E)^{-1} = S_{A,-B}(E)$. In [20] it was shown that the knowledge of the S-matrix at a fixed energy, $E_0$ say, uniquely fixes the boundary conditions. Here we will provide an explicit solution to this inverse problem. For known $S = S_{A,B}(E_0)$ let

$$A' = -\frac{1}{2} (S - \mathbb{I}), \quad B' = \frac{1}{2i \sqrt{E_0}} (S + \mathbb{I}).$$

(5)

Then by (4) one has $(A', B') = (CA, CB)$ with $C = (A + i \sqrt{E_0} B)^{-1}$. This proves that $S = S_{A,B}(E_0)$ indeed uniquely fixes the boundary condition. We can even say more. Indeed, observe that $(A', B')$ defined by (5) satisfies the two relations

$$A' B'^\dagger = \frac{1}{2i \sqrt{E_0}} (S^\dagger - S), \quad A' + i \sqrt{E_0} B' = \mathbb{I},$$

where the first relation is a simple consequence of unitarity. From the first relation we can also directly read off that $A' B'^\dagger$ is selfadjoint and from the second that $(A', B')$ has maximal rank equal to $n$. Thus we have proved the following

**Theorem 1.** For any unitary $n \times n$ matrix $S$ and any energy $E_0 > 0$ there are unique boundary conditions $(A, B)$ such that $S_{A,B}(E_0) = S$. More generally the relation

$$S_{A,B}(E) = \left( (\sqrt{E} - \sqrt{E_0}) S + (\sqrt{E} + \sqrt{E_0}) \right)^{-1} \cdot \left( (\sqrt{E} + \sqrt{E_0}) S + (\sqrt{E} - \sqrt{E_0}) \right)$$

(6)

holds for all $E > 0$.

Indeed, the relation (5) follows from $S_{A,B}(E) = S_{A',B'}(E)$ for all $E > 0$ and from relation (4). Since $E_0$ was arbitrary this in particular gives the relation

$$S_{A,B}(E) = \left( (\sqrt{E} - \sqrt{E_0}) S_{A,B}(E_0) + (\sqrt{E} + \sqrt{E_0}) \right)^{-1} \cdot \left( (\sqrt{E} + \sqrt{E_0}) S_{A,B}(E_0) + (\sqrt{E} - \sqrt{E_0}) \right)$$

(7)

for all $E$ and $E_0 > 0$. In particular this relation may be used as a test to verify if the S-matrix indeed results from boundary conditions in the way described here.

As an illustration with possible applications to quantum computers in mind we consider the some elementary gates usually discussed in this context (see e.g. [16]). Thus
we will view a vertex with \( n \) wires entering as a quantum gate with the wires viewed as channels. In particular the output channels are the same as the input channels. Therefore in addition to quantum transmission from one channel into a different one there will also be reflection from a channel into itself. These reflection amplitudes correspond to the notion of backpropagation in classical information theory.

It is important to realize that here we are dealing with a one-particle theory. In fact, the notion of a particle is introduced here for the following reason. In the concrete setup of classical computers one deals with signals, which are localized in space and time. But in quantum (field) theory and with the appropriate modifications this is one of the notions used to describe particles in terms of wave packets. In the quantum mechanical formulation incoming signals at gates result in outgoing signals and this corresponds to looking at scattering theory and the associated unitary S-matrix. In particular in our approach the vertices act like classical external potentials for which the associated quantum scattering theory has been discussed extensively (see e.g. \([41]\)). Here the dimension of the space of incoming plane waves at energy \( E \) is equal to \( n \), the number of wires entering the vertex. This contrasts with the usual discussion of quantum gates with \( n \) input and \( n \) (different) output channels, where the Hilbert space has dimension equal to \( 2^n \) and replaces the set of classical information containing \( n \) bits. This dimension reflects the tensor product structure (\( n \) factors, each being two-dimensional) of the underlying theory. The tensor product structure is essential for the notion of entanglement, the main ingredient for quantum computation. It is entanglement makes the drastic difference as compared with classical computation. The exponential dependence of the dimension on \( n \) is another reason for the attractiveness of quantum computing. The underlying picture in this case is therefore given by a multi-particle quantum theory, recall for example the discussion of the Einstein-Podolsky-Rosen paradox. A reconciliation of our discussion with the tensor product structure will need further investigations but again, our main motivation was to propose a possible physical realization of unitary operators associated to elementary quantum gates.

Our approach may also be adapted to the situation where we consider nonrelativistic electrons with spin moving through the wires and with boundary conditions possibly allowing for spin flips. Now for \( n \) wires the Hilbert space of incoming plane waves at fixed energy will have dimension equal to \( 2n \). As mentioned in the introduction we will not discuss the experimental feasibility of designing such vertices with a given boundary condition. Also we will not discuss to what extent the dynamics given by the Laplace operator \( \Delta(A,B) \) may serve as an approximation to the dynamics of a real particle (like an electron, say) in concrete wires, where for example one is also confronted with the problem of localization and the resulting exponential decay in space of some eigenfunctions due to the presence of impurities (see e.g. \([25]\) for a discussion on this point) and which may prevent the transmission (see \([21]\)).

**Example 1.** In what follows the energy \( E \) will be fixed at \( E_0 \). Consider the one-dimensional unitary matrix given as a phase \( \exp(i\chi) \) (\( n = 1 \)). Then the Robin boundary condition \( \cos \phi \psi(0) + \sin \phi \psi'(0) = 0 \) with \( \phi \) chosen such that

\[
e^{i\chi} = \frac{-cos \phi - i\sqrt{E_0} \sin \phi}{cos \phi + i\sqrt{E_0} \sin \phi}
\]

solves this problem for one wire. Next consider the \( 2 \times 2 \) unitary, idempotent so-called Hadamard matrix (\( n = 2 \))

\[
\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.
\]
Then the boundary conditions are given by

\[
A = \frac{1}{2} \begin{pmatrix}
1 - \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
-\frac{1}{\sqrt{2}} & 1 + \frac{1}{\sqrt{2}}
\end{pmatrix},
\]

\[
B = \frac{1}{2i\sqrt{E_0}} \begin{pmatrix}
1 + \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
\frac{1}{\sqrt{2}} & 1 - \frac{1}{\sqrt{2}}
\end{pmatrix}.
\]

Note that both \(A\) and \(B\) have vanishing determinant.

Finally consider the real, unitary \(4 \times 4\) matrix (the XOR gate, which is a special Toffoli gate, also called a controlled-NOT ("CNOT")) \((n = 4)\)

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}.
\]

The corresponding boundary conditions are now given as

\[
A = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & \frac{1}{2} & -\frac{1}{2} \\
0 & \frac{1}{2} & \frac{1}{2}
\end{pmatrix},
\]

\[
B = \frac{1}{2i\sqrt{E_0}} \begin{pmatrix}
2 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & 1 & 1
\end{pmatrix}.
\]

Again both \(A\) and \(B\) have vanishing determinant.

The S-matrix at a given energy and resulting from connecting such (elementary) gates is obtained from the S-matrices at the same energy of these individual gates and the lengths connecting them by what we called the generalized star product \([20, 23]\), because it generalizes the star product in classical network theory (see \([38, 39]\)). Although associative this composition rule is nonlinear due to the presence of reflection amplitudes. In the context of potential (quantum) scattering theory on the line an equivalent formulation of the star product also figures under the name Aktosun formula (see e.g. \([1, 4, 13, 14, 19]\)) and there it is an easy consequence of the multiplicative property of the fundamental solution of the Schrödinger equation for a given energy and which is a \(2 \times 2\) matrix (see \([19]\)). In the theory of mesoscopic systems and multichannel conductors this has also been known for a long time and there it is called the multiplicativity of the transfer matrix, which is conjugate to the fundamental solution (see e.g. \([53, 1, 2, 13, 14, 29, 49, 5, 10]\)). In this context we would also like to mention that the problem of how to connect gates in a concrete way without feedback problems (back propagation) due to the presence of reflection amplitudes seems to be well known (see e.g. \([1, \text{p. 3458}], 25\)) but to the best of our knowledge as yet no concrete proposal has been made, even on the conceptual level. Thus so far ordinary matrix multiplication has been used as the composition rule when connecting several gates (see e.g. \([4]\) and the references quoted there). This is in analogy to the notion of straightline programming in information theory.
3 Experimental determination of the S-matrix

In this section we will address the general problem to what extent scattering experiments fix the S-matrix. In what follows the quantum wire will be arbitrary, i.e. it may contain an arbitrary number of external and internal lines and with an arbitrary number of vertices (see [20] for details). First we recall that the matrix elements $S_{jk}(E)$ introduced in (3) have the physical interpretation of transmission coefficients ($j \neq k$) and reflection coefficients ($j = k$) into channel $j$ for an incoming plane wave of energy $E$ in channel $k$. Hence their absolute values are observable. On the other hand if one prepares an incoming wave packet $\phi(\cdot; E)$ to be of the form

$$\phi_k(x; E) = \lambda_k e^{-i\sqrt{E}x}$$

with arbitrary complex amplitudes $\lambda_k \in \mathbb{C}$ ($1 \leq k \leq n$), then the resulting transmission amplitudes into channel $j$ are of the form

$$\sum_{k=1}^{n} \lambda_k S_{jk}(E), \quad (8)$$

whose absolute values in principle are observable. But an easy argument implies the following. By a relabeling of the channels if necessary the S-matrix may be decomposed into a direct sum as

$$S_{A,B}(E) = \bigoplus_{m=1}^{M} S_{A,B}^m(E) \quad (9)$$

for all $E > 0$, where $M$ is supposed to be maximal with $1 \leq M \leq n$. Here the $S_{A,B}^m(E)$ are unitary $k_m \times k_m$ matrices with $\sum k_m = n$. Indeed, since $S_{A,B}(E)$ is real analytic in $E > 0$ any of its matrix elements is either identically equal to zero or vanishes on at most a denumerable set without accumulation points. This implies that such a maximal decomposition (8) exists and is unique. From the point of view of boundary conditions this means that $(A,B)$ may be chosen to have a corresponding maximal decomposition. This means that actually one has a disconnected graph (see [20] for further details). Now experiments fix $S_{A,B}(E)$ up to a phase factor matrix $\exp(i\chi(E))$, where

$$\exp(i\chi(E)) = \bigoplus_{m=1}^{M} \exp(i\chi_m(E)) \mathbb{I}. \quad (10)$$

So assume now that experimentally one has measured the S-matrix for all energies in the form $\tilde{S}(E)$ which agrees with $S_{A,B}(E)$ up to a phase factor matrix $\exp(i\chi(E))$, i.e. the relation $S_{A,B}(E) = \exp(i\chi(E))\tilde{S}(E)$ holds for as yet undetermined phase factors $\exp(i\chi_m(E))$, $1 \leq m \leq M$. In particular note that the decomposition (8) is observable, i.e. $\tilde{S}(E)$ has a decomposition of the same form. Since we know that $S_{A,B}(E)$ is real analytic in $\sqrt{E} > 0$ we may as well assume $\tilde{S}(E)$ to be real analytic by fitting with a phase factor matrix if necessary. But then the phase factor matrix $\exp(i\chi(E))$ is also real analytic. In particular if the graph has one vertex only then by (8) this results in the following relation for the phase factor matrix

$$\exp(i\chi(E)) = \tilde{S}(E)^{-1} \left(\sqrt{E} - \sqrt{E_0}\right) \exp(i\chi(E_0)) \tilde{S}(E_0) + \left(\sqrt{E} + \sqrt{E_0}\right)^{-1}$$

$$\cdot \left(\left(\sqrt{E} + \sqrt{E_0}\right) \exp(i\chi(E_0)) \tilde{S}(E_0) + \left(\sqrt{E} - \sqrt{E_0}\right)\right) \quad (11)$$

for all $E$ and $E_0$. Now fix $E_0$. If there is a solution, then (11) shows that $\exp(i\chi(E))$ is completely determined in terms of the “initial condition” $\exp(i\chi(E_0))$ for all $E$. On the
other hand in order to find a solution one has to choose $\exp(i\chi(E_0))$ in such a way that the r.h.s. of (11) is a phase factor matrix for all $E > 0$ in the sense of (10). However, this procedure does not lead to a unique solution in general as may be seen from looking at Robin boundary conditions given as

$$A_{jk} = \delta_{jk} \cos \phi_k, \ B_{jk} = \delta_{jk} \sin \phi_k$$

resulting in an S-matrix of the form

$$S_{jk}(E) = -\delta_{jk} \cos \phi_k - i\sqrt{E} \sin \phi_k \cos \phi_k + i\sqrt{E} \sin \phi_k.$$  \hspace{1cm} (12)

Then one can essentially only achieve

$$\tilde{S}_{jk}(E) = \delta_{jk}$$

by experiments and any initial condition leads to a solution. This general lack of uniqueness is reminiscent of a similar situation in scattering theory ([9, 33, 26, 18, 28], see also e.g. [27]).

However, there is a way out to find the phases of the S-matrix. The idea is to enlarge the graph by components for which the associated S-matrices $S_{\text{aux}}(E)$ are supposed to be known. The enlarged graph will give rise to an S-matrix $S_{\text{new}}(E)$, which is obtained from the original S-matrix $S(E)$, $S_{\text{aux}}(E)$ and the lengths of the new internal lines (which also are supposed to be known) via the generalized star product [20, 23]. By varying $S_{\text{aux}}(E)$ and measuring the absolute values of the matrix elements of $S_{\text{new}}(E)$, we may infer the phases of the matrix elements of $S(E)$. This strategy is inspired by a familiar procedure in quantum computation, where one analyzes the effect of a black box (an “oracle”) by combining the black box with another box, whose effect is known (see e.g. [34] and the references quoted there).

We start with the case where we want to determine the phase of the reflection amplitude $S_{ii}(E)$. If $S_{ii}(E) = 0$, there is nothing to prove, so we will assume $S_{ii}(E) \neq 0$. On the external line labeled by $i$ we introduce an additional vertex at a distance $a_i$ from the vertex where the line ends. There we introduce arbitrary boundary conditions which result in an arbitrary $2 \times 2$ unitary S-matrix $S_{\text{aux}}(E)$ by our previous discussion. By the techniques of the generalized star product the resulting S-matrix $S_{\text{new}}(E)$ is obtained from $S(E)$, $S_{\text{aux}}(E)$ and the length $a_i$ such that in particular

$$S_{\text{new}}^{ii}(E) = U_{22} + U_{21} S_{ii}(E) (1 - S_{ii}(E) U_{11})^{-1} U_{12}. \hspace{1cm} (12)$$

Here the $U_{kl}$, $k, l = 1, 2$ are the matrix elements of the unitary $2 \times 2$ matrix

$$U = \begin{pmatrix} e^{i\sqrt{E}a_i} & 0 \\ 0 & 1 \end{pmatrix} S_{\text{aux}}(E) \begin{pmatrix} e^{i\sqrt{E}a_i} & 0 \\ 0 & 1 \end{pmatrix}. $$

In the article [21] using a “Born series” expansion we explain the physical intuition behind the generalized star product, from which in particular (12) may easily be obtained. In [23] we shall provide a rigorous proof that the generalized star product indeed provides the right factorization. Since $S_{\text{aux}}(E)$ and $a_i$ are supposed to be known, $U$ is also known and may be chosen arbitrary in the unitary group $U(2)$. Thus $S_{\text{new}}^{ii}(E)$ is a function of $S_{ii}(E)$ and $U$ and by measurements $|S_{\text{new}}^{ii}(E)|$ and $|S_{ii}(E)|$ are known. Actually $S_{\text{new}}^{ii}(E) = \exp(2i\sqrt{E}a_i) S_{ii}(E)$ for the special case when

$$S_{\text{aux}}(E) = S_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$
the “unit matrix” with respect to the generalized star product.

Write \( S_{ii}(E) = \exp(i\phi) |S_{ii}(E)| \). Thus

\[
|S_{ii}^{\text{new}}(E)| = \left| U_{22} + U_{21}S_{ii}(E)|e^{i\phi}(1 - |S_{ii}(E)|e^{i\phi}U_{11})^{-1}U_{12} \right|
\]

is known for all \( U \) and the aim is to determine \( \phi \). Now any \( U \in U(2) \) may be written as

\[
U = \begin{pmatrix} e^{i(\chi+\rho)} & e^{i(\chi+\rho)}(1 - \rho^2)^{1/2} \\ e^{i(\chi+\rho)}(1 - \rho^2)^{1/2} & e^{i(\chi+\rho)}(1 - \rho^2)^{1/2} \end{pmatrix}
\]

with \( 0 \leq \rho \leq 1 \). Therefore

\[
|\rho - (1 - \rho^2)|S_{ii}(E)|(e^{-i(\phi+\chi+\tau)} - |S_{ii}(E)|\rho)^{-1} | (13)
\]

is known. Now choose \( \rho \) so small that \( 2\rho^2|S_{ii}(E)| < |S_{ii}(E)| - \rho \). Then (13) is easily seen to be maximal for \( \exp(i(\phi+\chi+\tau)) = -1 \). Thus tuning \( \chi \) and \( \tau \) and hence \( S_{aux}^E \) while keeping \( \rho \) fixed, such that \( |S_{ii}^{\text{new}}(E)| \) becomes maximal, fixes \( \phi \) as was claimed. An alternative way to determine \( \phi \) is to consider

\[
S_{ij}^{\text{new}}(E) = S_{ij}(E)(1 - S_{ii}(E)U_{11})^{-1}U_{12}
\]

with \( i \neq j \) under the same situation. This procedure therefore is only possible if the graph considered has at least two external lines. Now

\[
|S_{ij}^{\text{new}}(E)| = |S_{ij}(E)|(1 - \rho^2)^{1/2} \left| e^{-i(\phi+\chi+\tau)} - |S_{ii}(E)|\rho \right|^{-1}
\]

becomes maximal when \( \exp(i(\phi+\chi+\tau)) = 1 \) and minimal when \( \exp(i(\phi+\chi+\tau)) = -1 \).

We turn to a discussion of the phases of the transmission amplitudes \( S_{ij}(E), \ i \neq j \). As discussed above (see (8)), by a suitable preparation of the incoming state as a superposition of plane waves of energy \( E \) in the incoming channels \( i \) and \( j \), we can measure \( |S_{ij}(E) + \lambda S_{ii}(E)| \) for all complex \( \lambda \). Since \( S_{ii}(E) \) is has already been determined, this fixes \( S_{ij}(E) \) for \( i \neq j \) provided \( S_{ii}(E) \neq 0 \). Now assume \( S_{ii}(E) = 0 \). Then we proceed as follows. By the same procedure as above we insert a vertex on the line labeled by \( i \) at a distance \( a_i' \) with an S-matrix \( S_{aux}^E \). In analogy to (12) we then obtain an S-matrix \( S(E)' \) with \( S_{ii}(E)' = U_{22}' = S_{aux}^E(E) \), which is non vanishing provided \( \rho' > 0 \). Then we can measure \( S_{ij}(E)' \) with the arguments used above. Now \( S(E)'_{ij} \) converges to \( \exp(i\sqrt{E}a_i')S_{ij}(E) \) when \( S_{aux}^E(E)' \) converges to \( S_0 \), so this determines \( S_{ij}(E) \). The appearance of the phase factor \( \exp(i\sqrt{E}a_i') \) is due to the fact that the insertion of the new vertex shifts the origin of the line labeled by \( i \) by the distance \( a_i' \). This concludes our proof that all matrix elements \( S_{ij}(E) \) may be obtained from scattering experiments performed in this way. Note that for this procedure only scattering experiments at fixed energy are necessary.

4 Description in terms of von Neumann’s extension theory

With the observations of the Section 2 we also may describe \( \Delta(A,B) \) defined on a graph with a single vertex and the resulting S-matrix from the viewpoint of von Neumann’s extension theory (see e.g. [40]). This extends the discussion in Appendix A of [20]. According to von Neumann’s theorem any self-adjoint extension \( \Delta \) of \( \Delta^0 \) can be uniquely
parameterized by a linear isometric isomorphism $W : \text{Ker}(-\Delta_0^\dagger - i) \to \text{Ker}(-\Delta_0^\dagger + i)$ according to the formula

$$\mathcal{D}(\Delta) = \left\{ \psi + \psi_+ + W\psi_+ \mid \psi \in \mathcal{D}(\Delta^0), \psi_+ \in \text{Ker}(-\Delta_0^\dagger - i) \right\},$$

$$-\Delta(\psi + \psi_+ + W\psi_+) = -\Delta^0 \psi + i\psi_+ - iW\psi_+.$$

We will describe $W$ in terms of a matrix $W$ by choosing particular bases in $\text{Ker}(-\Delta_0^\dagger - i)$ and $\text{Ker}(-\Delta_0^\dagger + i)$ respectively.

Namely we choose $u_j \in \text{Ker}(-\Delta_0^\dagger - i)$ and $v_j \in \text{Ker}(-\Delta_0^\dagger + i)$, $j = 1, \ldots, n$ to be given as

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

One can easily verify that $\{u_j\}_{j=1}^n$ and $\{v_j\}_{j=1}^n$ are orthonormal bases for $\text{Ker}(-\Delta_0^\dagger - i)$ and $\text{Ker}(-\Delta_0^\dagger + i)$, respectively. Thus $W$ is the unitary matrix representation of $W$ with respect to these bases $\{u_j\}_{j=1}^n$ and $\{v_j\}_{j=1}^n$, i.e.

$$Wu_j = \sum_{k=1}^n W_{kj} v_k.$$  

In Appendix A of [20] it was shown that for $\Delta = \Delta(A, B)$ the matrix $W = W_{A,B}$ was given as

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

But this means that given any unitary matrix $W$ describing a selfadjoint extension in the sense of von Neumann in the basis described above, and using the pair $(A', B')$ given as $(A', B') = (CA, CB)$ with $C = \sqrt{2}(A - 1/\sqrt{2}(1 + i)B)^{-1} = \sqrt{2}(A - \exp(i\pi/4)B)^{-1}$ to describe the boundary conditions, we have $W = -\mathbb{I} - iB'$ as well as $W = \mathbb{I} - \sqrt{2}A' + B'$ giving $A'$ and $B'$ in terms of $W$ as

$$A' = -e^{-i\pi/4}W + e^{i\pi/4}\mathbb{I}$$
$$B' = i(W + \mathbb{I}).$$

Therefore the S-matrix $S_W(E)$ for a selfadjoint extension given in terms of $W$, and which has a matrix representation $W$ in the above bases, takes the form

$$S_W(E) = - \left( (-e^{-i\pi/4} + \sqrt{E})W + (e^{i\pi/4} - \sqrt{E})\mathbb{I} \right)^{-1} \cdot \left( (-e^{-i\pi/4} + \sqrt{E})W + (e^{i\pi/4} + \sqrt{E})\mathbb{I} \right).$$  

(14)

As a consistency check note that $S_W(E)$ is unitary for all $E > 0$ since $W$ is unitary. Also $W = -\mathbb{I}$ corresponds to Dirichlet boundary conditions with $S_{A=1, B=0}(E) = -\mathbb{I}$ for all $E > 0$. This last relation may of course be inverted to give the matrix $W$ in terms of the S-matrix at any energy. Indeed

$$W = \left( (e^{i\pi/4} - \sqrt{E})S(E) + (e^{i\pi/4} + \sqrt{E})\mathbb{I} \right) \cdot \left( (e^{-i\pi/4} + \sqrt{E})S(E) + (e^{-i\pi/4} - \sqrt{E})\mathbb{I} \right)^{-1}.$$  

(15)
In particular the right hand side is independent of the energy $E$ so this may serve as another test that the S-matrix indeed results from boundary conditions in the way described above.

**Acknowledgements:** The authors would like to thank David Tomanek for informative discussions concerning nanotubes and an anonymous referee for helpful critical remarks.
References

[1] T. Aktosun, “A factorization of the scattering matrix for the Schrödinger equation and for the wave equation in one dimension”, J. Math. Phys. 33, 3865 – 3869 (1992).

[2] T. Aktosun, M. Klaus, and C. van der Mee, “Factorization of scattering matrices due to partitioning of the potentials in one-dimensional Schrödinger-type equations”, J. Math. Phys. 37, 5897 – 5915 (1996).

[3] M.P. Anantram, Jie Han, and T.R. Govindan, “Transport in (10,10) carbon nanotubes with defects”, in A. Aviram and M. Ratner (Eds.), Molecular Electronics: Science and Technology, Ann. NYAS, Vol. 852, New York, 1998, p. 169 – 177.

[4] A. Barenco, C.H. Bennett, R. Cleve, D.P. DiVincenzo, N. Margolus, P. Shor, T. Sleator, J. Smolin, and H. Weinfurter, “Elementary gates for quantum computation”, Phys. Rev. A 52, 3457 – 3467 (1995).

[5] C.W.J. Beenakker, “Random theory of quantum transport”, Rev. Mod. Phys. 69, 731 – 808 (1997).

[6] M. Büttiker, “Four-terminal phase coherent conductance”, Phys. Rev. Lett. 57, 1761 – 1764 (1986).

[7] J.C. Charlier, T.W. Ebbesen, and Ph. Lambin, “Structural and electronic properties of pentagon-heptagon pair defects in carbon nanotubes”, Phys. Rev. B 53, 11108 – 11113 (1996).

[8] L. Chico, V.H. Crespi, L.X. Benedict, S.G. Louie, and M.L. Cohen, “Pure carbon nanoscale devices: Nanotubes heterojunctions”, Phys. Rev. Lett. 76, 971 – 974 (1996).

[9] J. H. Chrichton, “Phase shift ambiguities for spin-independent scattering”, Il Nuovo Cimento 45 A, 256 – 258 (1966).

[10] S. Datta, Electronic Transport in Mesoscopic Systems, Cambridge University Press, Cambridge, 1995.

[11] O.N. Dorokhov, “Transmission coefficient and the localization length of an electron in N bound disordered chains”, JETP Lett. 36, 318 – 321 (1982); Erratum: JETP Lett. 36, 458 (1982).

[12] O.N. Dorokhov, “Electron localization in a multichannel conductor”, Sov. Phys. JETP 58, 606 – 615 (1983).

[13] O.N. Dorokhov, “On the coexistence of localized and extended electronic states in the metallic phase”, Solid State Commun. 51, 381 – 384 (1984).

[14] O.N. Dorokhov, “Solvable model of multichannel localization”, Phys. Rev. B 37, 10526 – 10541 (1988).

[15] D.M. Eigler and E.K. Schweizer, “Positioning single atoms with a scanning tunneling microscope”, Nature 344, 524 – 526 (1990).

[16] N.I. Gerasimenko, The inverse scattering problem on a noncompact graph, Teor. Mat. Fiz. 75, 187 – 200 (1988) (Russian).
[17] S. Iijima, T. Ichihashi, and Y. Ando, “Pentagons, heptagons and negative curvature in graphite microtubule growth”, *Nature* **356**, 776 – 780 (1992).

[18] C. Itzykson and A. Martin, “Phase-shift ambiguities for analytic amplitudes”, *Il Nuovo Cimento* **17 A**, 245 – 287 (1973).

[19] V. Kostrykin and R. Schrader, “Scattering theory approach to random Schrödinger operators in one dimension”, *Rev. Math. Phys.* **11**, 187 – 242 (1999).

[20] V. Kostrykin and R. Schrader, “Kirchhoff’s rule for quantum wires”, *J. Phys. A: Math. Gen.* **32**, 595 – 630 (1999).

[21] V. Kostrykin and R. Schrader, “One-dimensional disordered systems and scattering theory”, preprint (1998); available from http://cartan.math.tu-berlin.de/abstracts/337.

[22] V. Kostrykin and R. Schrader, Determination of the scattering amplitudes of Schrödinger operators from the cross sections, a new approach”, *Lett. Math. Phys.* **48**, 197 – 200 (1999).

[23] V. Kostrykin and R. Schrader, “The generalized star product and the factorization of the scattering matrices on graphs”, in preparation.

[24] R. Landauer, “Electrical resistance of disordered one-dimensional lattices”, *Philos. Mag.* **21**, 863 – 867 (1970).

[25] R. Landauer, “The physical nature of information”, *Phys. Letters A* **217**, 188 – 193 (1996).

[26] A. Martin, “Construction of the amplitude from the differential cross-section”, *Nuovo Cimento* **59 A**, 131 – 152 (1969).

[27] A. Martin, *Scattering theory: Unitarity, Analyticity and Crossing*, Lecture Notes in Physics, Vol. 3, Berlin, Springer, 1969.

[28] A. Martin, “Relations between the modulus and the phase of scattering amplitudes”, in *Proceedings of the International Congress of Mathematicians*, Vancouver, 1974, p. 387 – 393.

[29] P.A. Mello, P. Pereyra, and N. Kumar, “Macroscopic approach to multichannel disordered conductors”, *Ann. Phys.* **181**, 290 – 317 (1988).

[30] M. Menon, D. Srivastava, “Carbon nanotube “T junctions”: Nanoscale metal-semiconductor-metal contact devices”, *Phys. Rev. Lett.* **79**, 4453 – 4456 (1997).

[31] G. Meyer, B. Neu, and K.-H. Rieder, “Controlled local manipulation of single molecules with the scanning tunneling microscope”, *Appl.Phys. A* **60**, 343 – 345 (1995).

[32] G. Meyer, S. Zöphel, and K.-H. Rieder, “Scanning tunneling microscopy manipulation of native substrate atoms: A new way to obtain registry information on foreign substrates”, *Phys. Rev. Lett.* **77**, 2113 – 2116 (1996).

[33] R. Newton, “Determination of the amplitude from the differential cross section by unitarity”, *J. Math. Phys.* **9**, 2050 – 2055 (1968).
[34] J. Preskill, A course on quantum computation; available from http://www.theory.caltech.edu/people/preskill/ph229.

[35] V.Ya. Prinz, V.A. Seleznev, V.A. Samoylov, and A.K. Gutakovsky, “Nanoscale engineering using controllable formation of ultra-thin cracks in heterostructures”, *Microelectronic Engineering* 30, 439 – 442 (1996).

[36] V.Ya. Prinz, V.A. Seleznev, and A.K. Guta, "Self-formed InGa/GaS Nanotubes: Concept, Fabrication, Properties", in the companion CD to *Proceedings of the 24th Int. Conference on the Physics of Semiconductors, Jerusalem, 1988*, D. Gershoni (Ed.), Singapore, World Scientific, 1999.

[37] M. Reck, A. Zeitinger, H.J. Bernstein, and P. Bertani, “Experimental realization of any discrete unitary operator”, *Phys. Rev. Lett.* 73, 58 – 61 (1994).

[38] R. Redheffer, “Difference equations and functional equations in transmission-line theory”, in E. F. Beckenbach (Ed.) *Modern Mathematics for the Engineer*, New York, McGraw-Hill, 1961.

[39] R. Redheffer, “On the relation of transmission line theory to scattering and transfer”, *J. Mathematics and Physics* 41, 1 – 41 (1962).

[40] M. Reed and B. Simon, *Methods of Modern Mathematical Physics, II: Fourier Analysis, Self-Adjointness*, New York, Academic Press, 1975.

[41] M. Reed and B. Simon, *Methods of Modern Mathematical Physics, III: Scattering Theory*, New York, Academic Press, 1979.

[42] R. Saito, G. Dresselhaus, and M.S. Dresselhaus, “Tunneling conductance of connected carbon nanotubes”, *Phys. Rev. B* 53, 2044 – 2050 (1996).

[43] M. Sassoli de Bianchi and M. Di Ventra, “On the number of states bound by one-dimensional finite periodic potentials”, *J. Math. Phys.* 36, 1753 – 1764 (1995).

[44] M. Sassoli de Bianchi, “Comment on “Factorization of scattering matrices due to partitioning of potentials in one-dimensional Schrödinger-type equations””, *J. Math. Phys.* 38, 4882 – 4883 (1997).

[45] M. Schatzmann, “On the eigenvalues of the Laplace operator on a thin set with Neumann boundary conditions”, *Applicable Analysis* 61, 293 – 306 (1996).

[46] P. W. Shor, “Quantum computing”, in *Proceedings of the International Congress of Mathematicians 1998 (Berlin)*, Extra Volume of *Documenta Mathematica, Journal der Deutschen Mathematischen Vereinigung*, 305 – 324 (1998).

[47] D. Srivastava, S. Saini, and M. Menon “Carbon nanotubes: Molecular electronics components”, in A. Aviram and M. Ratner (Eds.), *Molecular Electronics: Science and Technology*, Ann. NYAS, Vol. 852, New York, 1998, p. 178 – 187.

[48] A. Steane, “Quantum computing”, *Rep. Prog. Phys.* 61, 117 – 173 (1998).

[49] A.D. Stone, P.A. Mello, K. Muttalib, and J.-L. Pichard, “Random Matrix Theory and Maximum Entropy Models for Disordered Conductors”, in B.L. Altshuler, P.A. Lee, and R.A. Webb (Eds.) *Mesoscopic Phenomena in Solids*, North Holland, Amsterdam, 1991, p. 369 – 447.
[50] J.A. Stroscio and D.M. Eigler, “Atomic and molecular manipulation with scanning tunneling microscope”, *Science* **254**, 1319 – 1326 (1992).

[51] R. Tamura and M. Tsukada, “Relation between the transition rates and the wavefunctions in carbon nanotubes junctions”, preprint *cond-math/9903279*.

[52] S.J. Tans, A.R.M. Verschueren, and C. Dekker, “Room temperature transistor based on a single carbon nanotube”, *Nature* **393**, 49 – 51 (1998).

[53] B.Y. Tong, “Electronic structure of one-dimensional binary alloys”, *Phys. Rev.* **175**, 710 – 722 (1968).

[54] P. Zeppenfeld, C.P. Lutz, and D.M. Eigler, “Manipulating atoms and molecules with a scanning tunneling microscope”, *Ultramicroscopy* **42-44**, 128 – 133 (1992).