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</thead>
<tbody>
<tr>
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</tr>
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</tbody>
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Inverse scattering problem for quantum graph vertices

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We demonstrate how the inverse scattering problem of a quantum star graph can be solved by means of diagonalization of the Hermitian unitary matrix when the vertex coupling is of the scale-invariant (or Fülöp-Tsutsui) form. This enables the construction of quantum graphs with desired properties in a tailor-made fashion. The procedure is illustrated on the example of quantum vertices with equal transmission probabilities.

Interest in the inverse scattering problem for quantum graphs [1–3] is twofold: These graphs are a prime example of solvable systems possessing nontrivial physical properties [4]. At the same time, the problem is also important because of its relevance to the design principle of nanowire-based single-electron devices.

In this paper, we consider the inverse scattering problem on a star graph with scale-invariant vertex coupling [5], which is an important subset among all the couplings preserving the scale-invariant coupling. We shall give the solution to the corresponding inverse scattering problem in the form of an eigenvalue problem of a Hermitian unitary matrix. In particular, we show that a subclass of the scale-invariant case, and we note that the corresponding scattering problem is given in terms of a diagonalization. From (3) we have

\[
\Psi(0) = I + S \quad \text{and} \quad \Psi'(0) = k(-I + S);
\]

we substitute into (1), which leads to the equation

\[
\begin{pmatrix}
I^{(m)} & T \\
T^\dagger & -I^{(n-m)}
\end{pmatrix}
\begin{pmatrix}
S
\end{pmatrix}
= \begin{pmatrix}
I^{(m)} & T \\
-T^\dagger & I^{(n-m)}
\end{pmatrix}.
\]

It is easy to observe from (4) that

\[
S = X_m^{-1}Z_m X_m,
\]

with the matrices $X_m, Z_m$ defined by

\[
X_m = \begin{pmatrix}
I^{(m)} & T \\
T^\dagger & -I^{(n-m)}
\end{pmatrix}, \quad Z_m = \begin{pmatrix}
I^{(m)} & 0 \\
0 & -I^{(n-m)}
\end{pmatrix}.
\]

We see that (5) can be viewed as a diagonalization formula of the Hermitian unitary matrix $S$ with a diagonalizing matrix of specific block diagonal form, $X_m$, which gives a prescription to obtain $T$ that defines the boundary condition from the scattering matrix $S$. In other words, solution of the our inverse scattering problem is given in terms of a diagonalization.

In practice, the procedure of obtaining $T$ by a diagonalization of $S$ can be cumbersome for large $n$, and there is an alternative simpler way. A calculation shows that (5) can be rewritten in the form

\[
S = -I^{(a)} + 2 \begin{pmatrix}
I^{(m)} \\
T^\dagger
\end{pmatrix}(I^{(m)} + TT^\dagger)^{-1}(I^{(m)} T).
\]
Let us divide $S$ into four submatrices $S_{11}, S_{12}, S_{21}$ and $S_{22}$ of size $m \times m, m \times (n-m), (n-m) \times m$, and $(n-m) \times (n-m)$, respectively, as follows:

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}. \quad (8)$$

The block matrices $S_{ij}$ are expressed in terms of $T$ as $S_{11} = -I^{(m)} + 2(I^{(m)} + TT^\dagger)^{-1}$, $S_{12} = 2(I^{(m)} + TT^\dagger)^{-1}T$, and $S_{22} = I^{(n-m)} - 2(I^{(n-m)} + T^\dagger T)^{-1}$. From here, one gets easily

$$T = (I^{(m)} + S_{11})^{-1}S_{12} = S_{21}(I^{(n-m)} - S_{22})^{-1}. \quad (9)$$

Hence, the algorithm to obtain the matrix $T$ characterizing the vertex is the following:

1. Take the scattering matrix $S$ and set $m = \text{rank}(S + I^{(m)})$.
2. Decompose $S$ according to (8). If necessary, change the numbering of the incoming edges so that $I^{(m)} + S_{11}$ is regular (i.e., it is always possible).
3. Calculate $T$ using (9).

We remark that the matrix $T$ obtained by the algorithm above naturally depends on the numbering of the edges we choose.

In the rest of the paper we demonstrate how the matrix $T$ is used for understanding the meaning of the coupling and for the construction of the vertex with prescribed scattering properties.

Recall that a star-shaped network with a potential at the node can tend in the zero-diameter limit to the star graph with coupling strengths is not involved any approximation. For small values of the length parameter $d$ we have $F_{ij} = 1 + O(d^2)$ and $G_{ij} = 1 + O(d^2)$; then we can show by a straightforward computation in the manner of [9] that the shrinking limit $d \to 0$ gives the desired coupling condition for the scale-invariant vertex (1).

With the procedure described above, it is possible to construct a star graph from any given scattering matrix of the considered class. Our previous result detailed in [11], which provides a reconstruction of the “free-like” scattering, is one such example, and it could be achieved more easily by the current method. Here, we will illustrate the application of the procedure on the following exemplary problem. Let us look at this question: Can one construct a quantum vertex for which the particle incoming from any line is transmitted to all other lines with equal probability? At first, we should ask about the existence condition for the scattering matrix of the form

$$S = \frac{1}{\sqrt{d^2 + n - 1}} \begin{pmatrix} d & \epsilon^{\phi_{i1}} & \cdots & \epsilon^{\phi_{in}} \\ \epsilon^{\phi_{i1}} & d & \cdots & \epsilon^{\phi_{in}} \\ \vdots & \ddots & \ddots & \vdots \\ \epsilon^{\phi_{i,n-1}} & \cdots & \epsilon^{\phi_{i,n-1}} & -d \end{pmatrix}. \quad (15)$$

where $R$ is the matrix whose elements equal the absolute values of the matrix elements of $Q$, i.e., $R = [r_{ij}] = [Q_{ij}]$; the $n \times n$ matrix $J^{(n)}$ has all its elements equal to one. This means that we have $v_i = \frac{1}{d}(1 - \sum_{l \leq m} r_{il})$ for $i > m$, and $v_i = \frac{1}{d}(\sum_{l > m} r_{il} - \sum_{1 \leq i \leq n, l < d} r_{il})$ for $i \leq m$.

The wave function $\psi(x) = \phi_i(x)$ on any internal edge with indices $(i, j)$ has to satisfy the relation

$$\left( \psi^\dagger(0) \frac{d}{\epsilon^x} \psi^\dagger(\frac{x}{\epsilon}) \right) - \frac{\epsilon^{\phi}}{d} \left( G(\frac{x}{\epsilon}) - F(\frac{x}{\epsilon}) \right) \left( \psi(0) \frac{d}{\epsilon^x} \psi(\frac{x}{\epsilon}) \right), \quad (12)$$

with $F(x) = x \cot x$ and $G(x) = x \csc x$. Combining (12) with the condition at the $i$th endpoint where we have the $\delta$ potential of strength $v_i$,

$$\psi'(0) + \sum_{j \neq i} \phi_j'(0) = v_i \psi_i(0), \quad (13)$$

we obtain the relations between the boundary values $\psi_i = \psi_i(0)$ and $\psi'_i = \psi'_i(0)$ in the form

$$d \psi'_i = \left( v_i d + \sum_{j \neq i} r_{ij} F_{ij} \right) \psi_i - \sum_{l \neq i} \epsilon^{\phi_{jl}} r_{ij} G_{ij} \psi_j. \quad (14)$$

These matrices have been recently examined in [13]. It has been proved that the parameter $d$ is always bounded from above by $\frac{\pi}{2} - 1$ (except for $n \leq 2$) and, moreover, that for most values of $d \in [0, \frac{\pi}{2} - 1]$, the existence of the corresponding...
matrix (15) is impossible if the order \( n \) is odd. By contrast, if \( n \) is even, then one can construct an \( S \) for infinitely many values of \( d \), in particular for any \( d \) from the interval \([\frac{5}{2} - 3, \frac{5}{2} - 1]\), or, under certain extra conditions, for all \( d \in [0, 1] \); for further details and explicit matrix constructions we refer to [13].

With a matrix of the type (15) in hand, we can proceed to the construction of the finite approximation. We will demonstrate it on two examples. We first look at the case of reflectionless scattering with uniform transmission to all the other edges. In other words, we ask whether there is a graph with the presence of a nonzero phase shift \( \chi \).

In our finite approximation of a star graph with no internal couplings.

The finite graph approximation is schematically illustrated in the left side of Fig. 1. Our second example is the equal-scattering graph, in which the scattering is uniform to all the edges including the one of the incoming particle. Such a matrix, called a symmetric Hadamard matrix, is known to exist for \( n = 2, 4, 8, 12, 16, 20, 24, \ldots \). An example of such \( S \) for \( n = 8 \) is given by

\[
S = \frac{1}{\sqrt{8}} \left( -I^{(3)} - 2J^{(3)} - 2J^{(3)} + J^{(3)} \right) .
\]

By applying (9), the corresponding \( T \) is easily calculated,

\[
T = -\gamma I^{(3)} + (1 + \gamma) J^{(3)},
\]

where \( \gamma = (\sqrt{5} - 1)/2 \) is the golden mean. Our finite approximation is specified by the following parameters:

\[
\begin{align*}
r_{12} &= r_{23} = r_{13} = 4 + 3\gamma, \\
r_{14} &= r_{25} = r_{36} = 1, \\
r_{15} &= r_{16} = r_{26} = r_{24} = r_{31} = r_{32} = 1 + \gamma, \\
r_{14} &= r_{45} = r_{46} = r_{56} = 0, \\
e^{i\chi_{ij}} &= e^{i\chi_{ij}} = 1, e^{i\chi_{ij}} = -1, e^{i\chi_{ij}} = 1 \text{ for all others},
\end{align*}
\]

and \( v_1 = v_2 = v_3 = -2v_4 \). The finite graph approximation is schematically illustrated in the right side of Fig. 1.

Finally, let us discuss the convergence of the described finite-size graph approximation. In Fig. 2, we display scattering matrix elements of the finite graph constructed to approximate the equal-scattering reflectionless matrix (16). They are calculated directly from (14). The scale of the wavelength \( k \) is given by \( 1/d \). The approximation can be seen to be quite good below \( kd < 0.2 \). Numerical analysis of other examples of different graphs gives essentially the same conclusion, namely that the described construction does represent a physical realization of scale-invariant vertex couplings.

Thus the problem of finding the desired property of scale invariance is turned into a mathematical question about a Hermitian unitary matrix, and the search for systems with \( S \) having interesting specifications other than those examined here should follow. Also, a study of the bound-state spectra is one thing we have completely neglected here; applications to nonquantum waves, including particularly electromagnetic and water waves, should be another interesting subject.

In our finite approximation of a star graph with no internal edges, we have actually studied the low-energy properties of semiclassical properties of quantum-graph spectra [12]. Let us inspect the example of
of graphs with internal edges all of which are connected to the external ones, which we might term depth-one graphs. The examination of depth-two graphs and beyond seems to be a natural future direction. Our result showing the full solution to the inverse scattering problem is, in a sense, a partial fulfillment of the hope that a quantum graph somehow could be a solvable model and useful design tool at the same time.

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