Exterior–interior duality for discrete graphs

2009 J. Phys. A: Math. Theor. 42 035101

(http://iopscience.iop.org/1751-8121/42/3/035101)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 035101 (13pp) doi:10.1088/1751-8113/42/3/035101

Exterior–interior duality for discrete graphs

Uzy Smilansky

Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel
and
School of Mathematics, Cardiff University, Cardiff, Wales, UK

E-mail: uzy.smilansky@weizmann.ac.il

Received 26 September 2008, in final form 12 November 2008
Published 9 December 2008
Online at stacks.iop.org/JPhysA/42/035101

Abstract
The exterior–interior duality expresses a deep connection between the Laplace spectrum in bounded and connected domains in $\mathbb{R}^2$, and the scattering matrices in the exterior of the domains. Here, this link is extended to the study of the spectrum of the discrete Laplacian on finite graphs. For this purpose, two methods are devised for associating scattering matrices to the graphs. The exterior–interior duality is derived for both methods.

PACS numbers: 05.45.Mt, 02.10.Ox

1. Introduction

The purpose of this paper is to introduce to the study of the Laplacian on discrete graphs a concept which found several applications in the spectral theory of the wave (and the Schrödinger) operator—the exterior–interior duality. It applies for wave equations on manifolds which can be partitioned into interior (assumed to be simply connected and compact) and exterior domains separated by a boundary. One considers now the wave equations in the two domains, subject to the same boundary conditions. The wave operator restricted to the interior has a pure point spectrum, while in the exterior the spectrum is continuous and a scattering operator can be defined. The restriction of the scattering operator on a particular value of the spectral parameter is the unitary (on shell) scattering matrix $S(\lambda)$. Its spectrum is confined to the unit circle. The exterior–interior duality asserts that the spectrum of the interior can be identified as those values of λ for which one of the eigenvalues of the S matrix approaches the value 1.

The exterior–interior duality was first discussed in the physics literature in [1–4]. It was presented in several versions, which differ in the geometry of the space where the scattering operator is defined. Consider, e.g., a compact domain $\Omega \subset \mathbb{R}^2$ and the wave equation subject to Dirichlet boundary conditions. In the exterior, the wave equation is subject to the same boundary conditions and Ω is treated as an obstacle. The scattering it induces is described in

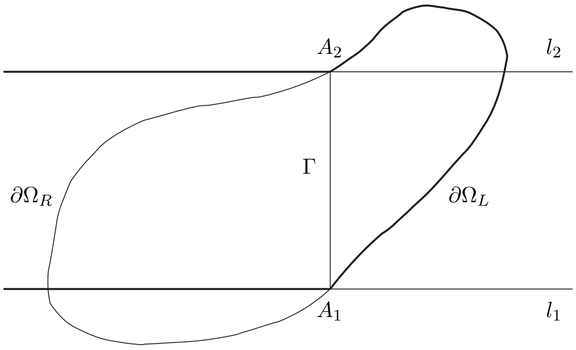

Figure 1. The domain and the added auxiliary channels which are used for the definition of the scattering matrix.

terms of the scattering matrix $S(\lambda)$. The exterior–interior duality ensures that the spectrum of the Dirichlet Laplacian in the interior is identified by the values of the spectral parameters where an eigenvalue of $S(\lambda)$ approaches unity. This was precisely formulated and proved in [5–7].

The wave-guide version that is closer to the present discussion can be crudely described as follows: consider a connected domain in $\mathbb{R}^2$ and impose Dirichlet boundary conditions on its boundary $\partial\Omega$, which is assumed to be smooth. The Dirichlet Laplacian has a discrete spectrum. To define an associated scattering system, choose on the boundary two arbitrary points A_1 and A_2 (see figure 1). Draw two parallel lines, l_1 through A_1 and l_2 through A_2 so that l_1 and l_2 are perpendicular to the chord $\Gamma = (A_2, A_1)$. Consider now the part of the boundary $\partial\Omega_L$ which starts at A_1 and is traversed in the positive mathematical sense as one goes from A_1 to A_2. The domain which is bounded by $\partial\Omega_L$ and by the half lines of l_1 and l_2 to the left of Γ is a semi-infinite channel, terminated at one of its ends by $\partial\Omega_L$. This domain will be denoted by L (for 'left') and its boundaries are drawn by darker lines. Impose Dirichlet conditions on the boundary of L and compute the scattering matrix $S_L(\lambda)$. Repeat the same construction for $\partial\Omega_R$ which is the part of the boundary which completes $\partial\Omega_L$ to the full boundary. The scattering matrix $S_R(\lambda)$ in the 'right' channel R is defined in the same way as above. (The domain boundaries are drawn with lighter lines.) The spectrum of the Laplacian in Ω is obtained by solving the secular equation

$$\det(I - S(\lambda)) = 0; \qquad S(\lambda) = S_L(\lambda)S_R(\lambda). \tag{1.1}$$

This equation expresses the essence of the exterior–interior duality: the spectral information in the interior is obtained from the scattering matrix computed for an appropriate exterior problem. This version and its variations were studied in the physics literature [1, 8, 9]. Only a few examples were studied with mathematical rigor [10].

The exterior–interior duality was discussed and proved for quantum graphs [11, 12].

The secular equation of type (1.1) has several theoretical and practical advantages which were used for various purposes in the study of the wave equation. In the following, analogous secular equations for the spectrum of the discrete Laplacian on graphs will be derived, thus extending the interior–exterior duality to the discrete case. There are two conceptual obstacles which should be cleared in order to carry out this program:

(i) Given a finite graph with a general connectivity, there is no natural way to convert it into a scattering problem analogous to the first version discussed above.

(ii) There is no natural definition for a 'boundary' on a compact graph, and if a boundary is defined, the meaning of boundary conditions has to be explained.

In the following section, the above difficulties will be addressed and the scattering matrices $S(\lambda)$ will be constructed in two different settings. The exterior–interior duality will be realized by deriving the corresponding secular equations of the form (1.1) for the spectrum of the graph.

A few applications will be presented in section 4.

The following notations and concepts will be used throughout the present work. A graph $\mathcal{G}$ is defined in terms of its vertex set $\mathcal{V}$ and edge (bond) set $\mathcal{E}$. The cardinality of these sets will be denoted by $V = |\mathcal{V}|$, $E = |\mathcal{E}|$. The graph topology is defined by the connectivity (adjacency) matrix C which is labeled by the vertex indices. It is a symmetric matrix whose i, j element counts the number of edges connecting the vertices i and j. The valency (degree) of a vertex is defined as the number of bonds which emanate from it, $v_i = \sum_j C_{i,j}$. The diagonal matrix $D = \mathrm{diag}(v_i)$ appears in the definition of the graph Laplacian:

$$\Delta = -C + D. \tag{1.2}$$

As explained above, and in a complete analogy with the example discussed in the introduction, the graph whose spectrum one wishes to compute will be extended so that it forms the 'interior graph' $\mathcal{G}^{(0)}$ in a scattering setting. All the quantities which are related to the 'interior' graph will be denoted by a superscript 0. For simplicity it is assumed to be connected and devoid of parallel bonds $\big(C^{(0)}_{i,j} \in \{0, 1\}\big)$ or loops $\big(C^{(0)}_{i,i} = 0\big)$.

2. Scattering on discrete graphs

In this section scattering on graphs will be defined using two different approaches. The first goes along the lines of [13], the second relies on the graph evolution operator defined in [14]. For the sake of completeness, some background material for each of the methods will be reviewed before the scattering matrices are presented.

2.1. Scattering into attached leads

In this setting, one attaches leads to the graph $\mathcal{G}^{(0)}$ and scattering is defined on the enlarged graph. A lead graph l is defined as a semi-infinite set of vertices $(l, 1), (l, 2), \ldots,$ which are connected linearly. A vertex is identified by a double index (l, i), l denotes the lead and i enumerates the vertex position on the lead. The lead connectivity (adjacency) matrix is $C^{(\mathrm{Lead})}_{(l,n),(l',n')} = w\delta_{l,l'}\delta_{|n-n'|,1}$, $n, n' \in \mathbb{N}^+$, where w stands for the number of parallel bonds which connect successive vertices. (All quantities related to the leads will be denoted by the superscript (Lead).) The spectrum of the lead Laplacian $\Delta^{(\mathrm{Lead})}_l$ and the corresponding eigenfunctions $\mathbf{f} = (f_{(l,1)}, f_{(l,2)}, \ldots)^\top$ satisfy

$$\begin{aligned}\big(\Delta^{(\mathrm{Lead})}_l \mathbf{f}\big)_{(l,n)} &= -w(f_{(l,n+1)} + f_{(l,n-1)}) + 2wf_{(l,n)} = \lambda f_{(l,n)} \quad \text{for} \quad n > 1,\\ &= -wf_{(l,2)} + wf_{(l,1)} = \lambda f_{(l,1)} \quad \text{for} \quad n = 1.\end{aligned} \tag{2.1}$$

The spectrum is continuous and supported on the spectral band $\lambda \in [0, 4w]$ (the conduction band). For any λ in the conduction band, there correspond two eigenfunctions which can be written as linear combinations of counter-propagating waves:

$$f^{(\pm)}_{(l,n)} = \xi_\pm^{n-1} \qquad \text{where} \quad \xi_\pm = 1 - \frac{\lambda}{2w} \pm \sqrt{\left(1 - \frac{\lambda}{2w}\right)^2 - 1} = \mathrm{e}^{\pm \mathrm{i}\alpha(\lambda)}. \tag{2.2}$$

For $\lambda > 4w$, $|\xi_-| > |\xi_+|$. The reason for constructing the leads with w parallel bonds is because the conduction band can be made arbitrarily broad. In the present application, an appropriate choice of w would be of the order of the mean valency in the interior graph, so the spectrum of $\mathcal{G}^{(0)}$ falls well within the conduction band.

A function that satisfies the boundary condition at $n = 1$ (the second line of (2.1)) is

$$f_{(l,n)} = f^{(-)}_{(l,n)} + s_l(\lambda) f^{(+)}_{(l,n)}, \tag{2.3}$$

where

$$s_l(\lambda) = -\frac{1-\xi_+}{1-\xi_-} = \xi_+, \quad |s_l(\lambda)| = 1 \qquad \text{for} \quad \lambda \in [0, 4w]. \tag{2.4}$$

The lead scattering amplitude $s_l(\lambda)$ provides the phase gained by scattering at the end of the lead (as long as λ is in the conduction band). It plays here the role of the scattering matrix which will be defined in the following.

Returning now to the interior graph $\mathcal{G}^{(0)}$ it is converted into a scattering graph by attaching to its vertices semi-infinite leads. At most one lead can be attached to a vertex, but not all vertices should be connected to leads. Let $\mathcal{L}$ denote the set of leads, and $L = |\mathcal{L}|$. The connection of the leads to $\mathcal{G}^{(0)}$ is given by the $V^{(0)} \times L$ 'wiring' matrix

$$W_{j,(l,1)} = \begin{cases} 1 & \text{if} \quad j \in \mathcal{V}^{(0)} \quad \text{is connected to } l \in \mathcal{L} \\ 0 & \text{otherwise.} \end{cases} \tag{2.5}$$

The number of leads which emanate from the vertex i is either 0 or 1 and is denoted by $d_i = \sum_{l\in\mathcal{L}} W_{i,(l,1)}$. Define also the diagonal matrix $\tilde{D} = \mathrm{diag}(d_i)$ so that

$$WW^\top = \tilde{D}; \qquad W^\top W = I^{(L)}, \tag{2.6}$$

where $I^{(L)}$ is the $L \times L$ unit matrix.

The scattering graph $\mathcal{G}$ is the union of $\mathcal{G}^{(0)}$ and the set of leads $\mathcal{L}$. Its vertex set is denoted by $\mathcal{V}$ and its connectivity matrix C is given by

$$\forall i, j \in \mathcal{V}, : C_{i,j} = \begin{cases} C^{(0)}_{i,j} & \text{if} \quad i, j \in \mathcal{V}^{(0)} \\ C^{(\mathrm{Lead})}_{i=(l,i),j=(l,j)} & \text{if} \quad l \in \mathcal{L} \\ wW_{i,j=(l,1)} & \text{if} \quad i \in \mathcal{V}^{(0)} \quad \text{and} \quad l \in \mathcal{L}. \end{cases} \tag{2.7}$$

As is usually done in scattering theory, one attempts to find eigenfunctions $\mathbf{f}$ of the discrete Laplacian of the scattering graph, subject to the condition that on the leads $l = 1, \ldots, L$ the wavefunction consists of counter propagating waves:

$$f_{(l,n)} = a_l \xi_-^{n-1} + b_l \xi_+^{n-1}, \qquad n \geqslant 1, \tag{2.8}$$

where a_l and b_l are the incoming and outgoing amplitudes. They are to be determined from the requirement that $\mathbf{f}$ is an eigenfunction of the scattering graph Laplacian. It will be shown below that this requirement suffices to provide a linear relationship between the incoming and outgoing amplitudes. The $L \times L$ scattering matrix $S^{(\mathrm{Lead})}(\lambda)$ is defined as the mapping from the incoming to the outgoing amplitudes:

$$\mathbf{b} = S^{(\mathrm{Lead})}(\lambda)\mathbf{a}. \tag{2.9}$$

To compute $S^{(\mathrm{Lead})}(\lambda)$, consider the action of the Laplacian on an eigenvector $\mathbf{f}$.

$$\begin{aligned} &\forall\, i \in \mathcal{V}^{(0)} : (\Delta\mathbf{f})_i = -\sum_{j\in\mathcal{V}^{(0)}} C^{(0)}_{i,j} f_j - w\sum_{l\in\mathcal{L}} W_{i,(l,1)} f_{(l,1)} + (D_i + wd_i) f_i = \lambda f_i. \\ &\forall\, l \in \mathcal{L} : (\Delta\mathbf{f})_{(l,1)} = -w\sum_{i\in\mathcal{V}^{(0)}} W^\top_{(l,1),i} f_i - wf_{(l,2)} + 2wf_{(l,1)} = \lambda f_{(l,1)}. \\ &(\Delta\mathbf{f})_{(l,n)} = -wf_{(l,n+1)} - wf_{(l,n-1)} + 2wf_{(l,n)} = \lambda f_{(l,n)}. \end{aligned} \tag{2.10}$$

The equations for $i \in \mathcal{V}^{(0)}$ (the first line in (2.10)) can be put in a concise form:

$$(\Delta^{(0)} + w\tilde{D} - \lambda I^{(V^{(0)})})\mathbf{f}^{(V^{(0)})} = wW\mathbf{f}_1^{(L)}, \tag{2.11}$$

where $I^{(V^{(0)})}$ is the unit matrix in $V^{(0)}$ dimension, $\mathbf{f}^{(V^{(0)})}$ is the restrictions of $\mathbf{f}$ on the vertices of the interior graph $\mathcal{G}^{(0)}$ and $\mathbf{f}_1^{(L)}$ is the L dimensional vector with components $f_{(l,1)}, l = 1, \ldots, L$. For λ away from the eigenvalues of $\Delta^{(0)} + w\tilde{D}$, the $V^{(0)} \times V^{(0)}$ matrix $R^{(0)}(\lambda)$ is defined as

$$R^{(0)}(\lambda) = (\Delta^{(0)} + w\tilde{D} - \lambda I^{(V^{(0)})})^{-1}. \tag{2.12}$$

Thus,

$$\mathbf{f}^{(V^{(0)})} = wR^{(0)}W\mathbf{f}_1^{(L)}. \tag{2.13}$$

Substituting into the second set of equations in (2.10) and using (2.8),

$$(-w^2W^\top R^{(0)}(\lambda)W + (2w - \lambda)I^{(L)})(\mathbf{a} + \mathbf{b}) = w(\mathbf{a}\xi_- + \mathbf{b}\xi_+). \tag{2.14}$$

This can be easily brought into the form (2.9). Using the fact that $2 - \lambda/w = \xi_- + \xi_+$ we get

$$S^{(\mathrm{Lead})}(\lambda) = -(wW^\top R^{(0)}(\lambda)W - \xi_- I^{(L)})^{-1}(wW^\top R^{(0)}(\lambda)W - \xi_+ I^{(L)}). \tag{2.15}$$

This is the desired form of the scattering matrix. It has a few important properties.

(i) As long as λ is in the conduction band, ξ_- and ξ_+ are complex conjugate and unitary. Since $W^\top R^{(0)}(\lambda)W$ is a symmetric real matrix, $S^{(\mathrm{Lead})}(\lambda)^\top = S^{(\mathrm{Lead})}(\lambda)$ and $S^{(\mathrm{Lead})}(\lambda)S^{(\mathrm{Lead})}(\lambda)^\dagger = I^{(L)}$, that is, $S^{(\mathrm{Lead})}(\lambda)$ is a symmetric and unitary matrix.

(ii) Once λ is outside the conduction band, $f_{(l,n)}^{(\pm)}$ are exponentially increasing or decreasing solutions—they are the analogs of the evanescent waves encountered in the study of wave guides. One of the reasons for the introduction of the w parallel bonds in the leads was to broaden the conduction band and avoid the spectral domain of evanescent waves. However, for the sake of completeness one observes that the scattering matrix as defined above can be analytically continued outside the conduction band by using (2.2) which is valid for any λ. The $S^{(\mathrm{Lead})}(\lambda)$ matrix outside the conduction band loses its physical interpretation, and it remains symmetric but is not any more unitary. However, it is a well-defined object, and can be used in the following for any real or complex λ. In the limit $\lambda \to \infty$, $S^{(\mathrm{Lead})}(\lambda) \to \xi_+ W^\top R^{(0)}(\lambda)W \approx \left(\frac{w}{\lambda}\right)^2 I^{(L)}$.

(iii) At the edges of the conduction band $\xi_\pm(\lambda = 0) = 1$; $\xi_\pm(\lambda = 4w) = -1$. Substituting into (2.15) one finds that at the band edges, $S^{(\mathrm{Lead})} = -I^{(L)}$.

(iv) The matrix $R^{(0)}(\lambda)$ is well defined for λ away from the spectrum of $\Delta^{(0)} + w\tilde{D}$. Approaching these values does not cause any problem in the definition of $S^{(\mathrm{Lead})}(\lambda)$ since there $S^{(\mathrm{Lead})} = -I^{(L)}$. However, for sufficiently large w the singularities of $R^{(0)}(\lambda)$ can be separated away from the domain where the spectrum of $\mathcal{G}^{(0)}$ is supported.

(v) The resonances are defined as the poles of the scattering matrix in the complex λ plane. They are the solution of the equation

$$z_{\mathrm{res}}(\lambda) = \det(wW^\top R^{(0)}(\lambda)W - \xi_- I^{(L)}) = 0. \tag{2.16}$$

The point $\lambda = 0$ is not a pole since $S^{(\mathrm{Lead})}(\lambda = 0) = -I^{(L)}$.

(vi) Finally, it might be instructive to note that the matrix $R^{(0)}(\lambda)$ is closely related to the discrete analog of the Dirichlet to Neumann map. This can be deduced from the following construction: add to each vertex $i \in \mathcal{V}^{(0)}$ a new auxiliary vertex $\tilde{i}$ connected exclusively to i. (Here we use $w = 1$ to make the analogy clearer.) Write the discrete Laplacian for the new graph and solve $(\Delta - \lambda I)\tilde{\mathbf{f}} = 0$, where $\tilde{\mathbf{f}}$ is a $2V^{(0)}$ dimensional vector, the first V entries correspond to the original vertices and the last V entries correspond to the auxiliary vertices: $\tilde{\mathbf{f}} = (\mathbf{f}, \mathbf{g})^\top$. Assuming that the values $g_{\tilde{i}}$ on the auxiliary vertices are given, the entries in $\mathbf{f}$ can be expressed as $\mathbf{f} = R(\lambda)\mathbf{g}$, where $R(\lambda)$ as defined in (2.12). To emphasize the connection to the Dirichlet to Neumann map, define $\psi = \frac{1}{2}(\mathbf{g}+\mathbf{f})$ (the 'boundary function') and $\partial\psi = (\mathbf{g}-\mathbf{f})$ (the 'normal derivative') then

$$\partial\psi = M(\lambda)\psi; \qquad M(\lambda) = 2(I^{(V^{(0)})} + R(\lambda))^{-1}(I^{(V^{(0)})} - R(\lambda)). \tag{2.17}$$

The Dirichlet to Neumann map is also defined in other applications of graph theory, see e.g., [16].

2.2. *Scattering into dangling bonds (evolution operator approach)*

An alternative construction of a scattering matrix follows naturally from the study of the evolution operator $U^{(0)}(\lambda)$ of the interior graph. It is a unitary matrix of dimension $2E^{(0)}$ which will be reviewed in the following paragraphs for the sake of completeness. (Details can be found in [14, 15]; see also [17–20] and references cited therein.)

Let $\mathbf{f} = (f_1, \ldots, f_{V^{(0)}})$ denote an eigenvector of the graph Laplacian $\Delta^{(0)}$ (1.2), corresponding to an eigenvalue λ. The bond b connecting the vertices i and j will be denoted by $b = (i, j)$. To each bond b one associates a *bond wavefunction*

$$\psi_b(x) = a_b\,\mathrm{e}^{\mathrm{i}\frac{\pi}{4}x} + \hat{a}_b\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}x}, \qquad x \in \{\pm 1\} \tag{2.18}$$

subject to the condition

$$\psi_b(1) = f_i, \qquad \psi_b(-1) = f_j. \tag{2.19}$$

Consider any vertex indexed by i of degree (valency) v_i and the bonds $(b_1, b_2, \ldots, b_{v_i})$ which emanate from i. The corresponding bond wavefunctions have to satisfy three requirements in order to form a proper eigenvector of $\Delta^{(0)}$.

(I) Uniqueness: The value of the eigenvector at the vertex i, f_i, computed in terms of the bond wavefunctions is the same for all the bonds emanating from i. The following $v_i - 1$ independent equalities express this requirement:

$$a_{b_1}\,\mathrm{e}^{\mathrm{i}\frac{\pi}{4}} + \hat{a}_{b_1}\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} = a_{b_2}\,\mathrm{e}^{\mathrm{i}\frac{\pi}{4}} + \hat{a}_{b_2}\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} = \cdots = a_{b_{v_i}}\,\mathrm{e}^{\mathrm{i}\frac{\pi}{4}} + \hat{a}_{b_{v_i}}\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}. \tag{2.20}$$

(II) $\mathbf{f}$ is an eigenvector of $\Delta^{(0)}$: At the vertex i, $\sum_{j=1}^{v_i} {\Delta^{(0)}}_{i,j} f_j = \lambda f_i$. In terms of the bond wavefunctions this reads

$$-\sum_{l=1}^{v_i}[a_{b_l}\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} + \hat{a}_{b_l}\,\mathrm{e}^{+\mathrm{i}\frac{\pi}{4}}] = (\lambda - v_i)\frac{1}{v_i}\sum_{m=1}^{v_i}[a_{b_m}\,\mathrm{e}^{\mathrm{i}\frac{\pi}{4}} + \hat{a}_{b_m}\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}]. \tag{2.21}$$

Together, (2.20) and (2.21) provide v_i homogeneous linear relations between the $2v_i$ coefficients $a_{b_m}, \hat{a}_{b_m}$. It is convenient to introduce at this point the following notation: let $d = (j, i), i, j \in \mathcal{V}^{(0)}$ denote a directed bond pointing from i to j. Then $o(d)$ $(t(d))$ stand for its origin i (terminus j) vertices, respectively. From now on, the amplitudes a_{b_m} and $\hat{a}_{b_m}$ which refer to propagating on the bond b_m in opposite directions will be denoted by a_d and $a_{\hat{d}}$ where $\hat{d}$ is the directed bond inverse to d. Using (2.20) and (2.21), the outgoing coefficients are expressed in terms of the incoming ones,

$$a_d = \sum_{d':t(d')=i} \sigma^{(i)}_{d,d'}(\lambda)a_{d'} \qquad \forall\, d : o(d) = i, \tag{2.22}$$

where

$$\sigma^{(i)}_{d,d'}(\lambda) = i\left(\delta_{\hat{d},d'} - \frac{2}{v_i}\frac{1}{1 - i\left(1 - \frac{\lambda}{v_i}\right)}\right). \tag{2.23}$$

The *vertex scattering matrices* $\sigma^{(i)}(\lambda)$ are the main building blocks of the present approach. A straightforward computation shows that for real λ the vertex scattering matrices are unitary and symmetric matrices.

(III) Consistency: The linear relation between the incoming and the outgoing coefficients (2.22) must be satisfied simultaneously at all the vertices. However, a directed bond (i, j) when observed from the vertex j is *outgoing*, while when observed from i it is *incoming*. This consistency requirement is implemented by introducing the *evolution operator* $U_{d',d}(\lambda)$ in the $2E^{(0)}$ dimensional space of directed bonds:

$$U_{d',d}(\lambda) = \delta_{t(d),o(d')}\sigma^{(t(d))}_{d',d}(\lambda). \tag{2.24}$$

The evolution operator is unitary $UU^{\dagger} = I^{(2E^{(0)})}$ for $\lambda \in \mathbb{R}$ due to the unitarity of its constituents $\sigma^{(i)}$. Denoting by $\mathbf{a}$ the $2E^{(0)}$ dimensional vector of the directed bond coefficients a_d defined above, the consistency requirement reduces to

$$U(\lambda)\mathbf{a} = \mathbf{a}. \tag{2.25}$$

This can be satisfied only for those values of λ for which

$$\det(I^{(2E^{(0)})} - U(\lambda)) = 0. \tag{2.26}$$

This result can be interpreted in the following way. The evolution operator $U(\lambda)$ is defined for any λ, and it maps the $2E^{(0)}$ dimensional vector space of amplitudes $\mathbf{a}$ to itself. The spectrum of $\Delta^{(0)}$ is identified as those values of λ for which there exist vectors which are *stationary* under the action of the mapping.

To construct a scattering operator for which $\mathcal{G}^{(0)}$ is the 'interior', add to the vertex set $\mathcal{V}^{(0)}$ another set of vertices denoted by $\mathcal{L}$ with $L = |\mathcal{L}|$. Connect $\mathcal{L}$ to a subset of $\mathcal{V}^{(0)}$ such that each $l \in \mathcal{L}$ is connected to a single vertex in $\mathcal{V}^{(0)}$, while a vertex in $\mathcal{V}^{(0)}$ can be connected to several vertices in $\mathcal{L}$. The vertices in $\mathcal{V}^{(0)}$ connected to $\mathcal{L}$ will be referred to as boundary vertices. The $V^{(0)} \times L$ 'wiring' matrix is defined similarly to the previous definitions (see (2.5)):

$$W_{j,l} = \begin{cases} 1 & \text{if} \quad j \in \mathcal{V}^{(0)} \quad \text{is connected to } l \in \mathcal{L} \\ 0 & \text{otherwise.} \end{cases} \tag{2.27}$$

The number of 'dangling bonds' which emanate from the vertex i is $d_i = \sum_{l\in\mathcal{L}} W_{i,l}$ and d_i can take any integer value or 0. The diagonal matrix with elements d_i will be denoted by $\tilde{D}$ and the identities (2.6) hold. The new graph $\tilde{\mathcal{G}}$ is of cardinality $\tilde{V} = V^{(0)} + L$ and it consists of the interior graph with L dangling bonds attached.

The evolution operator for $\tilde{\mathcal{G}}$ can be written in a block form as

$$\tilde{U} = \begin{pmatrix} \Sigma & \Omega & 0 \\ 0 & 0 & \rho^{(\text{out})} \\ \Omega^{\text{tr}} & \rho^{(\text{in})} & 0 \end{pmatrix}, \tag{2.28}$$

which is a $2(E^{(0)} + L) \times 2(E^{(0)} + L)$ unitary matrix arranged in the following way. The first $2E^{(0)}$ rows and columns are labeled by the indices of the directed bonds which belong to the interior graph $\mathcal{G}^{(0)}$. The last $2L$ rows and columns are labeled by the indices of the directed dangling bonds. The first L correspond to *incoming* bonds pointing from $\mathcal{L}$ to $\mathcal{V}^{(0)}$, the other L indices correspond to *outgoing* bonds from $\mathcal{V}^{(0)}$ to $\mathcal{L}$. The $2E^{(0)} \times 2E^{(0)}$ upper left block denoted by Σ is obtained by modifying the evolution operator for the interior graph: the vertex scattering matrices (2.23) are modified by replacing the original valency v_i by the modified valencies $\tilde{v}_i = v_i + d_i$. The rectangular $2E^{(0)} \times L$ matrix Ω consists of elements of the vertex scattering matrices between incoming dangling bonds and directed bonds in $\mathcal{G}^{(0)}$ which emanate from boundary vertices in $\mathcal{V}^{(0)}$. Ω^{tr} provides the scattering matrix elements for the time reversed transitions, from the directed bonds in $\mathcal{G}^{(0)}$ to the outgoing dangling bonds. The $L \times L$ matrix $\rho^{(\mathrm{out})}$ consists of matrix elements from outgoing to incoming dangling bonds which occur at the dangling vertices $\mathcal{L}$. Using (2.23) with $v_l = 1$, we get

$$\rho^{(\mathrm{out})}_{d',d} = -i\frac{1+i(1-\lambda)}{1-i(1-\lambda)}\delta_{o(d'),t(d)}W_{o(d'),t(d)}. \tag{2.29}$$

The $L \times L$ matrix $\rho^{(\mathrm{in})}$ consists of matrix elements from incoming to outgoing dangling bonds which occur at the boundary vertices. They are computed using (2.23) with $\tilde{v}_i = v_i + d_i$. Note the number of dangling bonds connected to the same vertex can exceed 1, and in these cases scattering to other dangling bonds may occur, as long as both the incoming and outgoing bonds are connected to the same vertex of $\mathcal{G}^{(0)}$. The four zero blocks correspond to transitions between bonds which do not follow each other. In particular, the second row of blocks in (2.28) has two zero entries, expressing the fact that incoming dangling bonds cannot follow neither interior bonds nor any incoming dangling bonds.

The unitarity of $\tilde{U}$ ensures the following relations between its components:

$$\begin{aligned}
&(a) \quad \Sigma\Sigma^\dagger + \Omega\Omega^\dagger = I^{(2E^{(0)})} \\
&(b) \quad \rho^{(\mathrm{out})}\rho^{(\mathrm{out})\dagger} = I^{(L)} \\
&(c) \quad \Omega^{\mathrm{tr}}\Omega^{\mathrm{tr}\dagger} + \rho^{(\mathrm{in})}\rho^{(\mathrm{in})\dagger} = I^{(L)} \\
&(d) \quad \Sigma\Omega^{\mathrm{tr}\dagger} + \Omega\rho^{\mathrm{in}\dagger} = 0
\end{aligned} \tag{2.30}$$

The evolution operator $\tilde{U}$ acts in the $2E^{(0)} + 2L$ dimensional space of amplitude vectors. Denote the $2E^{(0)}$ amplitudes which refer to directed bonds in $\mathcal{G}^{(0)}$ by $\mathbf{a}$ and the amplitudes associated with the incoming/outgoing dangling bonds by $\mathbf{b}^{(-/+)}$, respectively. The consistency condition (2.25) which determines the spectrum of $\tilde{\mathcal{G}}$ reads now

$$\begin{pmatrix} \Sigma & \Omega & 0 \\ 0 & 0 & \rho^{(\mathrm{out})} \\ \Omega^{\mathrm{tr}} & \rho^{(\mathrm{in})} & 0 \end{pmatrix}\begin{pmatrix} \mathbf{a} \\ \mathbf{b}^{(-)} \\ \mathbf{b}^{(+)} \end{pmatrix} = \begin{pmatrix} \mathbf{a} \\ \mathbf{b}^{(-)} \\ \mathbf{b}^{(+)} \end{pmatrix}. \tag{2.31}$$

To define a scattering matrix, one has to obliterate the requirement that scattering occurs at the dangling vertices. This is achieved by replacing $\rho^{(\mathrm{out})}$ by a 0 block in $\tilde{U}$. By doing so, the rank of $\tilde{U}$ is reduced by L. Thus, the resulting equations do not determine a spectrum. Rather, they can be solved for every value of λ, and yield a linear relation between the amplitudes of the outgoing and incoming dangling bonds:

$$\begin{aligned}
&\mathbf{b}^{(+)} = (\rho^{(\mathrm{in})} + \Omega^{\mathrm{tr}}(I^{(2E^{(0)})} - \Sigma)^{-1}\Omega)\mathbf{b}^{(-)} \doteq S^{(D)}(\lambda)\mathbf{b}^{(-)} \\
&S^{(D)}(\lambda) = \rho^{(\mathrm{in})}(\lambda) + \Omega^{\mathrm{tr}}(\lambda)(I^{(2E^{(0)})} - \Sigma(\lambda))^{-1}\Omega(\lambda).
\end{aligned} \tag{2.32}$$

The $L \times L$ matrix $S^{(D)}(\lambda)$ (the superscript 'D' stands for dangling) provides the scattering amplitudes between incoming and outgoing dangling bonds. It is meromorphic in λ, has a finite number of poles in the lower half plane, and is unitary on the real λ-axis. These statements can be easily checked by using the explicit form of the matrix elements of $\tilde{U}(\lambda)$ and the identities (2.30). The main advantage of $S^{(D)}(\lambda)$ over the matrix $S^{(\mathrm{Lead})}(\lambda)$ defined in (2.15) is that it depends solely on the properties of the interior graph, and its definition is free from restrictions or special features due to the properties of the leads.

3. The exterior–interior duality

In the present section, two versions of the exterior–interior duality will be formulated corresponding to the two ways by which scattering was defined above. The conversion of a graph into a scattering graph can be done in many ways—the vertices connected to leads or dangling bonds can be chosen arbitrarily. It will be shown here that any scattering matrix can be used to extract information about the spectrum of the 'interior' graph. However, there exists a unique construction which provides the entire spectrum of the interior. Namely, when all the vertices are connected to leads (in the first setting) or dangling bonds (one per vertex, in the second setting): $L = V^{(0)}$ and $W_{i,l} = I^{(V^{(0)})}$. Under these conditions the secular equations

$$\det(I^{(V^{(0)})} - S(\lambda)) = 0, \qquad \text{with} \qquad S = \xi_- S^{(\mathrm{Lead})} \qquad \text{or} \qquad S = S^{(D)} \tag{3.1}$$

provide the complete spectrum of the interior graph with multiplicities.

3.1. The exterior–interior duality for scattering to leads

Equations (2.10) form the basis of this discussion. They can be solved for any value of λ and they provide the building blocks for constructing the scattering matrix $S^{(\mathrm{Lead})}(\lambda)$. Consider the subset (2.11) of these equations. If for a given λ the corresponding vectors $\mathbf{f}^{(V^{(0)})}$ and $\mathbf{f}_1^{(L)}$ which solve (2.10) also satisfy

$$\tilde{D}\mathbf{f}^{(V^{(0)})} = W\mathbf{f}_1^{(L)} \qquad \text{and} \qquad \mathbf{f}^{(V^{(0)})} \neq 0, \tag{3.2}$$

then $\mathbf{f}^{(V^{(0)})}$ is an eigenvector of the interior graph Laplacian with an eigenvalue λ. If the leads are not connected to all the vertices, that is $L < V^{(0)}$, the kernel of $\tilde{D}$ is not empty. Hence, it is possible that the condition $\tilde{D}\mathbf{f}^{(V^{(0)})} = W\mathbf{f}_1^{(L)}$ is satisfied trivially by $\mathbf{f}^{(V^{(0)})}$ which is in the right kernel of $\tilde{D}$, and $\mathbf{f}_1^{(L)} = 0$. Such cases have to be excluded from the following derivation and therefore, in general, the equation to be derived below provides only a sufficient spectral condition. However, if one connects every vertex to a lead, this problem does not arise and a proper secular equation can be derived, as will be shown in the following.

As long as λ is away from the singularities of $R^{(0)}(\lambda)$, one can proceed and obtain from $\tilde{D}\mathbf{f}^{(V^{(0)})} = W\mathbf{f}_1^{(L)}$

$$(w\tilde{D}R^{(0)} - I^{(V^{(0)})})W\mathbf{f}_1^{(L)} = 0. \tag{3.3}$$

Using (2.6) one finds that (3.3) is equivalent to requiring a non trivial solution for the equation

$$W(wW^{\top}R^{(0)}(\lambda)W - I^{(L)})\mathbf{f}_1^{(L)} = 0. \tag{3.4}$$

Thus, it is sufficient but not necessary for λ to be in the spectrum if it is a zero of the function

$$z_R(\lambda) = \det(wW^{\top}R^{(0)}(\lambda)W - I^{(L)}). \tag{3.5}$$

However, when all the vertices are connected to leads, $W = I^{(L)} = I^{(V^{(0)})}$, $\tilde{D} = I^{(V^{(0)})}$ and $R^{(0)}(\lambda) = (\Delta^{(0)} - (\lambda - w)I^{(V^{(0)})})^{-1}$. Substituting into (3.5), one gets

$$z_R(\lambda) = (-1)^{V^{(0)}} \frac{\det(\Delta^{(0)} - \lambda I^{(V^{(0)})})}{\det(\Delta^{(0)} - (\lambda - w)I^{(V^{(0)})})}. \tag{3.6}$$

At this point the importance of the parameter w becomes clear: the spectrum of the Laplacian coincides with the zeros of $z_R(\lambda)$ only if there are no accidental overlaps with the poles of $R^{(0)}(\lambda)$. Thus, one should choose w so that the spectrum of $(\Delta^{(0)} + wI^{(V^{(0)})})$ exceeds the maximum of the spectrum of $\Delta^{(0)}$. For v regular graphs taking $w > 2v$ is sufficient. Using (2.15) one writes

$$wW^{\top}R^{(0)}(\lambda)W = (I^{(L)} + S^{(\mathrm{Lead})}(\lambda))^{-1}(\xi_+ I^{(L)} + \xi_- S^{(\mathrm{Lead})}(\lambda)). \tag{3.7}$$

Substituting into (3.5) yields the secular equation

$$z_{Ld}(\lambda) = \det(I^{(L)} - s_l^{-1}(\lambda)S^{(\mathrm{Lead})}(\lambda)) = \det(I^{(L)} - \xi_- S^{(\mathrm{Lead})}(\lambda)) = 0. \tag{3.8}$$

This is the desired result, since it determines the spectrum of the interior graph in terms of the scattering matrix $S^{(\mathrm{Lead})}(\lambda)$ and the free lead scattering matrix $s_l(\lambda)$ (2.4). It is analogous both in form and in content to the exterior–interior secular equation which was introduced in the introduction (1.1).

3.2. Exterior–interior duality for scattering to dangling bonds

The scattering matrix $S^{(D)}(\lambda)$ will be used to compute the spectrum of the interior graph $\mathcal{G}^{(0)}$. For this purpose, consider the action of the Laplacian of the extended graph $\tilde{\mathcal{G}}$. Denote by f_j the components of an eigenvector on a vertex $j \in \mathcal{V}^{(0)}$, and by g_k the component of the same eigenvector on a dangling vertex $k \in \mathcal{L}$. Then

$$\forall i : -\sum_{j \in \mathcal{G}^{(0)}} C_{i,j} f_j - \sum_{l=1}^{L} W_{i,l} g_l + (v_i + d_i) f_i = \lambda f_i. \tag{3.9}$$

λ is an eigenvalue of the interior graph, corresponding to an eigenvector $\mathbf{f} = (f_1, \ldots, f_{V^{(0)}})$, if for every $i \in \mathcal{V}^{(0)}$

$$\sum_{l=1}^{L} W_{i,l} g_l = d_i f_i, \tag{3.10}$$

and $\mathbf{f} \neq 0$. Consider a single boundary vertex j with $d_j \neq 0$. Expressing the eigenfunction on the dangling bonds in terms of the incoming and outgoing amplitudes (2.18):

$$\begin{aligned} &\forall k : W_{j,k} = 1, \qquad f_j = b_k^{(-)} \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} + b_k^{(+)} \mathrm{e}^{+\mathrm{i}\frac{\pi}{4}}, \\ &g_k = b_k^{(-)} \mathrm{e}^{+\mathrm{i}\frac{\pi}{4}} + b_k^{(+)} \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}. \end{aligned} \tag{3.11}$$

The upper line above imposes $d_j - 1$ linear relations between the amplitudes. Substituting (3.11) into (3.10) results in one more linear relation. Thus, one gets for each j exactly d_j linear relations between the incoming and outgoing amplitudes on the dangling bonds connected to the interior vertex j. Solving them for each j separately and combining the individual relationships gives

$$\mathbf{b}^{(+)} = S^{(0)} \mathbf{b}^{(-)}; \qquad S^{(0)}_{k,l} = \sum_{j \in \mathcal{V}^{(0)}} W_{j,k} W_{j,l} \left(\frac{1-i}{d_j} + i\delta_{k,l} \right). \tag{3.12}$$

This λ independent matrix of dimension $L \times L$ is bloc diagonal, with blocs of dimensions d_j. It is easy to check that each block (and hence the entire matrix) is unitary and symmetric. When only one dangling bond is connected to a vertex, $d_j = 1$ and the corresponding $S^{(0)}_{k,k} = 1$.

The requirement (3.12) has to be combined now with the relation (2.32) which is valid for all λ. This implies that λ is an eigenvalue of the Laplacian on the interior graph if there exists a non trivial solution for the equation

$$\mathbf{b}^{(+)} = S^{(D)}(\lambda) (S^{(0)})^{\dagger} \mathbf{b}^{(+)}, \tag{3.13}$$

in other words, if λ is a zero of the secular function:

$$z_D(\lambda) = \det(I^{(L)} - S^{(D)}(\lambda)(S^{(0)})^{\dagger}). \tag{3.14}$$

The derivation above follows from the requirement that (3.10) is satisfied for $\mathbf{f} \neq 0$. This can be guaranteed only when a single dangling bond is connected to each vertex. In this case, $S^{(0)} = I^{(V_0)}$ and the secular equation (3.14) expresses the exterior–interior duality in the present setting.

4. Examples and applications

In this section a few examples and applications which will illustrate the exterior–interior duality will be discussed.

4.1. Scattering on a single lead connected to a graph

Consider a single lead connected to one of the vertices of $\mathcal{G}^{(0)}$ which is denoted by $i = 1$. Following (2.12), (2.15),

$$R_{1,1}(\lambda) \doteq W^{\top} R(\lambda) W = \frac{G_{1,1}(\lambda)}{1 + wG_{1,1}(\lambda)},$$
$$G_{1,1}(\lambda) \doteq ((\Delta^{(0)} - \lambda I^{(0)})^{-1})_{1,1} = \sum_{r=1}^{V^{(0)}} \frac{\left|f_1^{(r)}\right|^2}{\lambda_r - \lambda}. \tag{4.1}$$

Clearly $G(\lambda)$ is the Green's function (resolvent) of the graph Laplacian. The one-dimensional scattering matrix reads

$$S^{(\mathrm{Lead})}(\lambda) = -\frac{wR_{1,1} - \xi_+}{wR_{1,1} - \xi_-}, \tag{4.2}$$

and the secular equation:

$$z_{Ld}(\lambda) = -\frac{1 + \xi_-}{wR_{1,1}(\lambda) - \xi_-}\frac{1}{1 + wG_{1,1}(\lambda)}. \tag{4.3}$$

This function has no poles for λ in the conduction band, and vanishes at the spectrum of $\Delta^{(0)}$(= the poles of the Green's function), provided that the corresponding residues do not vanish. This cannot be guaranteed since the component of an eigenvector can vanish on any number of vertices. Such eventualities cannot be excluded and therefore the proper secular equation has to be constructed by connecting all the vertices to leads.

4.2. Composition

Consider the two graphs $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$ with vertex sets $\mathcal{V}^{(i)}$ of cardinality $V^{(i)}$ and connectivity matrices $C^{(i)}$, $i = 1, 2$. Connect the two graphs by an arbitrary number of leads $(j, i), i \in \mathcal{V}^{(1)}, j \in \mathcal{V}^{(2)}$ but avoid parallel edges. Denote the number of connecting edges by L. The connection between the two graphs is given by the matrix:

$$\tilde{C}_{i,j} = \begin{cases} 1 & \text{if} \quad i \in \mathcal{V}^{(1)}, \qquad j \in \mathcal{V}^{(2)} \text{ are connected.} \\ 0 & \text{otherwise.} \end{cases} \tag{4.4}$$

The purpose is to obtain a secular equation for the composite graph $G^{(0)} = \mathcal{G}^{(1)} \cup \mathcal{G}^{(2)}$ with the connectivity matrix

$$\tilde{C}^{(0)} = \begin{pmatrix} C^{(1)} & \tilde{C} \\ \tilde{C}^{\top} & C^{(2)} \end{pmatrix}. \tag{4.5}$$

Consider the graph $\mathcal{G}^{(1)}$ say, and regard for the moments the bonds which connect it to $\mathcal{G}^{(2)}$ as dangling bonds. The corresponding wiring matrix is $\tilde{C}$, and one can write an L dimensional scattering matrix $S^{(1)}(\lambda)$ for this system by using the 'dangling bond' construction. Similarly, the scattering matrix $S^{(2)}(\lambda)$ which is also L dimensional can be written for $\mathcal{G}^{(2)}$. Denote by $\mathbf{a}$ and $\mathbf{b}$ the L dimensional vectors of amplitudes for incoming waves to $\mathcal{V}^{(1)}$. The consistency requirement of section (2.2) requires that

$$\mathbf{b} = S^{(1)}(\lambda)\mathbf{a}; \qquad \mathbf{a} = S^{(2)}(\lambda)\mathbf{b} \Rightarrow \mathbf{b} = S^{(1)}(\lambda)S^{(2)}(\lambda)\mathbf{b}, \tag{4.6}$$

so that a sufficient condition for λ to be in the spectrum of $\mathcal{G}^{(0)}$ is that it is a solution of the equation

$$\det(I^{(L)} - S^{(1)}(\lambda)S^{(2)}(\lambda)) = 0. \tag{4.7}$$

This is the analog of the example given in the introduction of the exterior–interior duality in $\mathbb{R}^2$.

As a simple corollary of this result, one can study the effect of adding a single vertex m of valency v_m to a given graph of cardinality V. Assuming that the new vertex is connected to the vertices $1, \ldots, v_m$, one computes the corresponding $v_m \times v_m$ scattering matrix $S^{(V)}$ from the original graph. $S^{(V)}$ plays the role of $S^{(1)}(\lambda)$ above. For $S^{(2)}(\lambda)$ one uses the vertex scattering matrix $\sigma^{(m)}$ (2.23). The resulting secular equation reads now

$$\det(I^{(v_{V+1})} - S^{(V)}(\lambda)\sigma^{(m)}(\lambda)) = 0. \tag{4.8}$$

The same problem can be addressed in a different way. With the same construction, one can compute the $R(\lambda)$ matrix (with $w = 1$). Connecting together all the v_m dangling bonds to a single vertex and setting the value of the wavefunction to f_m at the vertex m, one finds for the values of the function on the m connected vertices:

$$f_j = f_m \sum_{k=1}^{v_m} R(\lambda)_{j,k}. \tag{4.9}$$

At the same time, to be an eigenvalue **f** must satisfy

$$-\sum_{j=1}^{v_m} f_j + v_m f_m = \lambda f_m. \tag{4.10}$$

Thus, the secular equation for the spectrum of the enlarged graph reads

$$\lambda = v_m - \sum_{k,j=1}^{v_m} R(\lambda)_{j,k}. \tag{4.11}$$

It is hoped that the few simple illustrations given above illustrate the advantages and potential applications of the exterior–interior duality in the present context.

Acknowledgments

I would like to thank Rami Band and Amit Godel for critical comments and suggestions, Dr Iwao Sato for carefully reading the manuscript, Yehonatan Elon and Idan Oren for helpful discussions and Professor Marco Marletta for his illuminating comments on the Dirichlet to Neumann map. This work was supported by the Minerva Center for nonlinear Physics, the Einstein (Minerva) Center at the Weizmann Institute and the Wales Institute of Mathematical and Computational Sciences (WIMCS). Grants from GIF (grant I-808-228.14/2003) and BSF (grant 2006065) are acknowledged.

References

[1] Doron E and Smilansky U 1992 Chaotic spectroscopy *Phys. Rev. Lett.* **68** 1255–58

[2] Doron E and Smilansky U 1992 Semiclassical quantization of chaotic billiards—a scattering theory approach *Nonlinearity* **5** 1055–84

[3] Dietz B and Smilansky U 1993 A scattering approach to the quantization of billiards—the inside–outside duality *Chaos* **3** 581–90

[4] Smilansky U 1995 Semiclassical Quantization of Chaotic Billiards—A Scattering Approach *The Les Houches Summer School on Mesoscopic Quantum Physics* ed E Akkermans, G Montambaux and J L Pichard (Amsterdam: Elsevier)

[5] Eckmann J P and Pillet C-A 1995 Spectral duality for planar billiards *Commun. Math. Phys.* **170** 283–313

[6] Eckmann J P and Pillet C-A 1995 Scattering phases and density of states for exterior domains *Ann. Inst. Henri Poincaré* **62** 383–99

[7] Dietz B, Eckmann J P, Pillet C-A, Smilansky U and Ussishkin I 1995 Inside–outside duality for planar billiards—a numerical study *Phys. Rev.* E **51** 4222–31

[8] Schanz H and Smilansky U 1995 Quantization of Sinai's billiard—a scattering approach *Chaos Solitons Fractals* **5** 1289–309

[9] Rouvinez C and Smilansky U 1994 A scattering approach to the quantization of Hamiltonians in 2 dimensions—application to the Wedge billiard *J. Phys.* A **28** 77

[10] Bruening J and Geyler V A 2003 Scattering on compact manifolds with infinitely thin horns *Doklady RAN* **389** 310–3 (Russian)
Bruening J and Geyler V A 2003 *J. Math. Phys.* **44** 371–405

[11] Kottos T and Smilansky U 1999 Periodic orbit theory and spectral statistics for quantum graphs *Ann. Phys.* **274** 76–124

[12] Kottos T and Smilansky U 2003 Quantum graphs: a simple model for chaotic scattering *J. Phys. A: Math. Gen.* **36** 3501–24

[13] Fedorov S and Pavlov B 2006 Discrete wave scattering on star-graph *J. Phys. A: Math. Gen.* **39** 2657–71

[14] Smilansky U 2007 Quantum chaos on discrete graphs *J. Phys. A: Math. Theor.* **40** F621–30

[15] Mizuno H and Sato I 2008 The scattering matrix of a graph *Electron. J. Comb.* **15** R96

[16] Curtis E B and Morrow J A 1991 The Dirichlet to Neumann map for a resistor network *SIAM J. Appl. Math.* **51** 1011–29

[17] Novikov S 1999 Schrödinger operators on graphs and symplectic geometry *Field Inst. Commun.* **24** 397–413

[18] Cattaneo C 1997 The Spectrum of the continuous Laplacian on a graph *Mh. Math.* **124** 215–35

[19] Exner P 1997 A duality between Schrödinger operators on graphs and certain Jacobi matrices *Ann. Inst. Henri Poincare* **66** 359–71

[20] Kuchment P 2004 Quantum graphs: I. Some basic structures *Waves Random Media* **14** S107–28