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Hermitian symplectic geometry and the factorization of the scattering matrix on graphs

M Harmer

Department of Mathematics, University of Auckland, Private Bag 92019, Auckland, New Zealand

E-mail: harmer@math.auckland.ac.nz

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Abstract. Hermitian symplectic spaces provide a natural framework for the extension theory of symmetric operators. Here we show that Hermitian symplectic spaces may also be used to describe the solution to the factorization problem for the scattering matrix on a graph, i.e. we derive a formula for the scattering matrix of a graph in terms of the scattering matrices of its subgraphs. The solution of this problem is shown to be given by the intersection of a Lagrange plane and a coisotropic subspace which, in an appropriate Hermitian symplectic space, forms a new Lagrange plane. The scattering matrix is given by a distinguished basis to the Lagrange plane.

Using our construction we are also able to give a simple proof of the unitarity of the scattering matrix as well as provide a characterization of the discrete eigenvalues embedded in the continuous spectrum.

1. Introduction

As is well known, Hermitian symplectic spaces provide a natural framework for the description of the extensions of symmetric operators [1, 4, 6]. Here we discuss another possible application of Hermitian symplectic spaces, namely to the problem of the factorization of the scattering matrix for the Schrödinger operator on a graph. Using the fact that the Wronskian is a Hermitian symplectic form, we construct a Hermitian symplectic space of solutions on the rays of the graph. We use the term asymptotic Hermitian symplectic space in analogy with the asymptotic symplectic space introduced by Novikov [5] in the case of the discrete Schrödinger operator on a graph (in [5] the Wronskian is defined so that it is a symplectic form). The value of this construction lies in the fact that the generalized eigenspace of a self-adjoint Schrödinger operator forms a Lagrange plane in this space. This allows us to easily prove the unitarity of the scattering matrix on the real axis in the spectral plane. Furthermore, we show that the scattering matrix plays the role of the unitary matrix which parametrizes Lagrange planes [1].

We also use this construction to consider the factorization problem for graphs; that is, we find a composition rule whereby the scattering matrix of a graph can be written in terms of the scattering matrices of its subgraphs. This has already been considered in two papers by Kostrykin and Schrader [3, 4] in the case of the Laplacian on a graph. We present a substantially different approach, based on the properties of the asymptotic Hermitian symplectic space, to what is essentially the same problem, the factorization of the Schrödinger operator on graphs. Using the asymptotic Hermitian symplectic space we can express in a simple way the generalized eigenspace of a graph in terms of the generalized eigenspaces of the subgraphs. As the scattering matrix is defined by a distinguished basis for these eigenspaces, this in effect

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provides us with a composition rule for the scattering matrix. In practice, however, we need some linear algebra (simplified by our description of the generalized eigenspace) to write the composition rule explicitly in terms of the scattering matrices.

Both our approach, and the approach used by Kostrykin and Schrader, give the same answer. However, we believe that our approach is sufficiently novel to provide some new insights. Our description of the composition rule also reveals a characterization of the discrete eigenvalues embedded in the continuous spectrum of the non-compact graph.

2. The Hermitian symplectic space of asymptotic solutions

Here we study a connected non-compact graph, Γ. We assume that Γ consists of a compact part, Γ_c, composed of p finite interior edges. Attached to arbitrary vertices of the compact part are n semi-infinite rays. Both p and n are finite. Functions on the graph are represented by elements of the Hilbert space

$$H(\Gamma) = \oplus_{i=1}^{n} L^2([0,\infty)) \oplus_{j=1}^{p} L^2([0,a_j])$$

where the a_j are the lengths of the interior edges. The elements of $H(\Gamma)$ are $(n+p)$-dimensional vector functions and the inner product on $H(\Gamma)$ is

$$(\phi,\psi)_\Gamma = \sum_{i=1}^{n} (\phi_i,\psi_i)_{L^2([0,\infty))} + \sum_{j=1}^{p} (\phi_{n+j},\psi_{n+j})_{L^2([0,a_j])}$$

where ϕ_i are the components of $\phi \in H(\Gamma)$.

Let us consider the symmetric Schrödinger operator, $\mathcal{L}_0$ in $H(\Gamma)$

$$\mathcal{L}_0\psi_i \equiv -\frac{\mathrm{d}^2\psi_i}{\mathrm{d}x_i^2} + q_i\psi_i \qquad \text{for} \quad i = 1,\ldots,n+p$$

with domain consisting of the smooth functions with compact support in the open intervals

$$D(\mathcal{L}_0) = \oplus_{i=1}^{n} C_0^\infty([0,\infty)) \oplus_{j=1}^{p} C_0^\infty([0,a_j]).$$

The potentials q_i are supposed to be continuous real-valued functions which are integrable with a finite first moment,

$$\int_{\Gamma_i} (1+x)|q_i(x)|\,\mathrm{d}x < \infty \tag{1}$$

where $\Gamma_i = [0,\infty]$ or $[0,a_i]$. It is easy to see that the deficiency indices of $\mathcal{L}_0$ are $(n+2p, n+2p)$. Consequently, we may parametrize the self-adjoint extensions of $\mathcal{L}_0$ by unitary matrices $\mathsf{U}(n+2p)$ or, for separated boundary conditions, by $\mathsf{U}(d(1)) \oplus \cdots \oplus \mathsf{U}(d(m))$ where $d(i)$ is the degree of the ith vertex of Γ.

We construct a Hermitian symplectic space the elements of which are solutions on the rays of the graph. This construction follows an analogous construction by Novikov [5] for the discrete Schrödinger operator on graphs. Let ψ' denote the derivative of ψ with respect to x.

Definition 1. *The 2-form $\langle\cdot,\cdot\rangle$, defined on functions on the* rays *of the graph*

$$\langle\phi,\psi\rangle \equiv \sum_{i=1}^{n} \left[\bar{\phi}_i\psi_i' - \bar{\phi}_i'\psi_i\right](x_i) \qquad x_i \in [0,\infty) \tag{2}$$

is a Hermitian symplectic form.

As it stands this form is not well defined, it depends on the points x_i chosen on each of the rays. If, however, we consider the set of generalized eigenfunctions of $\mathcal{L}_0^\star$ on the rays for spectral parameter λ,

$$H_{2n}(\Gamma, \mathcal{L}_0, \lambda) = \left\{\phi \in \oplus_{i=1}^n C^2_{\mathrm{loc}}([0,\infty));\; -\frac{\mathrm{d}^2\phi_i}{\mathrm{d}x_i^2} + q_i\phi_i = \lambda\psi_i\right\}$$

we see that the form is independent of x_i—due to the constancy of the Wronskian. Obviously $H_{2n}(\Gamma, \mathcal{L}_0, \lambda)$ is a $2n$-dimensional vector space. We note, in particular, that the functions from $H_{2n}(\Gamma, \mathcal{L}_0, \lambda)$ do not obey any specific boundary conditions at the vertices. Below we may assume that the graph, Γ, and the potentials, $\mathcal{L}_0$, are given and simply write $H_{2n}(\lambda)$ or H_{2n}.

Proposition 1. *The vector space of generalized eigenfunctions on the rays $H_{2n}(\Gamma, \mathcal{L}_0, \lambda)$ for real λ equipped with the Hermitian symplectic form (2) is a Hermitian symplectic space, called the asymptotic Hermitian symplectic space.*

To prove this statement we only need to show that the form is non-degenerate [1], which is easy to see if we consider the basis of standard solutions $\{\theta_i, \phi_i\}^n$, i.e. the solutions which satisfy the boundary conditions

$$\theta_i\big|_0 = 1 \qquad \theta_{i,x}\big|_0 = 0$$
$$\phi_i\big|_0 = 0 \qquad \phi_{i,x}\big|_0 = 1$$

on ray i and are zero on the other rays. Furthermore, we note that this basis is canonical,

$$\langle\theta_i, \phi_j\rangle = \delta_{ij} = -\langle\phi_i, \theta_j\rangle$$
$$\langle\theta_i, \theta_j\rangle = 0 = \langle\phi_i, \phi_j\rangle$$

so H_{2n} is a canonical Hermitian symplectic space [1] (for brevity we just use the term Hermitian symplectic space here).

More interesting are bases constructed from the Jost solutions. We denote by $f_{\pm,j} \in H_{2n}(\lambda)$ the elements which are zero on all the rays except the jth one where they coincide with the Jost solution with asymptotic behaviour

$$f_{\pm,j} \simeq \mathrm{e}^{\pm \mathrm{i}kx_j}$$

for x large and where $\lambda = k^2$. The fact that our 2-form is defined using complex conjugation† complicates the evaluation of it on the Jost solutions. We have

$$\begin{aligned}\langle f_{+,i}, f_{+,j}\rangle &= 2\mathrm{i}k\delta_{ij} = -\langle f_{-,i}, f_{-,j}\rangle \\ \langle f_{+,i}, f_{-,j}\rangle &= 0 = \langle f_{-,i}, f_{+,j}\rangle\end{aligned} \tag{3}$$

but only for $\lambda > 0$ or $k \in \mathbb{R}$.

We also construct a canonical basis using the Jost solutions; consider

$$\psi_{0,j} = \frac{f_{+,j} + f_{-,j}}{2} \qquad \chi_{0,j} = \frac{f_{+,j} - f_{-,j}}{2ik}$$

where $j = 1, \ldots, n$. It is easy to see that this is a canonical basis, for all real λ (unlike the relations for the Jost solutions).

Now let us suppose that we have defined $\mathcal{L}$, a self-adjoint extension of $\mathcal{L}_0$, on the graph. The generalized eigenfunctions of $\mathcal{L}$ are (not necessarily square-integrable) solutions of the eigenvalue equation $\mathcal{L}\phi = \lambda\phi$. We emphasize that such a ϕ is defined on the whole of Γ

† The operation $f^\dagger(k) = \bar{f}(\bar{k})$ appears to be more natural in the definition of the Wronskian [1, 2]. As we will mainly be considering $\lambda > 0$ or $k \in \mathbb{R}$, we will not use this here.

(not just the rays) and obeys some self-adjoint boundary conditions at the nodes of Γ. By considering the restriction to the rays of the graph, a generalized eigenfunction of $\mathcal{L}$ may be thought of as an element of $H_{2n}(\lambda)$.

Lemma 1. *Given a self-adjoint extension $\mathcal{L}$, the generalized eigenspace of $\mathcal{L}$ at some real λ forms an isotropic subspace in $H_{2n}(\lambda)$.*

Proof. We formally consider the boundary form of generalized eigenfunctions ϕ and ψ

$$(\mathcal{L}\phi, \psi)_\Gamma - (\phi, \mathcal{L}\psi)_\Gamma = \sum_{i=1}^{n} \left[\bar{\phi}_i \psi_i' - \bar{\phi}_i' \psi_i\right]\big|_0 - \sum_{j=1}^{p} \left[\bar{\phi}_{n+j} \psi_{n+j}' - \bar{\phi}_{n+j}' \psi_{n+j}\right]\big|_0^{a_j}. \tag{4}$$

The self-adjoint boundary conditions are described by the vanishing of this form. Furthermore, the second sum on the right-hand side vanishes by the constancy of the Wronskian on the edges so we are left with

$$\sum_{i=1}^{n} \left[\bar{\phi}_i \psi_i' - \bar{\phi}_i' \psi_i\right]\big|_0 = \langle \phi, \psi \rangle = 0. \tag{5}$$

This completes the proof. □

The analogous statement for the discrete operator is proved in theorem 3 of [5]. In fact, Novikov shows in this theorem that the eigenspaces form Lagrange planes for any complex value of λ. In our case, the fact that the generalized eigenspaces form Lagrange planes for any real λ is a simple corollary of the following lemma:

Lemma 2. *Given a self-adjoint extension $\mathcal{L}$, the vector space of generalized eigenfunctions of $\mathcal{L}$ at real eigenvalue λ and with support on the rays of the graph is n dimensional.*

Proof. Let us consider the boundary form on Γ, equation (4). We know that this defines a non-degenerate Hermitian symplectic form in the $2(n+2p)$-dimensional space of boundary values and hence a Hermitian symplectic space which we denote, in the proof of this lemma, as $H_{2(n+2p)}$ [1, 4]—we emphasize that we are considering the space of boundary values, not the asymptotic Hermitian symplectic space defined above. It is clear that the self-adjoint boundary conditions are associated with $(n+2p)$-dimensional Lagrange planes in this space. Let us denote by P the $(n+2p)$-dimensional Lagrange plane in $H_{2(n+2p)}$ associated with our chosen self-adjoint $\mathcal{L}$.

Now let us consider an arbitrary interior edge indexed by i of length a. This edge is identified with the interval $[0, a]$. We say that a boundary condition $\psi \in H_{2(n+2p)}$ matches on this edge if

$$\begin{pmatrix} \psi_i|_a \\ \psi_i'|_a \end{pmatrix} = \begin{pmatrix} \theta_i|_a & \phi_i|_a \\ \theta_i'|_a & \phi_i'|_a \end{pmatrix} \begin{pmatrix} \psi_i|_0 \\ \psi_i'|_0 \end{pmatrix}.$$

Here $\psi_i|_0$ and $\psi_i'|_0$ are the components of $\psi \in H_{2(n+2p)}$ corresponding to one endpoint of edge i, $\psi_i|_a$ and $\psi_i'|_a$ are the components of $\psi \in H_{2(n+2p)}$ corresponding to the other endpoint of edge i, $\phi_i(\lambda)$ and $\theta_i(\lambda)$ are the standard solutions on edge i and λ is fixed in the hypothesis.

It is clear that the boundary conditions on edge i match iff there is a solution of $(\mathcal{L}-\lambda)f = 0$ on i, namely

$$f(x, \lambda) = \psi_i|_0 \theta_i(x, \lambda) + \psi_i'|_0 \phi_i(x, \lambda)$$

whose boundary values at the ends of edge i are the same as the relevant components of $\psi \in H_{2(n+2p)}$.

The set of boundary conditions matching on all p interior edges of Γ and with support only on these interior edges form an isotropic subspace in $H_{2(n+2p)}$ which we denote by N. This fact is equivalent to the fact that the Wronskian of two generalized eigenfunctions is constant,

$$\langle \phi, \psi \rangle = \sum_{j=1}^{p} \left[\bar{\phi}_{n+j} \psi'_{n+j} - \bar{\phi}'_{n+j} \psi_{n+j} \right] \Big|_0^{a_j} = 0.$$

Here the 2-form is the Hermitian symplectic form in the space of *boundary conditions* [4]. The dimension of N is $2p$—there are two independent solutions for each edge. On the other hand, $N^\perp$ consists of the set of boundary conditions which match on each of the interior edges but which may be arbitrarily prescribed on the rays.

First, let us consider $P \cap N^\perp$. These are boundary conditions which 'match' ($N^\perp$), as well as satisfy the self-adjoint boundary conditions associated with $\mathcal{L}(P)$. Consequently, each element of $P \cap N^\perp$ can be identified with a generalized eigenfunction of $\mathcal{L}$ on the graph Γ. However, these boundary conditions may also describe solutions with support confined to the interior edges of the graph, and we are only interested in solutions with support on the rays.

To pick only those solutions with support on the rays we should consider $N^\perp/N$. By lemma 5 (in the appendix) this is a Hermitian symplectic space of dimension $2n$ and may be identified with the set of boundary conditions with support on the rays. Consequently, if we consider the projection of $P \cap N^\perp$ into $N^\perp/N$ we get only those eigenfunctions with support on the rays and we know from theorem 2 (in the appendix) that this space has dimension n.

□

This, along with the fact that Lagrange planes are maximal isotropic subspaces, gives us the desired result.

Corollary 1. *Given the self-adjoint extension $\mathcal{L}$, the space of generalized eigenfunctions of $\mathcal{L}$ at real eigenvalue λ and with support on the rays of the graph forms a Lagrange plane in $H_{2n}(\lambda)$.*

Following Novikov we have an immediate application of these observations in the following proof of the unitarity of the scattering matrix for $\lambda > 0$ or real k.

Suppose that we have an n-dimensional basis for the space of generalized eigenfunctions of the form

$$\psi_i = f_{-,i} + \sum_j S_{ij} f_{+,j}.$$

We call S_{ij} the scattering matrix. Then since the generalized eigenspace forms an isotropic subspace

$$0 = \langle \psi_i, \psi_j \rangle = \left\langle f_{-,i} + \sum_l S_{il} f_{+,l},\ f_{-,j} + \sum_m S_{jm} f_{+,m} \right\rangle = 2\mathrm{i}k \left[\sum_{l,m} \bar{S}_{il} S_{jm} \delta_{lm} - \delta_{ij} \right]$$

where we have used equation (3) for real k. Hence, the scattering matrix is unitary for $\lambda > 0$ or real k.

The original idea for this proof can be found in corollary 2 of [5] where the author uses it to prove the *symmetry* of the scattering matrix (this is due to the fact that Novikov uses *symplectic* geometry).

Similarly, we can find a condition for the symmetry of the scattering matrix. In the paper by Kostrykin and Schrader [4] the authors show that if the boundary conditions of an operator can be expressed using real matrices then the scattering matrix is symmetric. In [1] we show that all self-adjoint boundary conditions can be parametrized by a unitary matrix U, the condition of Kostrykin and Schrader is equivalent to the symmetry $U = U^T$ of U, which may also be written as the condition $\phi \in D(\mathcal{L}) \Leftrightarrow \bar{\phi} \in D(\mathcal{L})$. Consequently, the form $\langle\bar{\psi}_i, \psi_j\rangle$ is also zero,

$$0 = \langle\bar{\psi}_i, \psi_j\rangle = \left\langle f_{+,i} + \sum_l \bar{S}_{il} f_{-,l}, f_{-,j} + \sum_m S_{jm} f_{+,m}\right\rangle = 2\mathrm{i}k\left[\sum_m S_{jm}\delta_{im} - \sum_l S_{il}\delta_{lj}\right]$$

showing that the scattering matrix is symmetric. This is analogous to Novikov's proof of the unitarity of the scattering matrix.

In the following sections we develop some new ideas based on Novikov's construction. In particular, we show a link between the scattering matrix and the Lagrange planes, and an application to the problem of the factorization of the scattering matrix.

3. The scattering matrix as a parameter of the Lagrange planes

We emphasize that for the remainder of this paper we will assume that $\lambda > 0$ or $k \in \mathbb{R}_0 \equiv \mathbb{R}/\{0\}$.

We have shown that the space of generalized eigenfunctions corresponds to a Lagrange plane, and that the Lagrange planes are parametrized by a unitary matrix [1]. It is not difficult to see that in the case of the asymptotic Hermitian symplectic space this unitary matrix is, in fact, the scattering matrix—for $\lambda > 0$. First, we need some appropriate notation; we define a new Hermitian symplectic form simply by dividing the old form by k,

$$\langle\phi, \psi\rangle \equiv \frac{1}{k}\sum_{i=1}^{n}\left[\bar{\phi}_i\psi_i' - \bar{\phi}_i'\psi_i\right](x_i) \qquad x_i \in [0, \infty).$$

This is a Hermitian symplectic form as long as k is real and non-zero. In terms of this new form the Jost solutions satisfy

$$\begin{aligned}\langle f_{+,i}, f_{+,j}\rangle &= 2\mathrm{i}\delta_{ij} = -\langle f_{-,i}, f_{-,j}\rangle \\ \langle f_{+,i}, f_{-,j}\rangle &= 0 = \langle f_{-,i}, f_{+,j}\rangle.\end{aligned} \tag{6}$$

However, the canonical basis $\psi_{0,i}$, $\chi_{0,i}$ defined above is no longer canonical. Instead we define the new canonical basis

$$\psi_{0,j} = \frac{f_{+,j} + f_{-,j}}{2} \qquad \chi_{0,j} = \frac{f_{+,j} - f_{-,j}}{2\mathrm{i}} \tag{7}$$

where $j = 1, \ldots, n$. We also use the notation

$$\xi_{0,j} = \psi_{0,j} \qquad \xi_{0,j+n} = \chi_{0,j}$$

where $j = 1, \ldots, n$ to denote these basis vectors. Let us denote by $\Pi_{0,n}$ the Lagrange plane spanned by the first n vectors of this basis. The precise relationship between the unitary matrices and the Lagrange planes is given in corollary 2 of [1]. Here this result becomes:

Theorem 1. *The Lagrange plane $\Pi_{0,n}$ can be made to coincide with Π_n, the Lagrange plane corresponding to the generalized eigenspace of a self-adjoint $\mathcal{L}$, by means of the Hermitian symplectic transformation of the form*

$$g = W^\star\hat{g}W = W^\star\begin{pmatrix} S & 0 \\ 0 & \mathbb{I}\end{pmatrix}W = \frac{1}{2}\begin{pmatrix} S+\mathbb{I} & \mathrm{i}(S-\mathbb{I}) \\ -\mathrm{i}(S-\mathbb{I}) & S+\mathbb{I}\end{pmatrix} \tag{8}$$

where S is the scattering matrix.

In particular, the canonical basis $\{\xi_{0,i}\}_{i=1}^{2n}$ *of equation (7) is taken into a canonical basis* $\{\xi_i\}_{i=1}^{2n}$

$$\xi_i = \sum_j^{2n} g_{ij}\xi_{0,j}$$

where the first n basis elements are the scattering wave solutions of $\mathcal{L}$ *and so form a basis for* Π_n.

Proof. We substitute for g and $\xi_{0,i}$ to obtain for $i = 1, \ldots, n$

$$\begin{aligned}\xi_i &= \frac{1}{2}\left[\sum_j^n (S + \mathbb{I})_{ij}\left(\frac{f_{+,j} + f_{-,j}}{2}\right) + \sum_j^n \mathrm{i}(S - \mathbb{I})_{ij}\left(\frac{f_{+,j} - f_{-,j}}{2\mathrm{i}}\right)\right] \\ &= \frac{1}{2}\left[\sum_j^n S_{ij} f_{+,j} + f_{-,i}\right] \equiv \psi_i\end{aligned}$$

which is the scattering wave solution. □

The remaining n terms of the new canonical basis, $\{\xi_i\}_{i=1}^{2n}$, are denoted

$$\chi_i = \xi_{i+n} = \frac{1}{2\mathrm{i}}\left[\sum_j^n S_{ij} f_{+,j} - f_{-,i}\right].$$

Clearly, this construction only works for $k \in \mathbb{R}_0$ when the scattering matrix is unitary. In [1] the matrix U plays the role of a unitary 'parameter' which we were free to choose in order to select self-adjoint boundary conditions and hence a Lagrange plane. Here the unitary matrix valued function $S(k)$ of course depends in some complicated way on the potentials on the edges and the boundary conditions at the vertices.

4. The factorization problem for the graph

Suppose that we are given two non-compact graphs Γ' and Γ'' with self-adjoint operators $\mathcal{L}'$ and $\mathcal{L}''$ defined on them and associated scattering matrices S' and S''. Consider the procedure of linking these graphs along p of their (truncated) rays to form a new graph Γ. We can obviously define a self-adjoint operator on Γ by using the boundary conditions and potentials of $\mathcal{L}'$ and $\mathcal{L}''$, we denote this by $\mathcal{L}$.

Given S' and S'' and the details of the linking, can we find the scattering matrix S of $\mathcal{L}$? We will show that it is possible to do so as long as the points at which rays are truncated in order to form a linking edge are outside of the support of the potential.

4.1. Matching of asymptotic solutions on linking edges

Consider a ray r' attached to Γ' and a ray r'' attached to Γ''. We want to connect these two rays together to form an edge of finite length in a new graph Γ.

We assume that the potentials on r' and r'' have finite support; $\mathrm{supp}(q_{r'}) \subset [0, a']$ and $\mathrm{supp}(q_{r''}) \subset [0, a'']$, respectively. We form the edges $e' = [0, a']$, $e'' = [0, a'']$ by truncating the rays r', r'' at a', a'', respectively and the two graphs are linked simply by joining these edges end to end, forming a new edge in the interior of Γ of length $a' + a''$.

Definition 2. *Given $\psi_{\Gamma'} \in H_{2m'}(\Gamma', \lambda)$ and $\psi_{\Gamma''} \in H_{2m''}(\Gamma'', \lambda)$ we say that these generalized eigenfunctions match on the edge formed by joining e' and e'' end to end if*

$$\psi_{\Gamma'}\big|_{a'} = \psi_{\Gamma''}\big|_{a''} \qquad \frac{d\psi_{\Gamma'}}{dx}\bigg|_{a'} = -\frac{d\psi_{\Gamma''}}{dx}\bigg|_{a''}. \tag{9}$$

That is, the eigenfunctions $\psi_{\Gamma'}$, $\psi_{\Gamma''}$ match if together they represent a solution on the augmented edge formed by joining e' and e'' end to end—this is different from the usage of the term 'match' in lemma 2 where instead of the asymptotic Hermitian symplectic space we were concerned with the space of boundary values. Nevertheless, there are formal similarities between elements of the asymptotic Hermitian symplectic space which match and elements of the Hermitian symplectic space of boundary values which match (although there is no possibility of confusion as they are different spaces) which is why we use the same term.

When considering linking edges it is natural to consider the sum

$$H_{2m}(\lambda) = H_{2m'}(\Gamma', \lambda) \oplus H_{2m''}(\Gamma'', \lambda)$$

here $m = m' + m''$. This is obviously also a Hermitian symplectic space with the form

$$\langle \phi_{\Gamma'} \oplus \phi_{\Gamma''}, \psi_{\Gamma'} \oplus \psi_{\Gamma''} \rangle \equiv \langle \phi_{\Gamma'}, \psi_{\Gamma'} \rangle_{\Gamma'} + \langle \phi_{\Gamma''}, \psi_{\Gamma''} \rangle_{\Gamma''}$$

where $\langle \cdot, \cdot \rangle_{\Gamma'}$ and $\langle \cdot, \cdot \rangle_{\Gamma''}$ are the Hermitian symplectic forms on Γ' and Γ'', respectively. Using this notation the condition for matching is expressed in the following lemma.

Lemma 3. *The element*

$$\psi = \psi_{\Gamma'} \oplus \psi_{\Gamma''} \in H_{2m}$$

matches on the edge formed by joining e' and e'' iff

$$\begin{aligned} \langle \psi_{\Gamma'} \oplus \psi_{\Gamma''}, \zeta f_{+,r'} \oplus f_{-,r''} \rangle &= 0 \\ \langle \psi_{\Gamma'} \oplus \psi_{\Gamma''}, f_{-,r'} \oplus \zeta f_{+,r''} \rangle &= 0 \end{aligned} \tag{10}$$

where $\zeta = e^{-ik(a'+a'')}$ and $f_{\pm,r'}$ and $f_{\pm,r''}$ are the Jost solutions on the rays $r' \in \Gamma'$ and $r'' \in \Gamma''$, respectively.

Proof. The Jost solutions $f_{\pm,r'}$ and $f_{\pm,r''}$ form a basis on the rays r' and r'' so we can write

$$\psi_{\Gamma'}\big|_{r'} = \alpha' f_{+,r'} + \beta' f_{-,r'} \qquad \psi_{\Gamma''}\big|_{r''} = \alpha'' f_{+,r''} + \beta'' f_{-,r''}.$$

Since the support of the potentials on the rays r' and r'' is within the intervals $[0, a']$ and $[0, a'']$, and remembering that the Jost solutions are continuous with continuous first derivatives, we see that

$$\begin{aligned} f_{\pm,r'}\big|_{a'} &= e^{\pm ika'} \qquad & \frac{df_{\pm,r'}}{dx}\bigg|_{a'} &= \pm ik e^{\pm ika'} \\ f_{\pm,r''}\big|_{a''} &= e^{\pm ika''} \qquad & \frac{df_{\pm,r''}}{dx}\bigg|_{a''} &= \pm ik e^{\pm ika''}. \end{aligned}$$

In order for equation (9) to be satisfied we need the following conditions:

$$\begin{aligned} \alpha' e^{ika'} + \beta' e^{-ika'} &= \alpha'' e^{ika''} + \beta'' e^{-ika''} \\ \alpha' e^{ika'} - \beta' e^{-ika'} &= -\left[\alpha'' e^{ika''} - \beta'' e^{-ika''}\right] \end{aligned}$$

or, solving for α' and β',

$$\bar{\zeta}\alpha' = \beta'' \qquad \beta' = \bar{\zeta}\alpha''.$$

On the other hand, using equation (6), we have

$$2\mathrm{i}\bar{\alpha}' = \langle \psi_{\Gamma'}, f_{+,r'} \rangle_{\Gamma'} \qquad -2\mathrm{i}\bar{\beta}' = \langle \psi_{\Gamma'}, f_{-,r'} \rangle_{\Gamma'}$$

$$2\mathrm{i}\bar{\alpha}'' = \langle \psi_{\Gamma''}, f_{+,r''} \rangle_{\Gamma''} \qquad -2\mathrm{i}\bar{\beta}'' = \langle \psi_{\Gamma''}, f_{-,r''} \rangle_{\Gamma''}$$

so equation (9) becomes

$$\zeta \langle \psi_{\Gamma'}, f_{+,r'} \rangle_{\Gamma'} = -\langle \psi_{\Gamma''}, f_{-,r''} \rangle_{\Gamma''}$$

$$-\langle \psi_{\Gamma'}, f_{-,r'} \rangle_{\Gamma'} = \zeta \langle \psi_{\Gamma''}, f_{+,r''} \rangle_{\Gamma''}$$

which, together with the fact that the Hermitian symplectic form is linear in its second argument, gives the desired result. □

Corollary 2. *The subspace of H_{2m} of elements with support confined to the rays r' and r'' and which match is an isotropic subspace with basis*

$$\left\{ \zeta f_{+,r'} \oplus f_{-,r''},\ f_{-,r'} \oplus \zeta f_{+,r''} \right\}.$$

Proof. The space of matching solutions is two dimensional since this is simply the space of solutions on the augmented edge of length $a'+a''$. The vectors we have given are independent—the Jost solutions f_+ and f_- are independent—all that remains is to show that they match, which is easily seen to be true if they are put into equation (10). Furthermore, the fact that these basis vectors satisfy equation (10) means that they are contained in their orthogonal complement, i.e. the subspace is isotropic. □

We consider linking p of the rays of Γ' with p of the rays of Γ''. Let us suppose that Γ' has $m' = n' + p$ rays, while Γ'' has $m'' = n'' + p$ rays. We also denote $m = m' + m''$, $n = n' + n''$ so that $m = n + 2p$.

We choose p of the rays of Γ' and p of the rays of Γ'' and consider the procedure of linking each ray of Γ' with a ray of Γ'' to form a new graph Γ. Let us denote by $N \subset H_{2m}$ the subset of elements with support confined to the linking rays and which match on the linking rays. Then, by a simple generalization of lemma 2, this subspace is isotropic with dimension $2p$ and we can write a basis for it in terms of the Jost solutions on the linking rays similar to the basis given in the lemma.

On the other hand, by lemma 3 the elements $\psi \in H_{2m}$ which match on each of the linking rays are just those elements $\psi \perp N$, i.e. the subspace $N^{\perp}$. In summary, suppose we choose p rays, $\{r_i'\}_{i=1}^{p}$, of Γ' and p rays, $\{r_i''\}_{i=1}^{p}$, of Γ'', and consider linking r_i' to r_i'' for each i to form the graph Γ. Then we have:

Corollary 3. *The subspace $N \subset H_{2m}$ of elements with support confined to the linking rays and which match on the linking rays is a $2p$-dimensional isotropic subspace with basis*

$$\left\{ \zeta_i f_{+,r_i'} \oplus f_{-,r_i''},\ f_{-,r_i'} \oplus \zeta_i f_{+,r_i''} \right\}_{i=1}^{p}$$

where $\zeta_i = \mathrm{e}^{-\mathrm{i}ka_i}$ and a_i is the length of the edge formed by joining r_i' and r_i''. Furthermore, $N^{\perp} \supset N$ consists of all of the elements of H_{2m} which match on the linking rays.

4.2. *Description of the Lagrange plane of generalized eigenfunctions for the linked graph* Γ

We suppose that on the graphs Γ' and Γ'' we have defined self-adjoint Schrödinger operators $\mathcal{L}'$ and $\mathcal{L}''$, respectively. In terms of these operators we can define the self-adjoint $\mathcal{L}$ on the graph Γ formed by linking Γ' and Γ'' as described above.

We recall that any generalized eigenfunction of $\mathcal{L}$ can be written as a generalized eigenfunction of $\mathcal{L}'$ on Γ' plus a generalized eigenfunction of $\mathcal{L}''$ on Γ'' such that these two functions match on all of the linking rays. This can be stated in terms of the asymptotic Hermitian symplectic space: associated with $\mathcal{L}'$ and $\mathcal{L}''$ are the Lagrange planes $\Pi_{m'} \subset H_{2m'}(\Gamma')$ and $\Pi_{m''} \subset H_{2m''}(\Gamma'')$, respectively. Furthermore, $\Pi_m = \Pi_{m'} \oplus \Pi_{m''} \subset H_{2m}$ is a Lagrange plane. Then the intersection of Π_m (the generalized eigenfunctions on Γ' and Γ'') and $N^{\perp}$ (the solutions which match on the linking rays) gives us the generalized eigenfunctions of $\mathcal{L}$ on Γ.

Really, we get a little bit more: $\Pi_m \cap N^{\perp}$ may also contain solutions which have support only on the linking edges, which, as we are only interested in solutions with support on the semi-infinite rays, need to be discarded. In fact, we should not look for a solution in the space H_{2m} as it is not a suitable asymptotic Hermitian symplectic space for the linked graph Γ. In particular, H_{2m} has too high a dimension; the linked graph Γ has $n = n' + n''$ rays so we should be working in an asymptotic Hermitian symplectic space of dimension $2n$. Consider the space $N^{\perp}/N$. It has dimension $2n$ (by lemma 5), moreover, it consists of solutions that match on all the linking rays. For this reason we state that $N^{\perp}/N$ is the asymptotic Hermitian symplectic space for the linked graph Γ.

We have established that $\Pi_m \cap N^{\perp}$ contains all of the generalized eigenfunctions of the operator $\mathcal{L}$ on the linked graph Γ plus, possibly, some solutions with support on just the linking rays. Projecting $\Pi_m \cap N^{\perp}$ onto $N^{\perp}/N$ eliminates solutions with support only on the linking rays and so will give us the generalized eigenspace of $\mathcal{L}$ on Γ which, by theorem 2 is a Lagrange plane.

Corollary 4. *The Lagrange plane* $(\Pi_m \cap N^{\perp})/N$ *in* $N^{\perp}/N$ *corresponds to the space of generalized eigenfunctions with support on the rays for the operator* $\mathcal{L}$ *on the graph* Γ.

It is easy to see that this description generalizes to the case where an arbitrary number of graphs are linked. In this case Π_m is defined as the direct sum of the Lagrange planes associated with each of these graphs and N is again an isotropic subspace which describes how the graphs are to be linked.

4.3. *Description of the scattering matrix for the linked graph* Γ

For the sake of convenience let us suppose that we are linking just two graphs Γ' and Γ'' (the case of an arbitrary number of graphs may be reduced to this case). As above, we assume that Γ' has m' rays and Γ'' m'' rays and that we have selected p rays of each graph to connect together. Consider the graph $\Gamma' \oplus \Gamma''$ and let us index the rays of this graph according to the scheme set out in figure 1.

The first p rays, which are part of graph Γ', are to be linked to the next p rays, which are part of graph Γ''. The last n rays in this scheme form the infinite rays of the linked graph Γ, the first n'' of these coming from Γ'' and the last n' coming from Γ'.

In order to make the calculations below clearer, we introduce the following index sets:

$$\begin{aligned} I &= \{1, \ldots, 2m\} \\ I_N &= \{1, \ldots, 2p\} \\ I_{N^{\perp}} &= \{1, \ldots, m, 2p + m + 1, \ldots, 2m\}. \end{aligned}$$

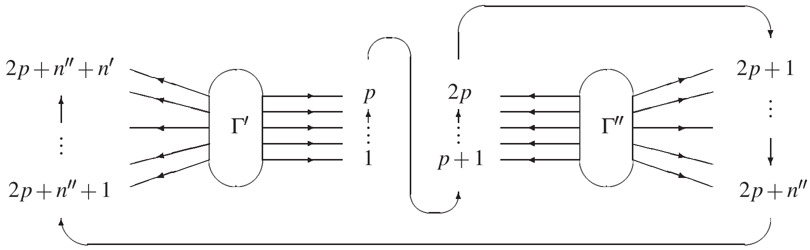

Figure 1. Labelling of the rays of the graphs.

We denote matrices in $\mathbb{C}^{m\times n}$ by $A_{(m,n)}$ and matrices in $\mathbb{C}^{n\times n}$ by $A_{(n)}$ where $\mathbb{I}_{(n)}$ is the unit matrix in $\mathbb{C}^{n\times n}$.

The Jost solutions $\{f_{\pm,i}\}_{i=1}^{m}$ and, as defined in equation (7), the canonical basis $\{\xi_{0,j}\}_{i=1}^{2m}$ are labelled in the obvious way according to the scheme of the figure.

We have self-adjoint $\mathcal{L}'$ and $\mathcal{L}''$ defined on Γ' and Γ'', respectively. Associated with these operators we have the Lagrange planes $\Pi_{m'}$, $\Pi_{m''}$ and canonical bases as described in theorem 1. Then $\Pi_{m'} \oplus \Pi_{m''}$ forms a Lagrange plane in H_{2m} with canonical basis $\{\xi_j\}_{j=1}^{2m}$ inherited from the canonical bases associated with $\Pi_{m'}$ and $\Pi_{m''}$. The indexing of the basis elements $\{\xi_j\}_{j=1}^{2m}$ follows the indexing given in figure 1. Specifically, suppose

$$S'_{(m')} = \begin{pmatrix} S'_{(p)} & S'_{(p,n')} \\ S'_{(n',p)} & S'_{(n')} \end{pmatrix}$$

is the scattering matrix for $\mathcal{L}'$ and

$$S''_{(m'')} = \begin{pmatrix} S''_{(p)} & S''_{(p,n'')} \\ S''_{(n'',p)} & S''_{(n'')} \end{pmatrix}$$

the scattering matrix for $\mathcal{L}''$ where the *ordering* of the entries follows the ordering described in the figure—in particular, the first p entries of each matrix correspond to the p rays which are to be linked. Then it is easy to see that the matrix g, which describes the transformation from the basis $\{\xi_{0,j}\}_{i=1}^{2m}$ to the basis $\{\xi_j\}_{j=1}^{2m}$ as in theorem 1, is of the form

$$g = W^\star \hat{g} W = W^\star \begin{pmatrix} S_{(m)} & 0 \\ 0 & \mathbb{I}_{(m)} \end{pmatrix} W$$

where, following figure 1

$$S_{(m)} = \begin{pmatrix} S'_{(p)} & 0 & 0 & S'_{(p,n')} \\ 0 & S''_{(p)} & S''_{(p,n'')} & 0 \\ 0 & S''_{(n'',p)} & S''_{(n'')} & 0 \\ S'_{(n',p)} & 0 & 0 & S'_{(n')} \end{pmatrix}. \tag{11}$$

We construct one more canonical basis, $\{\xi_{N,j}\}_{j=1}^{2m}$, which allows us to express the isotropic subspace N in simple terms. Recalling corollary 3, we see that the $2p$ elements defined by

$$\xi_{N,j} = \frac{\zeta_j f_{+,j} + f_{-,p+j}}{2} \qquad \xi_{N,j+p} = \frac{\zeta_j f_{+,p+j} + f_{-,j}}{2}$$

where $j = 1, \dots, p$, $\zeta_j = \mathrm{e}^{-\mathrm{i}ka_j}$ and a_j is the length of the jth linked edge, form a basis for N. Now we extend this to a canonical basis by defining the following n elements as identical to the elements of the canonical basis $\{\xi_{0,j}\}_{j=1}^{2m}$

$$\xi_{N,j} = \xi_{0,j} = \frac{f_{+,j} + f_{-,j}}{2}$$

where $j = 2p+1, \dots, m$. Then these elements span a Lagrange plane which, after theorem 1, has associated with it the 'scattering matrix'

$$T_{(m)} = \begin{pmatrix} \begin{matrix} 0 & \zeta_{(p)} \\ \zeta_{(p)} & 0 \end{matrix} & 0 \\ 0 & \mathbb{I}_{(n)} \end{pmatrix} \tag{12}$$

where $\zeta_{(p)}$ is a diagonal matrix with the entries on the diagonal being ζ_i. It is then a simple matter to see that the matrix

$$g_N = W^\star \hat{g}_N W = W^\star \begin{pmatrix} T_{(m)} & 0 \\ 0 & \mathbb{I}_{(m)} \end{pmatrix} W$$

takes the canonical basis $\{\xi_{0,j}\}_{j=1}^{2m}$ into a new canonical basis $\{\xi_{N,j}\}_{j=1}^{2m}$. We have already shown that the linear span

$$N = \bigvee_{j\in I_N} \{\xi_{N,j}\}$$

and it is not difficult to see, using the fact that this is a canonical basis, that

$$N^\perp = \bigvee_{j\in I_{N^\perp}} \{\xi_{N,j}\}.$$

In order to obtain the scattering matrix for the linked graph we first express ξ_j in terms of the $\xi_{N,j}$. Since

$$\xi_i = \sum_{j=1}^{2m} g_{ij}\xi_{0,j} \qquad \xi_{N,i} = \sum_{j=1}^{2m} g_{N,ij}\xi_{0,j}$$

we can write

$$\xi_i = \sum_{j,k=1}^{2m} g_{ij} g^\star_{N,jk} \xi_{N,k} = \sum_{j=1}^{2m} h_{ij}\xi_{N,j} \tag{13}$$

where

$$h = W^\star \hat{h} W = W^\star \begin{pmatrix} S_{(m)} T^\star_{(m)} & 0 \\ 0 & \mathbb{I}_{(m)} \end{pmatrix} W.$$

We use this equation to find an n-dimensional canonical basis for $(\Pi_m \cap N^\perp)/N$. Clearly, any such basis can be written, modulo elements of N, as a linear combination of $\{\xi_j\}_{j=1}^{m}$—since this set spans $\Pi_m \supset (\Pi_m \cap N^\perp)$. So there is a matrix R in $\mathbb{C}^{n\times m}$ so that the (representative in $\Pi_m \cap N^\perp$ of the) ith basis element of $(\Pi_m \cap N^\perp)/N$ is

$$\sum_{j=1}^{m} R_{ij}\xi_j = \sum_{j=1}^{m}\sum_{l=1}^{2m} R_{ij} h_{jl} \xi_{N,l} \tag{14}$$

Here $i = 1, \dots, n$. What are the properties of the matrix R?

(a) We can write the matrix R in the form

$$R = \begin{pmatrix} \rho_{(n,2p)} & \mathbb{I}_{(n)} \end{pmatrix}. \tag{15}$$

First, we know that the subspace $N^{\perp}/N$ can be represented by the space

$$\bigvee_{j \in I_{N^{\perp}} \setminus I_N} \{\xi_{N,j}\} = \bigvee_{j \in I_{N^{\perp}} \setminus I_N} \{\xi_{0,j}\}.$$

Furthermore, $(\Pi_m \cap N^{\perp})/N$ is a Lagrange plane in this space. Therefore, by theorem 1, there is a unitary matrix $S_{(n)}$ such that the ith basis element of the Lagrange plane has the form

$$\frac{1}{2}\left[\sum_j S_{(n),ij} f_{+,j} + f_{-,i}\right].$$

Here i and j take values in the range $\{2p+1, \ldots, m\}$. However, this is equivalent to equation (15). Really, the only way to ensure that $f_{-,i}$ occur only 'on the diagonal' is to have $\mathbb{I}_{(n)}$ in R, as shown.

(b) In order for these basis elements to be in $\Pi_m \cap N^{\perp}$ we need the coefficients of $\xi_{N,l}$ for $l \in I \setminus I_{N^{\perp}}$ in equation (14) to be zero.

Let us express the matrix h in the following form:

$$h = \begin{pmatrix} A_{(m)} & B_{(m)} \\ -B_{(m)} & A_{(m)} \end{pmatrix} = \begin{pmatrix} A_{(2p)} & A_{(2p,n)} & B_{(2p)} & B_{(2p,n)} \\ A_{(n,2p)} & A_{(n)} & B_{(n,2p)} & B_{(n)} \\ -B_{(2p)} & -B_{(2p,n)} & A_{(2p)} & A_{(2p,n)} \\ -B_{(n,2p)} & -B_{(n)} & A_{(n,2p)} & A_{(n)} \end{pmatrix}. \tag{16}$$

Using this representation, condition II can be expressed as

$$\rho_{(n,2p)} B_{(2p)} + B_{(n,2p)} = 0$$

i.e.

$$\rho_{(n,2p)} = -B_{(n,2p)} B_{(2p)}^{-1}.$$

This gives us the matrix R so we can write

$$Rh = \big(-B_{(n,2p)} B_{(2p)}^{-1} A_{(2p)} + A_{(n,2p)}, \quad -B_{(n,2p)} B_{(2p)}^{-1} A_{(2p,n)} + A_{(n)}, \quad 0, \\ -B_{(n,2p)} B_{(2p)}^{-1} B_{(2p,n)} + B_{(n)} \big).$$

We are not interested in the first $n \times 2p$ block of this matrix as this represents the coefficients of the terms in N. Let us write the second and fourth block as A and B, respectively. Then from condition I, along with theorem 1, we see that

$$A = \tfrac{1}{2}(S_{(n)} + \mathbb{I}_{(n)}) \qquad B = \tfrac{1}{2}\mathrm{i}(S_{(n)} - \mathbb{I}_{(n)})$$

where, as above, $S_{(n)}$ is the desired scattering matrix of $\mathcal{L}$ on Γ. In other words, the scattering matrix is

$$S_{(n)} = A - \mathrm{i}B = A_{(n)} - \mathrm{i}B_{(n)} - B_{(n,2p)}B^{-1}_{(2p)}(A_{(2p,n)} - \mathrm{i}B_{(2p,n)})$$

$$= \begin{pmatrix} S''_{(n'')} & 0 \\ 0 & S'_{(n')} \end{pmatrix} + \begin{pmatrix} S''_{(n'',p)}\bar{\zeta}_{(p)} & 0 \\ 0 & S'_{(n',p)}\bar{\zeta}_{(p)} \end{pmatrix} \begin{pmatrix} \mathbb{I}p & -S'_{(p)}\bar{\zeta}_{(p)} \\ -S''_{(p)}\bar{\zeta}_{(p)} & \mathbb{I}p \end{pmatrix}^{-1}$$

$$\times \begin{pmatrix} 0 & S'_{(p,n')} \\ S''_{(p,n'')} & 0 \end{pmatrix}$$

$$= \begin{pmatrix} S''_{(n'')} & 0 \\ 0 & S'_{(n')} \end{pmatrix} + \begin{pmatrix} S''_{(n'',p)} & 0 \\ 0 & S'_{(n',p)} \end{pmatrix} \begin{pmatrix} \zeta_{(p)} & -S'_{(p)} \\ -S''_{(p)} & \zeta_{(p)} \end{pmatrix}^{-1}$$

$$\times \begin{pmatrix} 0 & S'_{(p,n')} \\ S''_{(p,n'')} & 0 \end{pmatrix}. \tag{17}$$

The inverse $B^{-1}_{(2p)}$ which appears above obviously may not always exist. In fact, $B_{(2p)}$ does not have an inverse iff $\Pi_m \cap N$ is non-empty, i.e. iff we can find solutions with no support on the external rays but support on the linking edges.

Lemma 4. *The matrix $B_{(2p)}$ does not have an inverse iff $\Pi_m \cap N$ is non-empty.*

Proof. Let us suppose that $B_{(2p)}$ does not have an inverse. That is we can find a non-zero vector a such that

$$a^T B_{(2p)} = 0.$$

Then, by equations (13) and (16), we obtain

$$\psi = a^T \cdot \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_{2p} \end{pmatrix} \in N^{\perp}.$$

Now ψ is clearly non-zero on the linking edges and has the form $\alpha_i f_{+,i}$ on the n external rays—this statement follows from the fact that the scattering waves ξ_i for $i = 1, \ldots, 2p$ have this form on the n external rays. Also ψ is a generalized eigenfunction for $\mathcal{L}$, since it is in $\Pi_m \cap N^{\perp}$. However, then, by theorem 1, all the $\alpha_i = 0$. Another way to see this is that, since ψ is a generalized eigenfunction, it belongs to a Lagrange plane and consequently

$$\langle \psi, \psi \rangle = 0$$

which is equivalent to all the $\alpha_i = 0$. This gives us

$$\psi \in \Pi_m \cap N \neq 0$$

as required.

The converse statement follows simply from

$$\xi_{N,i} = \sum_{j=1}^{2m} h^{\star}_{ij}\xi_j.$$

This completes the proof. □

This condition provides a means of identifying discrete eigenvalues embedded in the continuous spectrum.

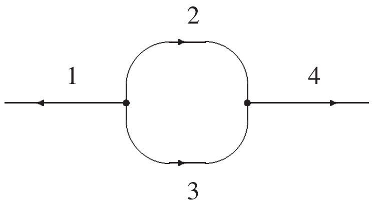

Figure 2. The graph from example 1.

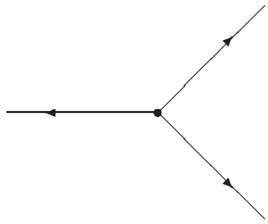

Figure 3. The 'Y' graph.

Corollary 5. *Given a graph* Γ *with m vertices we split* Γ *into m subgraphs* $\Gamma_{d(1)}, \ldots, \Gamma_{d(m)}$*, each consisting of just one vertex with* $d(i)$ *rays attached—here* $d(i)$ *is the degree of the ith vertex of* Γ*. Then the zeros of the determinant of the matrix* $B_{(2p)}$ *for the set of subgraphs* $\Gamma_{d(1)}, \ldots, \Gamma_{d(m)}$ *give the discrete eigenvalues embedded in the continuous spectrum.*

As we have mentioned above, equation (17) for the scattering matrix is the same, in essence, as the equation given in the paper by Kostrykin and Schrader [3, 4]. In this paper the authors consider how the scattering matrix for the Laplacian on a graph may be expressed in terms of the scattering matrices of its subgraphs. Introducing a potential, as in the case of the Schrödinger operator, does not introduce anything essentially new (as long as we assume, as we have done, that the potentials have compact support and that we do not truncate rays inside the support). Nevertheless, our approach is sufficiently novel, we believe, to be of independent interest. Kostrykin and Schrader also note the presence of an inverse matrix in their formula (analogous to our matrix $B_{(2p)}^{-1}$) and refer to the condition of this inverse not existing as *condition A*.

Example 1. *Consider the graph in figure 2 with potential equal to zero on all the edges, the internal edges of equal length a and flux-conserved boundary conditions, that is*

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

The arrows indicate the orientation of the edges.

We can reconstruct the scattering matrix of the graph of figure 2 by linking two 'Y' graphs, depicted in figure 3, according to the scheme of this section.

It is easy to see that the scattering matrices of such graphs have the form

$$S' = S'' = \begin{pmatrix} -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{pmatrix}.$$

So we obtain

$$\begin{aligned}
S'_{(n')} &= S''_{(n'')} = \begin{pmatrix} -\frac{1}{3} \end{pmatrix}\\
S'_{(n',p)} &= S''_{(n'',p)} = \begin{pmatrix} \frac{2}{3} & \frac{2}{3} \end{pmatrix} = S'^{T}_{(p,n')} = S''^{T}_{(p,n'')}\\
S'_{(p)} &= S''_{(p)} = \begin{pmatrix} -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} \end{pmatrix}
\end{aligned}$$

and, furthermore,

$$\begin{pmatrix} S''_{(n'')} & 0 \\ 0 & S'_{(n')} \end{pmatrix} = \begin{pmatrix} -\frac{1}{3} & 0 \\ 0 & -\frac{1}{3} \end{pmatrix}$$

$$\begin{pmatrix} S''_{(n'',p)} & 0 \\ 0 & S'_{(n',p)} \end{pmatrix} = \begin{pmatrix} \frac{2}{3} & \frac{2}{3} & 0 & 0 \\ 0 & 0 & \frac{2}{3} & \frac{2}{3} \end{pmatrix}$$

$$\begin{pmatrix} 0 & S'_{(p,n')} \\ S''_{(p,n'')} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \frac{2}{3} \\ 0 & \frac{2}{3} \\ \frac{2}{3} & 0 \\ \frac{2}{3} & 0 \end{pmatrix}.$$

Then from

$$\begin{pmatrix} \zeta_{(p)} & -S'_{(p)} \\ -S''_{(p)} & \zeta_{(p)} \end{pmatrix} = \begin{pmatrix} \zeta & 0 & \frac{1}{3} & -\frac{2}{3} \\ 0 & \zeta & -\frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & -\frac{2}{3} & \zeta & 0 \\ -\frac{2}{3} & \frac{1}{3} & 0 & \zeta \end{pmatrix}$$

where of course $\zeta = e^{-ika}$, we can easily show that

$$\begin{pmatrix} \zeta_{(p)} & -S'_{(p)} \\ -S''_{(p)} & \zeta_{(p)} \end{pmatrix}^{-1} = \frac{\zeta}{(9\zeta^2 - 1)(\zeta^2 - 1)}$$
$$\times \begin{pmatrix} 9\zeta^2 - 5 & -4 & -(3\zeta + \bar{\zeta}) & 2(3\zeta - \bar{\zeta}) \\ -4 & 9\zeta^2 - 5 & 2(3\zeta - \bar{\zeta}) & -(3\zeta + \bar{\zeta}) \\ -(3\zeta + \bar{\zeta}) & 2(3\zeta - \bar{\zeta}) & 9\zeta^2 - 5 & -4 \\ 2(3\zeta - \bar{\zeta}) & -(3\zeta + \bar{\zeta}) & -4 & 9\zeta^2 - 5 \end{pmatrix}.$$

Putting all of these into equation (17) gives us the following form for the scattering matrix:

$$S = \frac{1}{\gamma} \begin{pmatrix} 3(\bar{\zeta} - \zeta) & 8 \\ 8 & 3(\bar{\zeta} - \zeta) \end{pmatrix}$$

where we have used $\gamma = 9\zeta - \bar{\zeta}$.

On the other hand, going back to the graph of figure 2, it is easy to see that this has a scattering wave solution of the form

$$\begin{aligned} \psi_1 &= e^{-ikx} + \frac{3(\bar{\zeta} - \zeta)}{\gamma} e^{ikx} \\ \psi_{2/3} &= \frac{2\bar{\zeta}}{\gamma} e^{-ikx} + \frac{6\zeta}{\gamma} e^{ikx} \\ \psi_4 &= \frac{8}{\gamma} e^{ikx}. \end{aligned}$$

This confirms the form for the scattering matrix.

Acknowledgment

The author would like to thank Professor B S Pavlov for his advice and many useful conversations.

Appendix

Consider a canonical Hermitian symplectic space H_{2m} with Lagrange plane Π_m and isotropic subspace N of dimension q. Then $N^{\perp}/N$ is a canonical Hermitian symplectic space of dimension $2n = 2(m-q)$ and $(\Pi_m \cap N^{\perp})$ projects to a Lagrange plane in $N^{\perp}/N$.

Lemma 5. *$N^{\perp}/N$ is a Hermitian symplectic space of dimension $2n$.*

Proof. Since the form is non-degenerate

$$\dim(N^{\perp}) = \dim(H_{2m}) - \dim(N) = 2m - q = 2n + q.$$

Now since $N \subset N^{\perp}$, $\dim(N^{\perp}/N) = \dim(N^{\perp}) - \dim(N)$, which gives us the result for the dimension. Clearly, the form inherited from H_{2m} is uniquely defined since

$$\langle \phi + n_1, \psi + n_2 \rangle = \langle \phi, \psi \rangle \qquad \phi, \psi \in N^{\perp} \quad n_1, n_2 \in N.$$

To see non-degeneracy suppose there is some non-zero $\phi \in N^{\perp}$ which satisfies

$$\langle \phi, \psi \rangle = 0 \qquad \forall \psi \in N^{\perp}.$$

However, this simply means that $\phi \in N$, i.e. ϕ is in the coset containing zero. □

Note that we have only shown that $N^{\perp}/N$ is a Hermitian symplectic space, not a canonical Hermitian symplectic space. In order to show that it is canonical we need only show (see [1]) that it contains a Lagrange plane:

Theorem 2. *The subspace $(\Pi_m \cap N^{\perp}) \subset N^{\perp}$ projects to a Lagrange plane in $N^{\perp}/N$.*

Proof. We denote, somewhat imprecisely, the projection of $(\Pi_m \cap N^{\perp})$ into $N^{\perp}/N$ by $(\Pi_m \cap N^{\perp})/N$. Clearly, $(\Pi_m \cap N^{\perp})/N$ is isotropic since Π_m is a Lagrange plane. We need only show that it has maximal dimension. Firstly,

$$\begin{aligned}\dim((\Pi_m \cap N^{\perp})/N) &= \dim(\Pi_m \cap N^{\perp}) - \dim(\Pi_m \cap N^{\perp} \cap N) \\ &= \dim(\Pi_m \cap N^{\perp}) - \dim(\Pi_m \cap N).\end{aligned}$$

Now, remembering that Π_m is a Lagrange plane, it is easy to see that

$$(\Pi_m \cap N^{\perp})^{\perp} = \Pi_m + N.$$

So

$$\dim(\Pi_m \cap N^{\perp}) = \dim(H_{2m}) - \dim(\Pi_m + N) = 2m - \dim(\Pi_m + N).$$

To proceed we use the basic vector space identity $\dim(P)+\dim(N) = \dim(P+N)+\dim(P\cap N)$, which gives us

$$\dim(\Pi_m \cap N^{\perp}) = 2m - [\dim(\Pi_m) + \dim(N) - \dim(\Pi_m \cap N)].$$

Putting this into our equation for $\dim((\Pi_m \cap N^{\perp})/N)$ gives

$$\begin{aligned}\dim((\Pi_m \cap N^{\perp})/N) &= 2m - [\dim(\Pi_m) + \dim(N) - \dim(\Pi_m \cap N)] - \dim(\Pi_m \cap N) \\ &= 2m - \dim(\Pi_m) - \dim(N) \\ &= m - q = n.\end{aligned}$$

This completes the proof. □

Due to the nature of this proof it appears that this result should also hold for symplectic geometry. We also note that these results are only used above in the case where $q = 2p$ is even, although they clearly hold for any integral q.

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