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# A remark on discrete wave scattering 

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#### Abstract

We consider the spectral problem for the adjacency matrix of a discrete stargraph composed of a compact cluster and a few semi-infinite periodic leads attached. Based on the spectral properties of the adjacency matrix we develop the Lax-Phillips scattering theory for the corresponding discrete wave equation.


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## 1. Introduction

Spectral methods are widely used for the study of transport phenomena on compact discrete graphs; see [1]. The spectrum of the adjacency matrix of a discrete compact graph consists of a finite number of eigenvalues, which implies typical features of the corresponding random walk on the graph. The simplest non-compact discrete star-graph is obtained by attaching semi-infinite periodic leads to a compact graph (a cluster). The spectrum of the corresponding adjacency matrix has an absolutely continuous component. The typical transport phenomenon observed on the non-compact star-graph is the transmission of an incoming signal from one semi-infinite lead to another across the cluster; see [2]. This defines a role of the discrete noncompact graph with periodic leads as a convenient model for the optical network constructed of photonic crystals; see for instance [3-6]. The corresponding adjacency matrix or perturbed adjacency matrix, with special boundary conditions at the nodes, can play the role of a typical Hamiltonian. The optical conductance is defined by the scattering matrix of the Hamiltonian, which is usually calculated based on the stationary approach with the spectral parameter on a spectral band.

In this paper, we study the interplay between the characteristics of the discrete spectrum (eigenvalues and the eigenfunctions) of the adjacency matrix of the cluster and the transmission of signals from one lead to another. In particular, we derive an exact formula for the Scattering matrix of the optical network in terms of Neumann-to-Dirichlet map (ND-map) of the cluster. We also suggest a non-stationary interpretation of the constructed stationary Scattering matrix
based on the discrete wave equation on the graph. The corresponding Lax-Phillips theory allows us to reveal the spectral meaning of resonances.

Our paper has the following structure. In the second section we introduce an analog of the ND-map of the cluster and construct the scattered waves and the scattering matrix of the star-graph. In the third section we discuss the resonance mechanism of transmission of signals across the cluster and calculate the approximate scattering matrix based on a local rational approximation of the ND-map. In the fourth section we consider the discrete wave-equation, introduce the relevant energy norm and describe an orthogonal pair of incoming and outgoing subspaces. In the fifth section we consider the non-stationary scattering problem on the stargraph in terms of the Lax-Phillips theory. In the conclusion we briefly discuss the scattering problem for leads with non-trivial periods. We postpone to forthcoming publications the thorough analysis of the problem of leads with non-trivial periods, which requires spectral theory of analytic functions on a multiply connected domain.

## 2. The discrete Schrödinger equation on a star-graph

Consider a non-compact graph $\Omega$ consisting of a compact part (cluster) $\Omega_{\mathrm{in}}$ and a few simplest semi-infinite periodic leads $\omega=\left\{\omega^{l}\right\}_{l=1}^{N}$ attached to some vertices $a_{r} \in \Omega_{\mathrm{in}}, r=$ $1,2, \ldots, N<\infty$. The simplest lead $\omega^{l}$ is a periodic lattice $\left\{b_{1}^{l}, b_{2}^{l}, b_{3}^{l}, \ldots\right\}$, where each node $b_{s}^{l}$ has two nearest neighbours $b_{s-1}^{l}, b_{s-1}^{l}$. Following [1], we consider the adjacency matrix $L$ of the graph $\Omega$ in the space of square summable wave vectors $\mathbf{U}=\left\{\mathbf{u}_{\text {in }}, \overrightarrow{\mathbf{u}}\right\}$. Here $\mathbf{u}_{\text {in }}=\left(u_{1}, u_{2}, u_{3}, \ldots, u_{M}\right)$ are complex coordinates of the inner component $\mathbf{u}_{\text {in }}$ of $\mathbf{U}$, defined at the vertices $a_{s}, s=1,2,3, \ldots, M, M \geqslant N$, and $\overrightarrow{\mathbf{u}}=\left(\mathbf{u}^{1}, \mathbf{u}^{2}, \mathbf{u}^{3}, \ldots, \mathbf{u}^{N}\right)$ is the set of $l_{2}$-vectors $\mathbf{u}^{l}=\left(u_{1}^{l}, u_{2}^{l}, u_{3}^{l}, \ldots\right)$ on the leads $\omega^{l}, l=1,2, \ldots, N$. The first component of $\mathbf{U}$ in the decomposition $l_{2}(\Omega)=l_{2}\left(\Omega_{\text {in }}\right) \oplus l_{2}(\omega)$ is finite-dimensional, $\operatorname{dim} l_{2}\left(\Omega_{\text {in }}\right)=M$, the second component is infinite-dimensional. If the lead $\omega^{k}$ is attached to the node $a_{k} \in \Omega_{\mathrm{in}}$, we impose on vectors $\mathbf{U}$ from the domain of the operator $L$ the boundary conditions $u_{\text {in }}\left(a_{k}\right)=u_{1}^{k}$, thus assuming that $b_{1}^{k} \equiv a_{k}, k=1,2, \ldots, N$. We introduce also the contact space $E_{\text {cont }}=E=C_{N}$ as a space of vectors constituted by the values of the wave vectors at the contact points $a_{k}$.

The adjacency matrix $L$ of the star-graph can be interpreted as a self-adjoint extension (see [7]) of the properly restricted orthogonal sum $L_{\text {in }} \oplus \sum_{k=1}^{N} l^{k}$ of the adjacency matrix of the cluster and ones of the leads $\omega^{k}$ :

$$
\mathbf{l u}=\left(\begin{array}{ccccccccc}
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \ldots \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \ldots \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & \ldots \\
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & \ldots \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & \ldots \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots
\end{array}\right)\left(\begin{array}{c}
u_{1} \\
u_{2} \\
u_{3} \\
u_{4} \\
u_{5} \\
\ldots
\end{array}\right)
$$

Though the restricted operator is not densely defined, the corresponding self-adjoint extension can be constructed based on [7].

We revisit (see for instance [8]) the spectral properties of the unperturbed operator $\mathbf{l}$ on a lead. It is self-adjoint in $l_{2}$ and has a simple absolutely continuous spectrum. The spectrum consists of a single spectral band $[-2,2]$ with eigenfunctions parametrized by the quasimomentum exponential $\Theta=\mathrm{e}^{\mathrm{i} p}$ with real quasi-momentum $p$ on the interval $0 \leqslant p<2 \pi$. The eigenfunctions $\Psi_{\lambda}$ are obtained as linear combinations $\Psi_{\lambda}=\left\{1+S, \Theta+S \bar{\Theta}, \Theta^{2}+S \bar{\Theta}^{2}, \ldots,\right\}$ of Bloch solutions $\chi_{ \pm}$

$$
\chi_{+}=\left(1, \Theta, \Theta^{2}, \Theta^{3}, \ldots\right), \quad \chi_{-}=\left(1, \bar{\Theta}, \bar{\Theta}^{2}, \bar{\Theta}^{3}, \ldots\right)
$$

of the homogeneous equation $\mathbf{I} \chi_{ \pm}=\lambda \chi_{ \pm}, \lambda=\Theta+\bar{\Theta}$. Substitution of the ansatz $\Psi_{\lambda}$ into the homogeneous equation $I \Psi_{\lambda}-\lambda \Psi_{\lambda}=0$ gives $S=-\bar{\Theta}^{2}$. It is convenient to use the quasimomentum exponential as a spectral parameter instead of $\lambda$. Then we may write $\Psi_{\lambda}=\Psi_{\Theta}$ where $\lambda=\Theta+\bar{\Theta}$ is a point on the spectrum and $|\Theta|=1$. The spectral decomposition of $\mathbf{I}$ is given by integration on the quasi-momentum exponential $\Theta$ in the positive direction over the unit circle $\Sigma$

$$
\begin{equation*}
\frac{1}{2 \pi \mathrm{i}} \int_{\Sigma}\left\langle\mathbf{u}, \Psi_{\theta}\right\rangle \Psi_{\Theta} \frac{\mathrm{d} \Theta}{\Theta}=\mathbf{u} . \tag{1}
\end{equation*}
$$

The formula (1) can easily be verified on the dense set of finite elements $\mathbf{u}$ and extended via closure to $L_{2}(\Sigma)$. The system of all eigenfunctions $\Psi_{\Theta}, 0 \leqslant p<2 \pi$ is over-complete. The corresponding system on the interval $0 \leqslant p<\pi$ is complete and orthogonal. Hence the spectral integral can be reduced to the integral over the upper semi-circle $\theta=\mathrm{e}^{\mathrm{i} p}, 0 \leqslant p<\pi$, which corresponds to the upper shore of the spectral band $[-2,2]$ (since $\lambda=\Theta+\bar{\Theta}$ ):

$$
\begin{equation*}
\frac{1}{\pi} \int_{0}^{\pi}\left\langle\mathbf{u}, \Psi_{\Theta}\right\rangle \Psi_{\Theta} \mathrm{d} p=\mathbf{u} \tag{2}
\end{equation*}
$$

or to the integral over the spectral parameter $\lambda$-the 'energy':

$$
\begin{equation*}
\frac{1}{2 \pi} \int_{-2}^{2}\left\langle\mathbf{u}, \Psi_{\Theta}\right\rangle \Psi_{\Theta} \frac{\mathrm{d} \lambda}{\sin p}=\mathbf{u} \tag{3}
\end{equation*}
$$

with $\lambda=2 \cos p, \sin p=\sqrt{1-\lambda^{2} / 4}$. More about spectral properties of discrete and continuous periodic operators can be found in [8] (see also references therein). The operator $L_{\text {out }}=\oplus \sum_{k=1}^{N} \mathbf{l}^{k}$ is defined in the space $l_{2}(E)$ of vectors $\overrightarrow{\mathbf{u}}=\left(\mathbf{u}^{1}, \mathbf{u}^{2}, \mathbf{u}^{3}, \ldots, \mathbf{u}^{N}\right)$ with coordinates $\left\{u_{s}^{l}\right\}=\vec{u}_{s} \in E=C_{N}, s=0,1,2, \ldots$. Hereafter we call the space $E$ a contact space. The expansion over the system of eigenvectors $\vec{\Psi}=\left\{\Psi^{k}\right\}_{k=1}^{N}$ is obtained as an orthogonal sum

$$
\begin{equation*}
\frac{1}{2 \pi \mathrm{i}} \int_{\Sigma}\left\langle\overrightarrow{\mathbf{u}}, \vec{\Psi}_{\Theta}\right\rangle \vec{\Psi}_{\Theta} \frac{\mathrm{d} \Theta}{\Theta}=\overrightarrow{\mathbf{u}} \tag{4}
\end{equation*}
$$

where the summation is extended over the standard basis $v_{s} \in E, \nu_{s}=\delta_{\mathrm{st}}, 1 \leqslant s, t \leqslant N$. We have also spectral expansions for $L_{\text {out }}$ similar to (2, 3):

$$
\begin{equation*}
\frac{1}{\pi} \int_{0}^{\pi} \sum_{\nu}\left\langle\overrightarrow{\mathbf{u}}, \vec{\Psi}_{\Theta}(\nu)\right\rangle \vec{\Psi}_{\Theta}(\nu) \mathrm{d} p=\overrightarrow{\mathbf{u}} \tag{5}
\end{equation*}
$$

and

$$
\begin{equation*}
\frac{1}{2 \pi} \int_{-2}^{2} \sum_{v}\left\langle\overrightarrow{\mathbf{u}}, \vec{\Psi}_{\Theta}(\nu)\right\rangle \vec{\Psi}_{\Theta}(\nu) \frac{\mathrm{d} \lambda}{\sin p(\lambda)}=\overrightarrow{\mathbf{u}} \tag{6}
\end{equation*}
$$

The resolvent and the scattered waves of the perturbed operator $L$ can be constructed via matching a linear combination of Bloch solutions of the homogeneous equation on the leads with an appropriate solution of the homogeneous equation on $\Omega_{\text {in }}$. If $\lambda$ does not belong to the spectrum of $L_{\mathrm{in}}$, then the inner component $\Psi_{\text {in }}$ of the scattered wave on $\Omega_{\mathrm{in}}$ is constructed as a linear combination of resolvent kernels $G\left(r, a_{s}, \lambda\right)$ of the cluster with poles at the contact points $a_{s}: G\left(r, a_{s}, \lambda\right):=G_{s}(r)$ where the leads $\omega^{s}$ are attached:

$$
\begin{equation*}
\Psi_{\mathrm{in}}=\sum_{s=1}^{N} \alpha_{s} G_{s} . \tag{7}
\end{equation*}
$$

See a similar construction of the scattering ansatz for quantum graphs in [9]. The Green function $G_{s}(t)$ satisfies the non-homogeneous equation on the cluster:

$$
L_{\mathrm{in}} G_{s}(t)-\lambda G(t)=\sum_{r \in U_{s}} G_{s}(r)-\lambda G_{s}(t)=\lambda_{s, t}
$$

Here the summation is over the 'star' $U_{s}$ of the nearest neighbours to the node $a_{s}$. The Kronecker symbol is defined in an obvious way: $\delta_{s, t}=0$ on all nodes $t \neq s$ in $\Gamma_{\text {in }}$; and it is equal to 1 at the node $a_{s}$. On the complement of the (discrete) spectrum $\sigma_{d}^{\text {in }}$ of $L_{\text {in }}$ the matrix $G_{\text {in }}(s, t, \lambda)$ coincides with the inverse matrix $\left(L_{\text {in }}-\lambda I\right)^{-1}$. In this paper, we construct the scattered wave $\Psi_{s}$ of the perturbed operator $L$ which is initiated by an incoming wave on the semi-infinite lead $\omega^{s}$ attached to the vertex $a_{s}$. The components $\psi_{s}^{t}$ of the scattered wave $\Psi_{s}$ on the leads $\omega^{t}, t \neq s$, are proportional to the Bloch solution

$$
\begin{equation*}
\psi_{s}^{t}=S_{s}^{t}\left(1, \bar{\Theta}, \bar{\Theta}^{2}, \bar{\Theta}^{3}, \ldots,\right) \tag{8}
\end{equation*}
$$

such that the complex conjugate $\bar{\psi}$ admits an analytic continuation on the spectral sheet $\Theta$, $|\Theta|<1$, of the spectral parameter as square-summable sequences $\bar{\psi}_{s}^{t}=\bar{S}_{s}^{t}\left(1, \Theta, \Theta^{2}, \ldots,\right)$. The component of the scattered wave on $\omega^{s}$ is constructed of two Bloch solutions,

$$
\begin{equation*}
\psi_{s}^{s}=\left(1, \Theta, \Theta^{2}, \ldots,\right)+S_{s}^{s}\left(1, \bar{\Theta}, \bar{\Theta}^{2}, \ldots,\right) . \tag{9}
\end{equation*}
$$

We introduce the matrix $\left\{G\left(a_{t}, a_{s}, \lambda\right)\right\}:=G$ consisting of the values of the Green functions of the inner operator $L_{\text {in }}$ on the contact points. It coincides with the restriction of the inverse matrix $\left(L_{\text {in }}-\lambda I\right)^{-1}$ onto the contact space $E$ :

$$
G=\left.P_{E}\left(L_{\text {in }}-\lambda I\right)^{-1}\right|_{E}
$$

Assume that the complete orthogonal system of all scattered waves, initiated by incoming waves from all leads, is constructed. We calculate the coefficients $\left\{S_{s}^{t}\right\}:=S$ which form the scattering matrix.

## Lemma 2.1.

$$
\begin{equation*}
S=-\frac{I+\Theta G}{I+\bar{\Theta} G} \tag{10}
\end{equation*}
$$

Proof. Consider the matching conditions for the components of the scattered wave $\Psi_{s}$ initiated from the lead $\omega^{s}$ :

$$
\begin{array}{ll}
\sum_{r=1}^{N} \alpha_{r} G(t, r)=S_{s}^{t}, & t \neq s \\
\sum_{r=1}^{N} \alpha_{r} G(s, r)=1+S_{s}^{s}, & t=s
\end{array}
$$

The equation $L \Psi_{s}-\lambda \Psi_{s}=0$ can be written as

$$
\alpha_{t}+S_{s}^{t} \bar{\Theta}=0, \quad t \neq s ; \quad \alpha_{s}+\Theta+S_{s}^{s} \bar{\Theta}=0, \quad t=s
$$

Eliminating $\alpha$ using the second pair of equations and the Kronecker symbol we can re-write the linear system for $S$ as

$$
I+S+\Theta G+\bar{\Theta} S G=0
$$

where $S:=\left\{S_{s}^{t}\right\}_{s, t=1}^{N}$. Then we have for the matrix of coefficients $S_{s}^{t}$ of the scattered waves $\Psi_{s}, s=1,2, \ldots, N$ :

$$
S=-\frac{I+\Theta G}{I+\bar{\Theta} G}
$$

Remark. The matrix $G$ plays a role of the Neumann-to-Dirichlet map [10, 11]-the multidimensional version of the Weyl-Titchmarsh-Krein function; see [12-16], which recently attracts attention of specialists in spectral analysis; see for instance [17-20]. The finitedimensional operator-function $S$ is the scattering matrix of $L$. The formula (10) is an analog of
the formula expressing the scattering matrix in terms of the Dirichlet-to-Neumann map; see [11]. For the one-dimensional versions of the formula, see also [21-23].

The scattering matrix is defined on the continuous spectrum $[-2,2]$ of the operator $L$, which coincides with the continuous spectrum of the non-perturbed operator $L_{\text {out }}$. This interval corresponds to the unit circle $|\Theta|=1$ in terms of the quasi-momentum exponential $\Theta=\mathrm{e}^{\mathrm{i} p}, 0 \leqslant p \leqslant 2 \pi$. Using the connection between the quasi-momentum and the spectral parameter, we conclude that the scattering matrix admits an analytic continuation onto the unit disc $|\Theta|<1$, probably with some poles. The unit disc corresponds to the spectral (physical) sheet of energy $\lambda=\Theta+\Theta^{-1}$. Then the scattering matrix can be continued by symmetry $S^{+}\left(\bar{\Theta}^{-1}\right)=S^{-1}(\Theta)$ onto the whole complex plane of $\Theta$, with a finite number of zeros and poles. The zeros at the points $\Theta_{s}$ inside the unit disc correspond to the eigenvalues $\lambda_{s}=\Theta_{s}+\left(\Theta_{s}\right)^{-1}$ of $L$. Due to symmetry the scattering matrix has also complex poles situated symmetrically to the zeros with respect to the unit circle. The complement $\{\Theta:|\Theta|>1\}$ of the unit disc corresponds to the 'non-physical sheet' of energy. There are also zeros of the analytic continuation of the scattering matrix on the non-physical sheet. Generally they are called resonances (see for instance [8]) and play an important role in scattering processes. We will discuss resonances in sections 3-5.

The spectral expansion of the operator $L$ includes, generally, a sum over the eigenvalues situated on the real axis outside $[-2,2]$, and an integral over the continuous spectrum. Embedded eigenvalues and singular continuous spectrum are absent. We omit the standard derivation of the spectral expansion. It is obtained via compression of the Riesz integral around the spectrum of $L$ to the real interval [-2, 2], taking into account the residues at the eigenvalues, and followed by the use of the Hilbert identity for the jump of the resolvent across the continuous spectrum. Here is the final formula:

$$
\mathbf{U}=\sum_{v} \Psi_{m}\left\langle\mathbf{U}, \Psi_{m}\right\rangle+\frac{1}{2 \pi} \int_{-2}^{2} \sum_{s=1}^{N} \Psi_{\Theta}^{s}\left\langle\mathbf{U}, \Psi_{\Theta}^{s}\right\rangle \frac{\mathrm{d} \lambda}{\sin p(\lambda)}
$$

The scattered waves $\Psi_{\Theta}^{s}$, constructed above via matching linear combination of Bloch waves to linear combinations of Green's functions of $L_{\text {in }}$ with poles at the contact points, can also be obtained from the asymptotic of the resolvent kernel $G(t, s)$ of the operator $L$ when $t \rightarrow \infty$ along the lead attached to the corresponding contact point $a_{s}$ :

$$
G(\tau, t) \approx \Psi_{\tau}^{s} G^{s}(t), \quad \text { when } \quad t \rightarrow \infty, t \in \omega^{s}
$$

Here $G^{s}(s)=G^{s}(\tau, s)$ is the Green function of the component of $L_{\text {out }}$ on the lead $\omega^{s}, \tau \in \omega^{s}$.
We also consider two simple examples which show that the Neumann-to-Dirichlet map may have different structure depending on the size of the contact space.

Example 1. Consider a non-compact graph consisting of three leads attached to the nodes $a_{1}, a_{2}, a_{3}$, of an equilateral triangle $\Omega_{\mathrm{in}}$. The adjacency matrix $L_{\text {in }}$ of the triangle is

$$
L_{\mathrm{in}}=\left(\begin{array}{lll}
0 & 1 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{array}\right)
$$

The eigenvalues are -1 , multiplicity 2 , and 2 , multiplicity 1 . The corresponding normalized eigenvectors are, respectively,

$$
\phi_{1}=\frac{1}{\sqrt{6}}\left(\begin{array}{c}
1 \\
-2 \\
1
\end{array}\right), \quad \frac{1}{\sqrt{2}}\left(\begin{array}{c}
1 \\
0 \\
-1
\end{array}\right), \quad \text { and } \quad \frac{1}{\sqrt{3}}\left(\begin{array}{l}
1 \\
1 \\
1
\end{array}\right) .
$$

Since $\Omega_{\mathrm{in}}$ coincides with the set of contact points, we see that the whole operator $L$ is split into an orthogonal sum of two trivial parts defined by the symmetry of the eigenfunctions of $L_{\mathrm{in}}$. The equation $I+\bar{\Theta} G=0$ splits into two equations in complex plane $\Theta, \bar{\Theta}=\Theta^{-1}$, which correspond to the eigenvalues $-1,2$ :

$$
\Theta+\frac{1}{-1-\Theta-\Theta^{-1}}=0, \quad \Theta+\frac{1}{2-\Theta-\Theta^{-1}}=0
$$

The first equation gives $\Theta=-1$. The singularity $\Theta=-1$ corresponds to the eigenvalue $\lambda_{1}=-2$. The second equation defines the resonance $\Theta=2$. The zeros at the origin $\Theta=0$ in the numerator and in the denominator of the formula (10) for the scattering matrix cancel each other and thus give no contribution to the resulting spectrum and resonances.

Example 2. Consider a ring $\Omega_{\text {in }}$ with $N$ equidistant nodes $\left\{\mathrm{e}^{2 \pi l / M}\right\}_{l=0}^{l=M-1}$. The eigenvalues of the adjacency matrix $L_{\text {in }}$ are $2 \cos 2 \pi m / N$, and the corresponding eigenvectors are $\Phi_{m}=\left\{1, \mathrm{e}^{2 \mathrm{i} \pi m / N}, \mathrm{e}^{2 \mathrm{i} \pi 2 m / N}, \mathrm{e}^{2 \mathrm{i} \pi 3 m / N}, \ldots\right\}, m=1,2,3 \ldots, N-1$. Assume that only one lead is attached to the ring at $a_{0}=1$. Then there is only one contact point, and the corresponding contact space and the ND-map are one-dimensional. The scattering matrix is

$$
\begin{aligned}
S(p) & =-\frac{1+\bar{\Theta} \sum_{m=0}^{N-1} \frac{1}{N}[2 \cos 2 \pi m / N-\Theta-\bar{\Theta}]^{-1}}{1+\Theta \sum_{m=0}^{N-1} \frac{1}{N}[2 \cos 2 \pi m / N-\Theta-\bar{\Theta}]^{-1}} \\
& =-\frac{N-\sum_{m=0}^{N-1}\left[\Theta-\mathrm{e}^{2 \pi \mathrm{i} m / N}\right]^{-1}\left[\Theta-\mathrm{e}^{-2 \pi \mathrm{i} m / N}\right]^{-1}}{N-\sum_{m=0}^{N-1}\left[\bar{\Theta}-\mathrm{e}^{2 \pi \mathrm{i} m / N}\right]^{-1}\left[\bar{\Theta}-\mathrm{e}^{-2 \pi \mathrm{i} m / N}\right]^{-1}} .
\end{aligned}
$$

The complex zeros of the numerator of the scattering matrix can be found numerically.

## 3. Resonance mechanism of conductance on discrete graphs

We begin this section with a brief review of the resonance mechanism of conductance in quantum networks with dynamics governed by a Schrödinger operator. Thin two-dimensional quantum network constructed of the quantum wires $\omega_{s}$, width $\delta$, and a quantum well $\Omega_{\mathrm{int}}$, with the diameter $d, \delta / d \ll 1$, is often modelled (see [24]) by the corresponding continuous one-dimensional star-graph constructed of one-dimensional leads and a point-wise vertex supplied with an appropriate boundary condition. In the non-resonance case, the boundary conditions at the vertices depend, in first approximation, on the ratio of the width of the wires and the diameters of the quantum wells; see [25]. A more detailed description of the realistic boundary condition may be obtained when taking into account subtle geometrical details of the contact [26]. For instance, it was commonly expected that the angles between the wires at the vertex play an essential role. On the other hand, one can expect that the transmission of signals across the quantum well is defined by the shape of the resonance eigenfunction. Based on the resonance mechanism of conductance one can derive an exact formula connecting the scattering matrix of the star-shaped network with the Dirichlet-to-Neumann map of the vertex quantum well. When replacing in this formula the Dirichlet-to-Neumann map by the corresponding local rational approximation, we obtained in [27] an approximate formula for the scattering matrix. In the simplest case of a single resonance eigenvalue the formula, in standard Dirac bra - ket notation is

$$
\begin{equation*}
S(\lambda) \approx-\frac{\frac{P_{+} \frac{\partial \varphi_{0}^{r}}{\partial n}}{\lambda-\lambda_{0}}\left\langle P_{+} \frac{\partial \varphi_{0}^{r}}{\partial n}\right.}{\lambda-\mathrm{i} p P_{+}} \underset{\frac{P_{+} \frac{\partial \varphi_{0}^{r}}{\partial n}}{\lambda-\lambda_{0}}\left\langle P_{+} \frac{\partial \varphi_{0}^{r}}{\partial n}\right.}{\lambda-\mathrm{i} p P_{+}}:=\mathbf{S}_{\mathrm{approx}}(\lambda) . \tag{11}
\end{equation*}
$$

Here $\lambda_{0}$ is the 're-normalized' resonance eigenvalue of the Schrödinger operator in $\Omega, p$ is the momentum of the electron, $\frac{\partial \varphi_{0}}{\partial n}$ is the normal current of the resonance eigenfunction at the bottom sections $\Gamma=\cup_{s=1}^{N} \gamma_{s}$ of the quantum wires, and $P=\oplus \sum_{s=1}^{N} P_{s}$ is the orthogonal projection onto the cross-section eigenfunctions of the open channels in the wires $\omega_{s}$. This permits us to extend, for thin networks, $\delta / d \ll 1$, the boundary condition at the vertex, to the resonance case via substitution of (11) into

$$
\mathrm{i} p\left[I-S_{\text {approx }}(\lambda)\right] \vec{\Psi}(0)=\left[I+S_{\text {approx }}(\lambda)\right] \vec{\Psi} /(0)
$$

This energy-dependent boundary condition shows that the resonance transmission across the vertex is in fact defined by the shape of the resonance eigenfunction, but not necessarily by the angles between the wires.

In the case of discrete graphs (optical networks) we do not have any analog of the small parameter $\delta / d$. Nevertheless we are able to describe the resonance nature of transmission across the cluster revealing the role of the shape of the corresponding resonance eigenfunction. We will do it by deriving an approximate formula from the exact formula (10) for the scattering matrix.

The scattering matrix of the star-graph (10) is presented in the form of the ratio of the matrix-functions $D=P_{E}+\Theta G$ and $D^{+}=P_{E}+\bar{\Theta} G$ :

$$
S=-D^{+} D^{-1}
$$

The resonances are complex vector zeros $\mu_{r}=\Theta_{r}+\Theta_{r}^{-1}$ of the scattering matrix: $S\left(\mu_{r}\right) v_{r}=0$. They coincide with the vector zeros of the numerator

$$
D\left(\mu_{r}\right) v_{r}=\left[P_{E}+\left.\Theta_{r} P_{E}\left(L_{\mathrm{in}}-\mu I\right)^{-1}\right|_{E}\right] v_{r}=0
$$

The resolvent of the finite-dimensional operator $L$ can be represented by the spectral series in terms of its eigenvalues $\lambda_{l}$ and eigenvectors $\varphi_{l}$ :

$$
\left(L_{\mathrm{in}}-\lambda I\right)^{-1}=\sum_{l} \frac{\left.\varphi_{l}\right\rangle\left\langle\varphi_{l}\right.}{\lambda_{l}-\lambda} .
$$

Assuming that $\lambda_{0}$ is a 'resonance' eigenvalue of $L$, with the resonance eigenvector $\varphi_{0}$, we can split the above spectral representation into the sum of the polar term and the remainder:

$$
\left(L_{\text {in }}-\lambda I\right)^{-1}=\frac{\left.\varphi_{0}\right\rangle\left\langle\varphi_{0}\right.}{\lambda_{0}-\lambda}+\sum_{l \neq 0} \frac{\left.\varphi_{l}\right\rangle\left\langle\varphi_{l}\right.}{\lambda_{l}-\lambda}:=\frac{\left.\varphi_{0}\right\rangle\left\langle\varphi_{0}\right.}{\lambda_{0}-\lambda}+\mathcal{K}_{0}(\lambda) .
$$

Then we represent the ND-map as

$$
\begin{align*}
G(\lambda) & =\frac{\left.P_{E} \varphi_{0}\right\rangle\left\langle P_{E} \varphi_{0}\right.}{\lambda_{0}-\lambda}+P_{E} \mathcal{K}_{0}\left(\lambda_{0}\right) P_{E}+P_{E}\left[\mathcal{K}_{0}(\lambda)-\mathcal{K}_{0}\left(\lambda_{0}\right)\right] P_{E} \\
& =G_{0}(\lambda)+P_{E}\left[\mathcal{K}_{0}(\lambda)-\mathcal{K}_{0}\left(\lambda_{0}\right)\right] P_{E} \tag{12}
\end{align*}
$$

Assume that $\left\|P_{E} \varphi_{0}\right\| \neq 0$. Then we introduce the normalized 'resonance contact vector'

$$
e_{0}=\left\|P_{E} \varphi_{0}\right\|^{-1} P_{E} \varphi_{0}
$$

and the corresponding orthogonal projections $P_{0}, P_{\perp}$, decomposing $P_{E}=P_{0} \oplus P_{\perp}$ :

$$
\begin{equation*}
\left.P_{0}=e_{0}\right\rangle\left\langle e_{0}, \quad P_{\perp}=P_{E} \ominus P_{0}\right. \tag{13}
\end{equation*}
$$

Lemma 3.1. If $\left\|P_{E} \varphi_{0}\right\| \neq 0$ and the operator $P_{\perp} \mathcal{K}_{0}\left(\lambda_{0}\right) P_{\perp}:=\mathcal{K}_{\perp \perp}$ is invertible in $P_{\perp} E$, then the sum $G_{0}$ of the first two terms on the right-hand side of (12) dominate the third term on a small real neighbourhood of the resonance eigenvalue $\lambda_{0}$.

Proof. Represent the first two terms of (12) via the orthogonal decomposition $P_{+}=P_{0} \oplus P_{\perp}$ (13) as a $2 \times 2$ matrix:

$$
\begin{align*}
G_{0}(\lambda) & =\left(\begin{array}{cc}
{\left[\frac{\left\|P_{E} \varphi_{0}\right\|^{2}}{\lambda_{0}-\lambda}+\operatorname{Trace} \mathcal{K}_{0}\left(\lambda_{0}\right) P_{0}\right] P_{0}} & P_{0} \mathcal{K}_{0}\left(\lambda_{0}\right) P_{\perp} \\
P_{\perp} \mathcal{K}_{0}\left(\lambda_{0}\right) P_{0} & P_{\perp} \mathcal{K}_{0}\left(\lambda_{0}\right) P_{\perp}
\end{array}\right) \\
& :=\left(\begin{array}{cc}
P_{0}\left[\frac{\left\|P_{E} \varphi_{0}\right\|^{2}}{\lambda_{0}-\lambda}+\mathcal{K}_{00}\right] & P_{0} \mathcal{K}_{0 \perp} \\
\mathcal{K}_{\perp 0} P_{0} & \mathcal{K}_{\perp \perp}
\end{array}\right) . \tag{14}
\end{align*}
$$

Denoting

$$
A=-\frac{\lambda_{0}-\lambda}{\left\|P_{E} \varphi_{0}\right\|^{2}-\left(\lambda_{0}-\lambda\right) \mathcal{K}_{00}} \mathcal{K}_{\perp 0} \mathcal{K}_{0 \perp}+\mathcal{K}_{\perp \perp}
$$

we represent the solution of the equation

$$
G_{0}(\lambda)\binom{u_{0}}{u_{\perp}}=\binom{f_{0}}{f_{\perp}}
$$

in the form

$$
\begin{align*}
& u_{\perp}=A^{-1}\left[-\frac{\lambda_{0}-\lambda}{\left\|P_{E} \varphi_{0}\right\|^{2}-\left(\lambda_{0}-\lambda\right) \mathcal{K}_{00}} \mathcal{K}_{\perp 0} f_{0}+f_{1}\right]  \tag{15}\\
& u_{0}=\frac{\lambda_{0}-\lambda}{\left\|P_{E} \varphi_{0}\right\|^{2}-\left(\lambda_{0}-\lambda\right) \mathcal{K}_{00}}\left[f_{0}-P_{0} \mathcal{K}_{0 \perp} u_{\perp}\right] .
\end{align*}
$$

We leave to the reader the explicit calculation of the inverse $G_{0}^{-1}(\lambda)$ based on (15). One can see that the inverse of (14) is uniformly bounded near $\lambda_{0}$, if $\left\|P_{E} \varphi_{0}\right\|^{2} \neq 0$ and $\mathcal{K}_{\perp \perp}$ is invertible. Hence

$$
\begin{equation*}
G(\lambda)=G_{0}(\lambda)\left\{I+G_{0}^{-1}(\lambda) P_{E}\left[\mathcal{K}_{0}(\lambda)-\mathcal{K}_{0}\left(\lambda_{0}\right)\right] P_{E}\right\} \tag{16}
\end{equation*}
$$

The second term in the curled brackets on the right-hand side of (16) is small near $\lambda_{0}$ due to the smoothness of $\mathcal{K}_{0}(\lambda)$.

Corollary. The sums of leading terms of the numerator and the denominator of the scattering matrix

$$
\begin{equation*}
P_{E}+\Theta G_{0}(\lambda):=D_{0}(\lambda), \quad P_{E}+\bar{\Theta} G_{0}(\lambda):=D_{0}^{+}(\lambda) \tag{17}
\end{equation*}
$$

are invertible on the upper and lower shores of the spectral band: $0<p<\pi, \pi<p<2 \pi$. This is derived from the symmetry of the matrix $G_{0}$ and positivity of the imaginary part of $\Theta$ on both shores of the spectral band.

Theorem 3.1. If the resonance eigenvalue is situated strictly inside the spectral band of $L$, and the conditions of the preceding statement (3.1) are fulfilled, then the expression (10) for the scattering matrix can be replaced, with a minor error, on a certain small real interval $\Delta_{0}$ centred at the resonance eigenvalue $\lambda_{0}$, by the approximate expression:

$$
\begin{equation*}
S(\lambda) \approx-\frac{P_{E}+\Theta G_{0}(\lambda)}{P_{E}+\bar{\Theta} G_{0}(\lambda)}:=S_{\text {approx }}(\lambda) \tag{18}
\end{equation*}
$$

The scattering matrix $S(\lambda)$ can be calculated on $\Delta_{0}$ via analytic perturbation procedure based on $S_{\text {approx }}(\lambda)$, with geometrically convergent series of successive approximations.

Proof. Due to the above Corollary both the numerator $D_{0}^{+}$and the denominator $D_{0}$ of $S_{\text {approx }}$ are invertible inside the spectral band; hence both of them dominate the remainder $G(\lambda)-G_{0}(\lambda)$
in a small real neighbourhood of the resonance eigenvalue:

$$
\left[G(\lambda)-G_{0}(\lambda)\right]\left(P_{E}+\Theta G_{0}(\lambda)\right)^{-1}=o(1)
$$

Hence

$$
\begin{equation*}
S(\lambda)=(I+o(1)) S_{\text {approx }}(\lambda)\left(I+o^{+}(1)\right)^{-1} \approx S_{\text {approx }}(\lambda) . \tag{19}
\end{equation*}
$$

If the small real interval $\Delta_{0}$ is selected such that for $\lambda \in \Delta_{0}$, we have $\|o(1)\|<1$, then, due to (19), the scattering matrix $S(\lambda)$ can be calculated on $\Delta_{0}$ via analytic perturbation procedure, based on $S_{\text {approx }}(\lambda)$, with geometrically convergent series of successive approximations.

The approximate scattering matrix may play a certain role in mathematical design of an optical network. In fact, the preceding theorem shows that the transmission of the signal with resonance energy in the star-graph across the cluster is essentially equivalent to the transmission of the signal on an auxiliary network constructed of the wires attached to a single resonance node supplied with the formal energy-dependent 'Hamiltonian':

$$
\mathbf{l}(\lambda) \overrightarrow{\mathbf{u}}=\left(\begin{array}{ccccccccc}
G_{0}(\lambda) & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \ldots  \tag{20}\\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \ldots \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & \ldots \\
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & \ldots \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & \ldots \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots
\end{array}\right)\left(\begin{array}{c}
\vec{u}_{1} \\
\vec{u}_{2} \\
\vec{u}_{3} \\
\vec{u}_{4} \\
\vec{u}_{5} \\
\ldots
\end{array}\right) .
$$

Here $\vec{u}_{s}=\left(u_{s}^{1}, u_{s}^{2}, u_{s}^{3}, \ldots, u_{s}^{N}\right)$. The corresponding auxiliary scattering matrix is $S_{\text {approx }}$. The energy-dependence of the Hamiltonian of the auxiliary network prevents us from using standard operator machinery for analysis of the corresponding dynamics. But we are also able to prove, that $S_{\text {approx }}$ coincides with the scattering matrix of a solvable model of the network, obtained via equipping the node with an appropriate 'inner structure'. We postpone the construction of the model to a forthcoming publication.

Note that both exact and approximate scattering matrices admit an analytic continuation with respect to $\Theta$ across the absolutely continuous spectrum $|\Theta|=1$ onto the non-physical sheet $|\Theta|>1$. Hereafter we consider the scattering matrix already continued on the whole complex plane $\Theta$ with appropriate singularities at the points symmetric to the zeros. The zeros of the scattering matrix on the physical sheet $|\Theta|<1$ are the eigenvalues of $L$. The zeros on the non-physical sheet are resonances. In the case when the graph has $N$ semi-infinite branches, these are vector zeros, that is,

$$
S(\mu) v_{\mu}=0, \quad v \in E, \quad \operatorname{dim} E=N
$$

Calculation of resonances is an important problem which generally cannot be solved based on self-adjoint theory. In the case of quantum networks there exists a small parameter-the ratio $\delta / d$-which permits us to calculate the resonances based on the asymptotic-the approximate scattering matrix-when $\delta / d \rightarrow 0$. We do not have any small parameter in the case of combinatoric graphs. Nevertheless one can formulate conditions which permit us to localize a resonance in a neighbourhood of the resonance eigenvalue. In this paper we will do the corresponding calculation for zeros of the approximate scattering matrix.

Theorem 3.2. The zeros of the approximate scattering matrix can be found from the equation

$$
\frac{\left\|P_{E} \varphi_{0}\right\|^{2}}{\lambda_{0}-\mu}+\mathcal{K}_{00}=-\Theta^{-1}+\mathcal{K}_{0 \perp}\left[\Theta^{-1}+\mathcal{K}_{\perp \perp}\right]^{-1} \mathcal{K}_{\perp 0}
$$

with $\Theta=\Theta_{\mu}: \mu=\Theta_{\mu}+\Theta_{\mu}^{-1}$.

Proof. Really, the vector zeros ( $\mu, e_{\mu}$ ) of the approximate scattering matrix coincide with the ones of the numerator $D_{0}(\mu) \mathrm{e}^{\mu}=0$ :

$$
\begin{align*}
& \left(\begin{array}{cc}
{\left[\Theta^{-1}+\frac{\left\|P_{E} \varphi_{0}\right\|^{2}}{\lambda_{0}-\mu}+\mathcal{K}_{00}\right] P_{0}} & P_{0} \mathcal{K}_{0 \perp} \\
\mathcal{K}_{\perp 0} P_{0} & \mathcal{K}_{\perp \perp}
\end{array}\right)\binom{\mathrm{e}_{0}^{\mu}}{\mathrm{e}_{\perp}^{\mu}} \\
& :=\left(\begin{array}{cc}
{\left[\Theta^{-1}+\frac{\left\|P_{E} \varphi_{\varphi}\right\|^{2}}{\lambda_{0}-\lambda}+\mathcal{K}_{00}\right] P_{0}} & P_{0} \mathcal{K}_{0 \perp} \\
\mathcal{K}_{\perp 0} P_{0} & \Theta^{-1}+\mathcal{K}_{\perp \perp}
\end{array}\right)\binom{\mathrm{e}_{0}^{\mu}}{\mathrm{e}_{\perp}^{\mu}}=0 . \tag{21}
\end{align*}
$$

Eliminating $\mathrm{e}_{\perp}^{\mu}$ we obtain an equation for $\mu$ :

$$
\begin{equation*}
\frac{\left\|P_{E} \varphi_{0}\right\|^{2}}{\lambda_{0}-\mu}+\mathcal{K}_{00}=-\Theta^{-1}+\mathcal{K}_{0 \perp}\left[\Theta^{-1}+\mathcal{K}_{\perp \perp}\right]^{-1} \mathcal{K}_{\perp 0} \tag{22}
\end{equation*}
$$

Here the inverse $\left[\Theta^{-1}+\mathcal{K}_{\perp \perp}\right]^{-1}$ exists for complex $\Theta=\Theta_{\mu}$ due to the symmetry of $\mathcal{K}_{\perp \perp}$. Choosing $\mathrm{e}_{0}^{\mu}=e_{0}$, we find $\mathrm{e}_{\perp}^{\mu}$ as

$$
\mathrm{e}_{\perp}^{\mu}=-\left[\Theta_{\mu}^{-1}+\mathcal{K}_{\perp \perp}\right]^{-1} \mathcal{K}_{\perp 0} e_{0} .
$$

If we choose $\Theta_{0}=\Theta\left(\lambda_{0}\right)$ as the first approximation for $\Theta_{\mu}$, then we obtain the first approximation for $\mu$ as

$$
\mu_{0} \approx \lambda_{0}+\frac{\left\|P_{E} \varphi_{0}\right\|^{2}}{\mathcal{K}_{00}-\mathcal{K}_{0 \perp}\left[\Theta_{0}^{-1}+\mathcal{K}_{\perp \perp}\right]^{-1} \mathcal{K}_{\perp 0}-\Theta_{0}^{-1}}
$$

One can prove that this approximation is correct, if the second term on the right-hand side of the formula is small.

The zeros of the numerator $D(\lambda)$ of the exact scattering matrix can be also localized via comparison with $D_{0}(\lambda)$, based on [28], if an appropriate domination condition

$$
\begin{equation*}
\sup _{\Sigma_{\varepsilon}}\left\|D_{0}^{-1}(\lambda) P_{E}\left[\mathcal{K}_{0}(\lambda)-\mathcal{K}_{0}\left(\lambda_{0}\right)\right] P_{E}\right\|<1 \tag{23}
\end{equation*}
$$

is fulfilled on some small circle $\Sigma_{\varepsilon}=\left\{\lambda:\left|\lambda-\mu_{r}\right|=\varepsilon\right\}$, centred at the zero $\mu_{r}$ of the approximate scattering matrix. The problem of localization of resonances/eigenvalues of $L$ for the star-graph with a certain geometry can be analysed based on straightforward computing for eigenvalues and eigenvectors of the operator $L_{\mathrm{in}}$.

## 4. The discrete wave equation

Once the spectral analysis of the adjacency matrix is completed, one can solve various dynamical problems on the graph $\Omega$. Denote by $\overrightarrow{\mathbf{u}}(t)$ a function on the graph which depends also on the discrete time variable $t=0, \pm 1, \pm 2, \ldots$, and takes complex values at the nodes on the compact subgraph $\Omega_{\mathrm{in}}$ and on the leads $\omega^{s}, s=1,2, \ldots, N$ :

$$
\overrightarrow{\mathbf{u}}(t)=\left\{\mathbf{u}_{\text {in }}(t), \mathbf{u}^{1}(t), \mathbf{u}^{2}(t), \mathbf{u}^{3}(t), \ldots, \mathbf{u}^{N}(t)\right\} .
$$

Consider the discrete wave equation on the graph $\Omega$

$$
\begin{equation*}
\mathbf{u}(t+1)+\mathbf{u}(t-1)=L \mathbf{u}(t) \tag{24}
\end{equation*}
$$

with the Cauchy data $\mathbf{U}(0)=\left(U_{0}(0), U_{1}(0)\right)$ fixed at the initial moment of time. Generally we consider also the Cauchy data $\mathbf{U}(t)=\left(U_{0}(t), U_{1}(t)\right)$ at the moment $t$ :

$$
U_{0}(t)=\mathbf{u}(t), \quad U_{1}(t)=\mathbf{u}(t+1)-\mathbf{u}(t-1)
$$

One can see that the compactly supported functions $\overrightarrow{\mathbf{u}}(t \pm s)$ on the leads represent incoming and outgoing waves. The energy dot-product associated with the adjacency matrix $L_{\text {out }}$ on the leads $\omega$

$$
[\mathbf{U}, \mathbf{V}]_{\varepsilon_{\text {out }}}=\frac{1}{2}\left\langle\left(4-L_{\text {out }}^{2}\right) U_{0}, V_{0}\right\rangle_{L_{2}(\omega)}+\frac{1}{2}\left\langle U_{1}, V_{1}\right\rangle_{L_{2}(\omega)}
$$

vanishes if $\mathbf{U}$ and $\mathbf{V}$ are the Cauchy data of incoming and outgoing waves, respectively, and is positive for $\mathbf{U}=\mathbf{V}$. Thus the restriction of the evolution defined by the discrete wave equation onto the outer space (supported by the wires) has the typical properties of the LaxPhillips unitary group; see [29]. In particular, it has an orthogonal pair of incoming and outgoing subspaces obtained by the closure in the energy-norm the liner hulls of all compactly supported Cauchy data of incoming and outgoing waves, respectively.

This structure is inherited also by the wave evolution (24) on the whole graph. To motivate this statement, let us introduce the dot-product in the space $\mathcal{E}$ of all Cauchy data of the wave equation (24):

$$
\begin{equation*}
[\mathbf{U}, \mathbf{V}]_{\varepsilon}=\frac{1}{2}\left\langle\left(4-L^{2}\right) U_{0}, V_{0}\right\rangle_{L_{2}(\Omega)}+\frac{1}{2}\left\langle U_{1}, V_{1}\right\rangle_{L_{2}(\Omega)} \tag{25}
\end{equation*}
$$

Generally the energy dot-product defined by the formula (25) is indefinite, since the operator $L$ may have discrete spectrum. If the spectrum of $L$ is absolutely continuous, then $[\mathbf{U}, \mathbf{V}]_{\varepsilon_{\text {wn }}}$ is positive for $\mathbf{U}=\mathbf{V}$. Hereafter we proceed under the assumption that the dot-product (25) is positive. The general case of the indefinite dot-product can be treated similarly to [31].

We represent $\mathcal{E}$ as an orthogonal sum of incoming and outgoing subspaces $\mathcal{D}_{\text {in }}, \mathcal{D}_{\text {out }}$ of Cauchy data supported on the leads and the co-invariant subspace $\mathcal{K}$

$$
\mathcal{K}:=\mathcal{E} \ominus\left[\mathcal{D}_{\text {in }} \oplus \mathcal{D}_{\text {out }}\right]
$$

Theorem 4.1. The discrete wave equation on the space of energy-normed Cauchy data is equivalent to the unitary group in $\mathcal{E}$ defined by the appropriate Dirac operator:

$$
\mathcal{U}:=\frac{1}{2}\left(\begin{array}{cc}
L & 1 \\
L^{2}-4 & L
\end{array}\right), \quad \mathcal{U}+\mathcal{U}^{-1}=\left(\begin{array}{ll}
L & 0 \\
0 & L
\end{array}\right) .
$$

The eigenfunctions of the absolutely-continuous spectrum of the generator $\mathcal{U}$ are represented as

$$
\begin{equation*}
\Phi_{\Theta}=\binom{\frac{1}{\Theta-\Theta^{-1}} \Psi_{\Theta}}{\Psi_{\Theta}} \tag{26}
\end{equation*}
$$

They correspond to the spectral points $\Theta=\mathrm{e}^{\mathrm{i} p}, 0 \leqslant p \leqslant 2 \pi: \mathcal{U} \Phi_{\Theta}=\Theta \Phi_{\Theta}$. The spectral representation of the transformation $\mathcal{U}$ is given by the formula

$$
\begin{aligned}
& \mathbf{U} \xrightarrow{\mathcal{J}}\left[\mathbf{U}, \Phi_{\Theta}\right]_{\mathcal{E}}:=(\mathcal{J} \mathbf{U})(\Theta), \\
& (\mathcal{J} \mathbf{U})(\Theta) \xrightarrow{\mathcal{J}^{-1}} \frac{1}{2 \pi \mathrm{i}} \int_{\Sigma_{1}} \Phi_{\Theta}(\mathcal{J} \mathbf{U})(\Theta) \frac{\mathrm{d} \Theta}{\Theta}=\mathbf{U} .
\end{aligned}
$$

Proof. The identity

$$
\mathcal{U}+\mathcal{U}^{-1}=\left(\begin{array}{ll}
L & 0 \\
0 & L
\end{array}\right)
$$

can be obtained by direct calculation. This means that all spectral objects for the operator $\mathcal{U}$, including the resolvent and the spectral expansion, can be constructed from the corresponding details of the operator $L$-see a similar calculation for the standard Lax-Phillips generator in [30]. In particular, the eigenfunctions of the absolutely continuous spectrum of the generator $\mathcal{U}$ can be obtained from the columns (26) of the scattered waves $\Psi_{\Theta}$ of $L$ in the course of the solution of the wave equation by the Fourier method. It is sufficient to verify that $\Phi_{\Theta}$ satisfies the homogeneous equation $\mathcal{U} \Phi_{\Theta}=\Theta \Phi_{\Theta}$ in the weak sense. We use the fact that $L \Psi_{\Theta}=\left(\Theta+\Theta^{-1}\right) \Psi_{\Theta}$, in the weak sense, as a functional on a dense domain of compactly supported elements in $l_{2}(\Omega)$. Then, using the equations $\left(L^{2}-4\right) \Psi_{\Theta}=\left(\Theta-\Theta^{-1}\right)^{2} \Psi_{\Theta}$ and $L \Psi_{\Theta}=\left(\Theta+\Theta^{-1}\right) \Psi_{\Theta}$, we obtain the desired statement. To prove the equivalence of the
unitary group to the original wave equation we substitute $\overrightarrow{\mathbf{u}}(t+1)+\overrightarrow{\mathbf{u}}(t-1)=L \overrightarrow{\mathbf{u}}(t)$ into $\mathcal{U}$. We obtain

$$
2 \overrightarrow{\mathbf{u}}(t+1)=\overrightarrow{\mathbf{u}}(t+1)+\overrightarrow{\mathbf{u}}(t-1)+\overrightarrow{\mathbf{u}}(t+1)-\overrightarrow{\mathbf{u}}(t-1)
$$

and

$$
2(\overrightarrow{\mathbf{u}}(t+2)-\overrightarrow{\mathbf{u}}(t))=L(\overrightarrow{\mathbf{u}}(t+1)+\overrightarrow{\mathbf{u}}(t-1))-4 \overrightarrow{\mathbf{u}}(t)+L \overrightarrow{\mathbf{u}}(t+1)-L \overrightarrow{\mathbf{u}}(t-1)
$$

Using $\overrightarrow{\mathbf{u}}(t+1)+\overrightarrow{\mathbf{u}}(t-1)=L \overrightarrow{\mathbf{u}}(t)$, again, we obtain the announced statement. The unitarity of the transformation $\mathcal{U}$ follows from the spectral representation.

## 5. Lax-Phillips semigroup and resonances

If the spectrum of the operator $\mathcal{U}$ is purely continuous, then the corresponding unitary group $\mathcal{U}^{l}$ exhibits all typical features of the simplest Lax-Phillips scattering system. In particular, it possesses an orthogonal pair of incoming and outgoing subspaces of the Cauchy data, supported by the leads, and the corresponding co-invariant subspace, supported by the cluster. The Lax-Phillips scattering matrix is obtained from the stationary scattering matrix S (see (10)) via complex conjugation on the spectrum,

$$
\mathbf{S}_{\mathrm{LPh}}(\Theta)=-\frac{1+\bar{\Theta} G}{1+\Theta G}
$$

and can be continued onto the whole complex plane of the quasi-momentum exponential $\Theta$ by the formula
$\mathbf{S}_{\mathrm{LPh}}(\Theta)=-\frac{1+\Theta^{-1} G}{1+\Theta G}=-\Theta \frac{\Theta+G}{1+\theta G}, \quad$ with $\quad G=G(\lambda)=G\left(\Theta+\Theta^{-1}\right)$.
The Lax-Phillips scattering matrix is analytic in the unit disc because the pair of incoming and outgoing subspaces supported by the leads is orthogonal; see [29]. Using the spectral representation for the Green function of $L_{\text {in }}$ in terms of eigenvectors $\varphi_{s}$ and eigenvalues $\lambda_{s}$,

$$
\begin{equation*}
G(\lambda)=\sum_{s=1}^{M} \frac{\left.P_{E} \varphi_{s}\right\rangle\left\langle P_{E} \varphi_{s}\right.}{\lambda_{s}-\lambda}, \tag{28}
\end{equation*}
$$

we obtain an equation for the resonances-vector zeros $\left(\Theta_{r}, \nu_{r}\right)$ of the Lax-Philips scattering matrix $\mathbf{S}_{\mathrm{LPh}}\left(\Theta_{r}\right) v_{r}=0$ in the unit disc $|\Theta|<1$ :

$$
\Theta v+\sum_{s=1}^{M} \frac{\left.P_{E} \varphi_{s}\right\rangle\left\langle P_{E} \varphi_{s}, v\right\rangle}{\lambda_{s}-\lambda}=0, \quad \text { with } \quad \lambda=\Theta+\Theta^{-1}
$$

From the solution of this equation we can observe the dependence of the resonances on the eigenvalues of $L_{\mathrm{in}}$ and on the projection $P_{E} \Psi_{s}$ of the eigenvectors onto the contact space $E$. This way the shape of the eigenvectors of $L_{\text {in }}$ defines the non-stationary transmission from one lead to another.

The matrix-function $\mathbf{S}_{\mathrm{LPh}}(\Theta)$ contains complete spectral information on dynamics defined by the wave equation. In particular, the incoming and outgoing subspaces of the corresponding unitary evolution group $\mathcal{U}^{t}$ are transferred, by the spectral representation $\mathcal{J}$, into $H_{-}^{2}, \mathbf{S}_{\mathrm{LPh}} H_{+}^{2}$ respectively, while the co-invariant subspace becomes $H_{+}^{2} \ominus \mathbf{S}_{\mathrm{LPh}} H_{+}^{2}:=\mathcal{K}$. The eigenvalues of the generator $\mathcal{T}$ of the Lax-Phillips semigroup [29]

$$
\mathcal{P}_{\mathcal{K}} \mathcal{U}^{t} \mid \mathcal{K}:=\mathcal{T}^{t}, \quad t=0,1,2 \ldots
$$

coincide with the zeros $\Theta_{s}$ of the Lax-Phillips scattering matrix and the eigenvectors-the resonance states-in the spectral representation $\mathcal{J}$ are simply $\mathbf{S}_{\mathrm{LPh}} \nu_{r}\left(\Theta_{r}-\Theta\right)^{-1}$. The biorthogonal system of eigenvectors of $\mathcal{T}$ consists of reproducing kernels $\left(1-\bar{\Theta}_{r} \Theta\right)^{-1}$; see
[32]. The completeness of the system of resonance states is equivalent to the absence of the singular factor in $\mathbf{S}_{\mathrm{LPh}}(\Theta)$ in the unit disc.

Corollary. The scattering matrix $\mathbf{S}_{\mathrm{LPh}}$ of the wave evolution with positive adjacency matrix is a Blaschke product. This is simply because the above formula (27) represents it as a ratio of two polynomials of $\Theta$, of the same degree. Hence the system of eigenvectors of the discrete spectrum of the semigroup $\mathcal{T}^{t}, t=0,1,2, \ldots$ is complete.

One can also explore, based on [33, 34], the joint completeness of eigenvectors of both semigroups $\mathcal{T}^{t},\left[\mathcal{T}^{+}\right]^{t}, t=0,1,2, \ldots$

## 6. Conclusion: general periodic leads

Generally, the spectrum of the adjacency matrix of the non-compact graph may have more sophisticated structure; see, for instance, [35]. In particular, the spectrum may be nonconnected if the leads have a richer period. Really, assume that an additional node is attached to each node $b_{k}$ of the lead considered in the previous section, such that the added node has only one nearest neighbour, the node $b_{k}$. Then the new lead will have two nodes on the minimal period and the adjacency matrix on the lead will act on the semi-infinite wave vector $\vec{u}=\left\{u_{2 l}, u_{2 l+1}\right\}_{l=0}^{\infty}$ as a semi-infinite periodic matrix:

$$
\{\mathbf{l} \vec{u}\}_{s}=\left\{u_{s-2}+u_{s+1}+u_{s+2}\right\}, \quad s=2 l \geqslant 2,\{\mathbf{l} \vec{u}\}_{s+1}=u_{s}
$$

The absolutely continuous spectrum of $\mathbf{l}$ consists of two spectral bands $\sigma(\mathbf{l})=[-\sqrt{3}-$ $1,-\sqrt{2}+1] \cup[\sqrt{2}-1, \sqrt{3}+1]$. The standard Lax-Phillips theory is not applicable to operators with non-connected band spectrum. But the wave equation, naturally associated with $\mathbf{I}$, permits us to define an appropriate Dirac operator in the corresponding energy-normed space of Cauchy data and develop a modified Lax-Phillips scattering theory based on the spectral theory of function on the double-connected domain $C \backslash \sigma(\mathbf{l})$ and the corresponding double, diffeomorphic to the torus; see [36]. In the general case of several spectral bands the relevant theory, including joint completeness of eigenvectors of an analog of the Lax-Phillips semigroup, can be developed based on recent results in spectral theory of functions on multiply connected domains; see [34, 37-39] and references therein. We postpone discussion of these interesting questions to a forthcoming publication.

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