Hermitian symplectic geometry and the Schrödinger operator on the graph

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Abstract

The theory of self-adjoint extensions is closely related to the theory of hermitian symplectic geometry [13, 9, 12]. Here we develop this idea, showing that it may also be used to consider symmetric extensions of a symmetric operator. Furthermore we find an explicit parameterisation of the Lagrange Grassmannian in terms of the unitary matrices $\mathsf{U}(n)$. This allows us to explicitly describe all self-adjoint boundary conditions for the Schrödinger operator on the graph in terms of a unitary matrix. We show that the asymptotics of the scattering matrix can be simply expressed in terms of this unitary matrix. Using the construction of the asymptotic hermitian symplectic space [11, 12] we derive a formula for the scattering matrix of a graph in terms of the scattering matrices of its subgraphs. This also provides a characterisation of the discrete eigenvalues embedded in the continuous spectrum.

1 Introduction

In the first section we consider the extension theory for the Schrödinger operator on the graph with trivial compact part. This is done using the well know connection between the self-adjoint extensions of a symmetric operator and the Lagrange planes of a hermitian[1] symplectic space [13, 9, 12]. It follows from von Neumann extension theory that the set of Lagrange planes is isomorphic to the set of unitary matrices $\mathsf{U}(n)$ where n is the deficiency index. However, to our knowledge, no explicit parameterisation of these Lagrange

[1] This terminology follows [9].

planes by the unitary matrices has been given in the literature. Here we investigate hermitian symplectic geometry and describe its connection with the theory of extensions, symmetric and self-adjoint. In particular we derive an explicit parameterisation of the Lagrange planes by unitary matrices and use this to describe all self-adjoint boundary conditions at the origin for the Schrödinger operator on the graph with trivial compact part. Furthermore, we show that the asymptotics of the scattering matrix may be written in terms of this unitary matrix and that the boundary conditions do not contribute to the discrete spectrum iff this unitary matrix is also hermitian.
We emphasise that although in von Neumann extension theory the self-adjoint extensions are also parameterised by unitary matrices, our approach differs in that it allows us to parameterise the self-adjoint *boundary conditions* for the Schrödinger operator on the graph in terms of unitary matrices (see [5] where self-adjoint extensions of the Schrödinger operator on the graph are described using von Neumann extension theory).

In the next section we discuss non-compact graphs formed from a compact graph with n semi-infinite rays attached. The tool we will use to investigate such graphs is the idea of an asymptotic hermitian symplectic space introduced by Novikov [12] in the case of the discrete Schrödinger operator on the graph. The value of this construction lies in the fact that the generalised 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. Furthermore we show that the scattering matrix has the rôle of the unitary matrix which parameterises Lagrange planes.

In the final section we consider the factorisation problem for graphs. That is, we will 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 done in the case of the Laplacean on a graph by Kostrykin and Schrader [9]. We present a substantially different approach, based on the construction of the asymptotic hermitian symplectic space, to what is essentialy the same problem, the factorisation of the Schrödinger operator on graphs.
Using the asymptoic hermitian symplectic space we can express in a simple way the generalised eigenspace of a graph in terms of the generalised eigenspaces of the subgraphs. As the scattering matrix is defined by a distinguished basis for these eigenspaces this, in effect, provides us with a composition rule for the scattering matrix. In practice, however, we need some linear algebra (simplified by our description of the generalised 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 characterisation of the discrete eigenvalues embedded in the continuous spectrum of the non-compact graph.

2 The Schrödinger Operator on the Graph with trivial Compact Part

Here we consider the non-compact graph cocsisting of n semi-axes connected at a single vertex, we denote such a graph by Γ_n. Functions on Γ_n may be represented by elements of the Hilbert space

$$H(\Gamma_n) = \oplus_{i=1}^{n} L^2([0,\infty)).$$

The elements of $H(\Gamma_n)$ are n-dimensional vector functions and the inner product on $H(\Gamma_n)$ is

$$\begin{aligned}(\phi,\psi) &= \sum_{i=1}^{n} (\phi_i,\psi_i)_{L^2([0,\infty))} \\ &= \sum_{i=1}^{n} \int_0^\infty \bar{\phi}_i \psi_i dx\end{aligned}$$

where ϕ_i are the components of ϕ.
Let us consider the symmetric Schrödinger operator, $\mathcal{L}_0$, in $H(\Gamma_n)$

$$\mathcal{L}_0 \psi_i \equiv -\frac{d^2\psi_i}{dx_i^2} + q_i(x_i)\psi_i \quad \text{for } i = 1,\ldots,n.$$

The potentials q_i are continuous real functions which are integrable with finite first moment, that is

$$\int_0^\infty (1+t)|q_i(t)|dt < \infty \tag{1}$$

for $i = 1,\ldots,n$. The domain of $\mathcal{L}_0$ is the set of smooth functions with compact suppport in the open interval

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

The claim that $\mathcal{L}_0$ is a symmetric operator in this Hilbert space (L^2) is a simple consequence of the assumed domain of $\mathcal{L}_0$ and integration by parts. Furthermore it is easy to see that the deficiency indices of $\mathcal{L}_0$ are (n,n). Consequently we may consider the self-adjoint extensions of $\mathcal{L}_0$ and indeed, using the results of Neumann extension theory [2] parameterise these extensions by the unitary matrices $\mathsf{U}(n)$.
The problem of finding self-adjoint *boundary conditions* for such an operator is discussed in detail in [9, 5]. In [9] all self-adjoint boundary conditions are

parameterised non-uniquely in terms of two n-th order matrices, A B, such that $(A\,B)$ is of maximal rank and $AB^\star = BA^\star$ is hermitian.
Here we will parameterise all of the self-adjoint boundary conditions at the origin in terms of a unitary matrix U using the well known connection between Lagrange planes and self-adjoint extensions [13, 9, 12]. The domain of a self-adjoint extension of a symmetric operator can be described as a set of elements for which the boundary form

$$\mathcal{J}(f,g) \equiv (\mathcal{L}_0^\star f, g) - (f, \mathcal{L}_0^\star g) \quad f,g \in \mathrm{Dom}(\mathcal{L}_0^\star) \tag{2}$$

vanishes identically—see [13] for a precise description. In other words the self-adjoint extensions can be identified with Lagrange planes while the boundary form $\mathcal{J}(\cdot,\cdot)$ is seen to be a hermitian symplectic form (a precise definition of these terms is given below). In the following sections we make explicit the connection between extension theory and hermitian symplectic geometry.

3 Hermitian symplectic geometry and extension theory

Many of the basic ideas in this section can be found in any standard text on symplectic geometry [3, 4, 6, 10]. However, when we consider the requirement of equal deficiency indices and the details of the parameterisation of Lagrange planes in a hermitian symplectic space the discussion differs from the standard symplectic case. In particular the Lagrange planes in hermitian symplectic geometry are parameterised by unitary matrices whereas they have different parameterisations in the standard symplectic geometry. Also, by our definition, a hermitian symplectic space need not be even dimensional or admit a canonical basis—unlike the symplectic case. Such an instance is seen to correspond to a symmetric operator with unequal deficiency indices.

We start with some basic definitions.

Definition 3.1 *The two-form $\langle\cdot,\cdot\rangle$, linear in the second argument and conjugate linear in the first argument, is a hermitian symplectic form if*

$$\langle\phi,\psi\rangle = -\overline{\langle\psi,\phi\rangle}.$$

It is clear that the boundary form of equation (2) is a hermitian symplectic form. We recall that the standard symplectic form obeys $\langle\phi,\psi\rangle = -\langle\psi,\phi\rangle$. We will use the prefix 'hermitian' to emphasise the distinction between these forms.

Definition 3.2 *We say that an m-dimensional ($m < \infty$) vector space H_m over $\mathbb{C}$ is a hermitian symplectic space if it has defined on it a nondegenerate hermitian symplectic form. By nondegenerate we mean that if ϕ obeys*

$$\langle\phi,\psi\rangle = 0 \quad \forall\psi \in H_m$$

then $\phi = 0$

This definition is completely analogous to the definition of the usual symplectic space over $\mathbb{C}$. It will turn out that for the cases in which we are interested $m = 2n$ is an even integer, as is the case in the usual symplectic geometry. We only consider the finite dimensional case here.

Definition 3.3 *We say that* $\phi, \psi \in H_m$ *are skew-orthogonal, denoted* $\phi \perp \psi$, *if*

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

Similarly we define the skew-orthogonal complement:

Definition 3.4 *Given a subspace* $N \subset H_m$, *we define the skew-orthogonal complement,* $N^\perp$, *as the subspace*

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

Since H_m is a vector space we can find a basis $\{e_i\}_{i=1}^m$ for it and use this basis to express the hermitian symplectic form as a matrix with entries

$$\omega_{ij} = \langle e_i, e_j \rangle. \tag{3}$$

By the definition of the form, the matrix ω is a skew-hermitian, $\omega = -\omega^\star$, nondegenerate matrix. Using ω and the inner product on $\mathbb{C}^m$ it is easy to see that the hermitian symplectic form can be written

$$\langle \phi, \psi \rangle = (\phi, \omega\psi) \tag{4}$$

where, on the right hand side, ϕ and ψ are written as vectors in $\mathbb{C}^m$ using the basis $\{e_i\}_{i=1}^m$ and $(\cdot, \cdot)$ is the inner product in $\mathbb{C}^m$.
In the usual symplectic case ω is skew-symmetric and as is well known a skew-symmetric matrix of odd order is degenerate—consequently symplectic spaces are even dimensional. In the hermitian symplectic case this restriction does not apply and therefore there is no obstruction to having hermitian symplectic spaces of odd dimension. The following is a basic result of symplectic geometry which also holds in the hermitian symplectic case.

Lemma 3.1 *Given a hermitian symplectic subspace* $V \subset H_m$, $V^\perp$ *is also hermitian symplectic,*

$$V + V^\perp = H_m$$

and these subspaces have trivial intersection.

Proof: It is clear that the intersection $V \cap V^\perp$ is empty. Supposing instead that there is a $v \in V \cap V^\perp$ then v is skew-orthogonal to all the elements of V and hence the form is degenerate on V which is a contradiction.
Since the matrix ω_{ij} is nondegenerate the dimension of $V^\perp$ is the codimension

of V. But since these two spaces do not intersect, by a simple argument of linear independence

$$V + V^{\perp} = H_m.$$

Now we suppose that the form is degenerate on $V^{\perp}$, so there is some element $z \in V^{\perp}$ so that

$$\langle z, u \rangle = 0 \quad \forall u \in V^{\perp}$$

and

$$\langle z, v \rangle = 0 \quad \forall v \in V.$$

But this would imply that the form is degenerate on H_m which is a contradiction. $\square$

This lemma also holds in the case of symplectic geometry and is usually used to show the existence of a canonical basis in the following manner: As we have shown, a symplectic space is an even dimensional vector space so we can find some basis $\{e_i\}_{i=1}^{2n}$ for it. Let us pick $p_1 = e_1$. Then, since the form is nondegenerate, there is an element $\hat{q}_1$ such that $\langle p_1, \hat{q}_1 \rangle \neq 0$ and hence we can normalise so that

$$\langle p_1, q_1 \rangle = 1.$$

We denote by V_1 the linear span of $\{p_1, q_1\}$. This is clearly a symplectic space so we may apply the above lemma to it which implies that $V_1^{\perp}$ is also symplectic. Repeating this process for $V_1^{\perp}$ allows us to construct a *canonical basis.*

Definition 3.5 *A basis $\{p_i, q_i\}_{i=1}^{n}$ which has the following propery*

$$\begin{aligned} \langle p_i, q_j \rangle &= \delta_{ij} = -\langle q_i, p_j \rangle \\ \langle p_i, p_j \rangle &= 0 = \langle q_i, q_j \rangle \end{aligned}$$

where δ_{ij} is the Kronecker delta is known as a canonical basis.

In the hermitian symplectic case such a construction fails. Firstly the dimension of the space need not be even, but even if it is the construction may still fail. Let us suppose that we have a basis $\{e_i\}_{i=1}^{2n}$ so that the skew-hermitian matrix ω has the form

$$\omega = (\langle e_i, e_j \rangle) = i\mathbb{I}_{(2n)}.$$

We denote by $\mathbb{I} = (\delta_{ij})$ or $\mathbb{I}_{(n)}$ the $n \times n$ unit matrix. This case is obviously prohibited in the symplectic case but acceptable in the hermitian symplectic case. Now if it were possible to find a canonical basis in this space then there would be a non-singular transformation of the basis, P, such that ω would be transformed to

$$P^{\star} \omega P = \mathrm{J}$$

where J, known as the canonical symplectic structure, is

$$\mathrm{J} = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}.$$

This is clearly not possible. We use the fact that any non-singular transformation can be written as the product of a unitary and a hermitian matrix, $P = UH$. Consequently

$$iH^2 = P^\star \omega P = J$$

and the left hand side is a matrix with eigenvalues only on the imaginary axis in the upper half plane. The right hand side, J, however, has eigenvalues $\pm i$ equally distributed between the upper and lower half planes. We conclude that in general a hermitian symplectic space may not have a canonical basis.

Lemma 3.2 *A hermitian symplectic space H_m is, up to a non-singular transformation of the basis, completely characterised by two integers, n_+, n_-, $n_+ + n_- = m$. Specifically the matrix ω associated with the hermitian symplectic form can be diagonalised to i times the square root of unity*

$$i\mathbb{I}_{(n_+,n_-)}.$$

Furthermore H_m admits a canonical basis iff $n_+ = n_-$.

Proof: A hermitian symplectic space is specified by the matrix ω up to a non-singular transformation of the basis, P. The matrix $-i\omega$ is hermitian and hence it can be diagonalised

$$-i\omega = UDU^\star$$

where D is a real diagonal matrix without zeroes on the diagonal (ω is non-degenerate). Let us choose the matrix H as the *positive* diagonal matrix so that $D^2 = H^4$. Then choosing the non-singular transformation of the basis, $P = UH^{-1}$ we get

$$P^\star \omega P = iH^{-1}U^\star UDU^\star UH^{-1} = i\mathbb{I}_{(n_+,n_-)}.$$

Here we use the usual notation

$$\mathbb{I}_{(n_+,n_-)} \equiv \begin{pmatrix} \mathbb{I}_{(n_+)} & 0 \\ 0 & -\mathbb{I}_{(n_-)} \end{pmatrix}$$

and n_+ is the number of positive eigenvalues of $-i\omega$ and n_- the number of negative eigenvalues. Clearly, when $n_+ = n_- = n$ we not only have an even dimensional hermitian symplectic space but we can find a canonical basis. This follows from the fact that the characteristic polynomial of $i\mathbb{I}_{(n,n)}$, ie. $(i-\lambda)^n(-i-\lambda)^n$, is up to a sign the same as the characteristic polynomial of J and hence we can easily find a non-singular transformation taking one to the other. □

Another characterisation of a hermitian symplectic space with canonical basis is iff we can choose a basis so that the matrix ω is real—in this case we use the arguments of usual symplectic geometry.

Let us relate this back to the hermitian symplectic space created by the boundary form, equation (2), of a symmetric operator with equal deficiency indices. Actualy this is not a hermitian symplectic space as defined above since the form is degenerate on $\mathrm{Dom}(\mathcal{L}_0) \subset \mathrm{Dom}(\mathcal{L}_0^\star)$, a simple consequence of the fact the $\mathcal{L}_0$ is symmetric. Picking any $f \in \mathrm{Dom}(\mathcal{L}_0)$, $g \in \mathrm{Dom}(\mathcal{L}_0^\star)$ we see

$$\begin{aligned}
\mathcal{J}(f,g) &= (\mathcal{L}_0^\star f, g) - (f, \mathcal{L}_0^\star g) \\
&= (\mathcal{L}_0 f, g) - (f, \mathcal{L}_0^\star g) \\
&= (f, \mathcal{L}_0^\star g) - (f, \mathcal{L}_0^\star g) \\
&= 0.
\end{aligned}$$

We recall the well known fact of operator theory[2] that the domain of $\mathcal{L}_0^\star$ can be expressed

$$\mathrm{Dom}(\mathcal{L}_0^\star) = \mathrm{Dom}(\mathcal{L}_0) + \mathcal{N}_{+i} + \mathcal{N}_{-i}$$

where these three subspaces are linearly independent. The eigenspaces

$$\mathcal{N}_{\pm i} \equiv \ker(\mathcal{L}_0^\star \pm i)$$

are known as the deficiency subspaces, $\mathcal{L}_0^\star$ being the adjoint of $\mathcal{L}_0$. We define the deficiency indices (n_+, n_-) to be the dimensions

$$n_\pm \equiv \dim \mathcal{N}_{\pm i}.$$

Clearly the restriction of the boundary form to the subspace $\mathcal{N}_{+i}+\mathcal{N}_{-i}$ defines a nondegenerate hermitian symplectic form. We claim:

Lemma 3.3 *The hermitian symplectic space formed by the boundary form $\mathcal{J}$ on $\mathcal{N}_{+i} + \mathcal{N}_{-i}$ is characterised, in the sense of the previous lemma, by the deficiency indices $n_\pm$.*

Proof: Suppose that we have orthonormal bases $\{f_{+,i}\}_{i=1}^{n_+}$, $\{f_{-,i}\}_{i=1}^{n_-}$ for $\mathcal{N}_{+i}$ and $\mathcal{N}_{-i}$ respectively. We use these bases to write the boundary form as a matrix. By orthogonality

$$\langle f_{+,i}, f_{-,j} \rangle = 0.$$

Since $f_{\pm,i}$ satisfy

$$\mathcal{L}_0^\star f_{\pm,i} \pm i f_{\pm,i} = 0$$

we have

$$\begin{aligned}
\langle f_{+,i}, f_{+,j} \rangle &= (\mathcal{L}_0^\star f_{+,i}, f_{+,j}) - (f_{+,i}, \mathcal{L}_0^\star f_{+,j}) \\
&= i(f_{+,i}, f_{+,j}) + i(f_{+,i}, f_{+,j}) \\
&= 2i\delta_{ij}.
\end{aligned}$$

Similarly we see

$$\langle f_{-,i}, f_{-,j} \rangle = -2i\delta_{ij}$$

so that the matrix ω takes the form

$$\omega = 2i\mathbb{I}_{(n_+,n_-)}. \qquad \Box$$

In particular, a symmetric operator with equal deficiency indices has associated with it an even dimensional hermitian symplectic space which admits a canonical basis.

Remark 3.1 *In the remainder of this paper we will always assume that we are working with a hermitian symplectic space which is even dimensional and admits a canonical basis.*

We return to the question of describing the self-adjoint extensions in the form of boundary conditions at the origin. As described in the paper of Pavlov [13] the self-adjoint extensions correspond to Lagrange planes which we now define precisely.

Definition 3.6 *The subspace $N \subset H_{2n}$ is isotropic if*

$$N \subset N^{\perp}$$

Let us assume that we have fixed some even dimensional basis and have found the corresponding skew-hermitian matrix ω from equation (3). The following are all basic results of symplectic geometry.

Lemma 3.4 *The subspace $N \subset H_{2n}$ is isotropic iff the subspaces N and ωN are orthogonal in the Euclidian sense.*

Proof: Follows directly from equation (4). $\Box$

Lemma 3.5 *The dimension, k, of an isotropic subspace $N \subset H_{2n}$ never excedes n.*

Proof: Since the operator ω on $\mathbb{C}^{2n}$ is nondegenerate, the dimensions of N and ωN are the same. Consequently $k + k \leq 2n$, that is, $k \leq n$. $\Box$

Definition 3.7 *An isotropic subspace $\Pi_n \subset H_{2n}$ of maximal dimension, that is dimension n, is called a Lagrange plane.*

Corollary 3.1 *If $\Pi_n \subset H_{2n}$ is a Lagrange plane then $\Pi_n^{\perp} = \Pi_n$*

Proof: Well Π_n and $\Pi_n^{\perp}$ both have dimension n, and $\Pi_n \subset \Pi_n^{\perp}$. $\Box$

It is clear that in order to have the existence of a Lagrange plane we need a hermitian symplectic space which admits a canonical basis. It is also easy to see that the first n elements of a canonical basis span a Lagrange plane. On the other hand isotropic subspaces may exist in hermitian symplectic spaces of odd dimension.

Definition 3.8 *A matrix g is known as a J-unitary or hermitian symplectic matrix if it satisfies*

$$g^\star J g = J.$$

Clearly, the transformation such a matrix induces on H_{2n}, when H_{2n} is expressed in terms of $\mathbb{C}^{2n}$ (equation (3)) using a canonical basis, preserves the hermitian symplectic form. We now prove some results which allow us to parameterise the set of Lagrange planes in H_{2n}, the Lagrange Grassmannian, denoted by Λ_n.

Lemma 3.6 *A given Lagrange plane $\Pi_{0,n}$ can be made to coincide with any other Lagrange plane Π_n by means of a hermitian symplectic transformation of the form*

$$g = \begin{pmatrix} A & B \\ -B & A \end{pmatrix} \qquad A, B \in \mathbb{C}^{n\times n} \tag{5}$$

where A and B satisfy

$$\begin{aligned} A^\star A + B^\star B &= \mathbb{I} & (6)\\ A^\star B &= B^\star A. & (7) \end{aligned}$$

Specifically, we are given a canonical basis $\{\xi_{0,i}\}_{i=1}^{2n}$, the first n elements of which span the Lagrange plane $\Pi_{0,n}$. Then we can find the hermitian symplectic transformation g such that the first n elements of the canonical basis $\{\xi_i\}_{i=1}^{2n}$ given by

$$\xi_i = \sum_{j=1}^{2n} g_{ij}\xi_{0,j}$$

span Π_n.

Proof: From remark 3.1 there always exists a canonical basis $\{\xi_{0,i}\}_{i=1}^{2n}$ and we choose $\Pi_{0,n}$ to be the span of the first n elements of this basis. Using this canonical basis we can, as mentioned above, identify H_{2n} with $\mathbb{C}^{2n}$ where the matrix $\omega = \mathrm{J}$. Now we consider another arbitrary Lagrange plane Π_n. Since Π_n is an n-dimensional subspace of $\mathbb{C}^{2n}$ (using the identification above) we can find a set of n orthonormal–*in the Euclidian sense using the inner product in* $\mathbb{C}^{2n}$–vectors which form a basis for Π_n. Let us denote this basis by $\{\xi_i\}_{i=1}^{n}$. Since the $\{\xi_{0,i}\}$ form a basis for H_{2n} there are matrices A and B such that

$$\xi_i = \sum_j^n A_{i,j}\xi_{0,j} + \sum_j^n B_{i,j}\xi_{0,j+n} \quad \text{for } i = 1\ldots n. \tag{8}$$

Furthermore, since the $\{\xi_i\}$ are assumed to be orthonormal, in the Euclidian sense, we immediately have equation (6). Using the fact that the $\{\xi_i\}$ form a Lagrange plane in equation (4) gives us the second equation (7). Together these two equations imply that g is a hermitian symplectic transformation. □

In fact, it is easy to see that the conditions, equations (6,7), which imply that g is a hermitian symplectic matrix are also equivalent to it being a unitary matrix. Hence it preserves the hermitian symplectic form and the Euclidian inner product. Let us denote by $\mathcal{G}$ the set of matrices of the form

$$\mathcal{G} = \left\{ g = \begin{pmatrix} A & B \\ -B & A \end{pmatrix} ;\ A, B \in \mathbb{C}^{n\times n},\ g \in \mathsf{U}(2n) \right\}$$

which occur in the above lemma. It is easy to see that $\mathcal{G}$ is a group under matrix multiplication. In order to classify Λ_n we need to find the stationary subgroup of $\mathcal{G}$, ie. the $\mathcal{H} \subset \mathcal{G}$, the elements of which take the Lagrange plane $\Pi_{0,n}$ into itself. But it is easy to see that in the notation of the above lemma these are just those matrices with $B = 0$. The stationary subgroup $\mathcal{H}$ is the set of matrices

$$\mathcal{H} = \left\{ h = \begin{pmatrix} C & 0 \\ 0 & C \end{pmatrix} ;\ C \in \mathbb{C}^{n\times n},\ h \in \mathsf{U}(2n) \right\}.$$

Lemma 3.7 *The set of Lagrange planes Λ_n is in one-to-one correspondence with the unitary group.*

$$\Lambda_n \simeq \mathcal{G}/\mathcal{H} \simeq \mathsf{U}(n)$$

Proof: The first isomorphism is by definition. To see the second we use the unitary matrix

$$W = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I} & i\mathbb{I} \\ i\mathbb{I} & \mathbb{I} \end{pmatrix}$$

Our choice of W is motivated by the fact that it diagonalises in 'blockwise' sense matrices of the form given by equation (5). Precisely

$$WgW^\star = W \begin{pmatrix} A & B \\ -B & A \end{pmatrix} W^\star = \begin{pmatrix} A - iB & 0 \\ 0 & A + iB \end{pmatrix}.$$

Since g is unitary so too is $WgW^\star$ and hence, $A - iB$ and $A + iB$ must also be unitary.
Now instead of considering the groups $\mathcal{G}$ and $\mathcal{H}$, we consider the unitarily equivalent groups

$$\hat{\mathcal{G}} = W\mathcal{G}W^\star = \left\{ \hat{g} = \begin{pmatrix} S & 0 \\ 0 & T \end{pmatrix} ;\ S, T \in \mathsf{U}(n) \right\}$$

and, since the elements of $\mathcal{H}$ are already on the diagonal,

$$\hat{\mathcal{H}} = W\mathcal{H}W^\star = \left\{ \hat{h} = \begin{pmatrix} C & 0 \\ 0 & C \end{pmatrix} ;\ C \in \mathsf{U}(n) \right\}.$$

It is easy to see that we can represent the set of cosets $\hat{\mathcal{G}}/\hat{\mathcal{H}}$ by the section from $\hat{\mathcal{G}}$ of matrices where the bottom right block is of the form $T = \mathbb{I}$, that is

$$\Lambda_n \simeq \hat{\mathcal{G}}/\hat{\mathcal{H}} \simeq \left\{ \hat{g} = \begin{pmatrix} U & 0 \\ 0 & \mathbb{I} \end{pmatrix} ;\ U \in \mathsf{U}(n) \right\}.$$

This establises the result. □

Corollary 3.2 *A given Lagrange plane can be made to coincide with any other Lagrange plane by means of a hermitian symplectic transformation of the form*

$$g = W^\star \hat{g} W = W^\star \begin{pmatrix} U & 0 \\ 0 & \mathbb{I} \end{pmatrix} W = \frac{1}{2} \begin{pmatrix} U+\mathbb{I} & i(U-\mathbb{I}) \\ -i(U-\mathbb{I}) & U+\mathbb{I} \end{pmatrix} \qquad (9)$$

where U is a unitary matrix.

4 Parameterisation of self-adjoint boundary conditions

We now consider the specific case of the Schrödinger operator on Γ_n or $\oplus_{i=1}^{n} L^2([0,\infty))$, ie. acting on vectors with n components. A simple calculation using integration by parts shows that the boundary form can be expressed

$$(\mathcal{L}_0^\star \psi, \phi) - (\psi, \mathcal{L}_0^\star \phi) = \sum_{j=1}^{n} [\bar{\psi}_i \phi_{i,x} - \bar{\psi}_{i,x} \phi_i]\big|_0 \qquad (10)$$

where the subscript $_x$ denotes differentiation with respect to x, and we use the notation $|_0$ to denote evaluation at $x=0$. Hence the boundary form may be thought of as acting in the $2n$-dimensional hermitian symplectic space, H_{2n}, of boundary values at the origin (the degenerate subspace $\mathrm{Dom}(\mathcal{L}_0)$ consists of just those elements with $\phi_i|_0 = \phi_{i,x}|_0 = 0$). Written in this way the form defines a canonical basis; the hermitian symplectic form defined by the boundary form is

$$\langle \psi, \phi \rangle = (\psi, \mathrm{J}\phi)$$

where on the right hand side the inner product is in $\mathbb{C}^{2n}$ and ψ, ϕ are vectors in $\mathbb{C}^{2n}$ of the form

$$(\psi_1|_0, \ldots, \psi_n|_0, \psi_{1,x}|_0, \ldots, \psi_{n,x}|_0)^T.$$

Let us represent this canonical basis explicitly by the elements $\{\xi_{0,i}\}_{i=1}^{2n} \in H_{2n}$ where for $i = 1, \ldots, n$, $\xi_{0,i}$ represents the boundary condition $\psi_i|_0 = 1$; and for $i = n+1, \ldots, 2n$ it represents the boundary condition $\psi_{i,x}|_0 = 1$. The first n and last n elements of a canonical basis each span a Lagrange plane—the first n basis vectors specify self-adjoint Neumann boundary conditions, and the last n basis vectors specify self-adjoint Dirichlet boundary conditions.

We fix a unitary matrix U and consider the associated self-adjoint boundary conditions/Lagrange plane. From corollary 3.2 the basis for the Lagrange plane defined by U is given by

$$\xi_i = \sum_{j=1}^{2n} g_{ij} \xi_{0,j} \quad \text{for } i = 1, \ldots, n,$$

where $\xi_{0,j}$ is defined above and g is defined by equation (9). Writing this in terms of boundary values we see that (up to a transposition) the set of self-adjoint boundary values is

$$(\psi_1|_0, \ldots, \psi_n|_0, \psi_{i,x}|_0, \ldots, \psi_{n,x}|_0)^T \in \operatorname{Ran} \begin{pmatrix} \frac{1}{2}(U+\mathbb{I}) \\ \frac{i}{2}(U-\mathbb{I}) \end{pmatrix}.$$

It is convenient to have the self-adjoint boundary *conditions*, ie. to have an expression in terms of the kernel rather than the range of a matrix. This is possible if we note that

$$\operatorname{Ran} \begin{pmatrix} \frac{1}{2}(U+\mathbb{I}) \\ \frac{i}{2}(U-\mathbb{I}) \end{pmatrix} \subset \ker \left(\frac{i}{2}(U^\star - \mathbb{I}),\ \frac{1}{2}(U^\star + \mathbb{I}) \right)$$

which follows from equation (7), that is

$$\left(\frac{i}{2}(U^\star - \mathbb{I}),\ \frac{1}{2}(U^\star + \mathbb{I}) \right) \begin{pmatrix} \frac{1}{2}(U+\mathbb{I}) \\ \frac{i}{2}(U-\mathbb{I}) \end{pmatrix} = 0. \tag{11}$$

Since both of these matrices are of maximal rank, ie. rank n, the dimension of both kernel and range is n which gives us equality. Consequently, the boundary conditions may be expressed

$$\frac{i}{2}(U^\star - \mathbb{I})\, \psi|_0 + \frac{1}{2}(U^\star + \mathbb{I})\, \psi_x|_0 = 0. \tag{12}$$

As far as we are aware this is a novel formulation of the self-adjoint boundary conditions. One of the advantages of the above formulation is that it is readily generalisable—we may parameterise the self-adjoint boundary conditions, using the boundary form equation (2), of any symmetric operator using this framework. Furthermore, in the case of non-equal deficiency indices, we may use this framework to parameterise the symmetric extensions of a symmetric operator—although in this case there are no Lagrange planes/self-adjoint extensions.

4.1 The asymptotics of the scattering matrix in terms of the boundary conditions

Here it is convenient for us to consider the problem for the Schrödinger operator on the graph with n rays as a matrix problem (with diagonal potential, see [8, 7]). Let us consider the set of n solutions of Schrödinger equation $\mathcal{L}\Xi = \lambda \Xi$ on the graph with boundary conditions at the origin

$$\Xi\Big|_0 = \frac{1}{2}(U+\mathbb{I}) \equiv A, \qquad \Xi_x\Big|_0 = \frac{i}{2}(U-\mathbb{I}) \equiv B. \tag{13}$$

Here we are assuming that Ξ is an $n \times n$ matrix with each column being a solution of Schrödinger equation on the graph such that the matrix satisfies the above equation at $x = 0$. It is clear that each column of Ξ satisfies the self-adjoint boundary conditions, ie. equation (12), and hence is an eigenvalue of the self-adjoint Schrödinger operator on the graph with boundary conditions prescribed by U.
Likewise we can define the Jost solutions, $F_\pm$, as the matrix of solutions of the homogeneous equation $\mathcal{L}F_\pm = \lambda F_\pm$, with asymptotic behaviour

$$\lim_{x\to\infty} F_\pm(x,k) \sim e^{\pm ikx}\mathbb{I},$$

and no prescribed behaviour at the origin. We will always denote $\lambda = k^2$. As the Jost solutions form a complete set of solutions we can write

$$\Xi(x,k) = F_-(x,k)M_-(k) + F_+(x,k)M_+(k). \tag{14}$$

In this notation we define the scattering wave solutions

$$\Psi(x,k) \equiv \Xi(x,k)M_-^{-1} = F_- + F_+S(k)$$

where $S(k)$ is known as the scattering matrix. The coefficients $M_\pm$ can be evaluated by taking the Wronskian of Ξ and F_+ or F_- [8]

$$M_\pm = \pm\frac{1}{2ik}\left[\mathsf{F}_\pm^\dagger B - \mathsf{F}_{\pm,x}^\dagger A\right]. \tag{15}$$

where $\mathsf{F}_\pm(k) \equiv F_\pm(0,k)$ are known as the Jost functions and † is the involution $Y^\dagger(x,k) \equiv Y^\star(x,\bar{k})$. The Wronskian of $\Xi^\dagger$ and Ξ

$$W\{\Xi^\dagger,\Xi\} = \left[\Xi^\dagger\Xi_x - \Xi^\dagger{}_x\Xi\right]\Big|_0 = A^\star B - B^\star A = 0,$$

is always zero. Moreover, if we write Ξ in terms of the scattering wave solutions

$$\begin{aligned} W\{\Xi^\dagger,\Xi\} &= M_-^\dagger W\{F_-^\dagger + S^\dagger F_+^\dagger, F_- + F_+S\}M_- \\ &= 2ikM_-^\dagger\left[-\mathbb{I} + S^\dagger S\right]M_- = 0. \end{aligned}$$

we see, since $S^\dagger = S^\star$ for $k \in \mathbb{R}$, that the scattering matrix is unitary for real k.
If we diagonalise U, and use the well known asympototics of the Jost functions [1, 8] in the above expression for $M_\pm$, we see that the scattering matrix has the following asymptotic behaviour:

Lemma 4.1 *Given the self-adjoint operator $\mathcal{L}$, with associated unitary matrix U defining the boundary conditions of $\mathcal{L}$, the scattering matrix of $\mathcal{L}$ has the asymptotics*

$$\lim_{k\to\infty} S(k) \sim \hat{U}$$

where $\hat{U}$ is a unitary hermitian *matrix $\hat{U} = \hat{U}^\star$ derived from U by applying the map*

$$z \mapsto \begin{cases} 1 & : z \in \mathbb{T} \setminus \{-1\} \\ -1 & : z = -1 \end{cases}$$

to the spectrum of U.

Here $\mathbb{T}$ is the unit circle in $\mathbb{C}$.

Proof: Let us diagonalise the matrix U. In this basis, using equation (15) and the well known asymptotics of the Jost functions, the asymptotic expression for the scattering matrix is a diagonal matrix with entries

$$\lim_{k\to\infty} - \left[(e^{i\varphi_j} - 1) + k(e^{i\varphi_j} + 1)\right] \left[(e^{i\varphi_j} - 1) - k(e^{i\varphi_j} + 1)\right]^{-1}.$$

where the $e^{i\varphi_j}$ are the (unitary) eigenvalues of U. There are two cases; when $e^{i\varphi_j} = -1$, this limit is clearly -1, and when $e^{i\varphi_j} \neq -1$ then the limit is 1. This completes the proof. □

Those boundary conditions which are defined by unitary matrices which are also hermitian matrices can be expressed by projections—the terms $\frac{1}{2}(U \pm \mathbb{I})$ are really orthogonal projections

$$\begin{aligned} P &= \frac{1}{2}(U + \mathbb{I}) \\ P^\perp &= \mathbb{I} - P = -\frac{1}{2}(U - \mathbb{I}). \end{aligned}$$

which follows simply from the fact that $U = U^\star = U^{-1}$. Using this notation and orthogonality we can write the boundary conditions, equation (12),

$$P^\perp\, \psi|_0 = 0, \qquad P\, \psi_x|_0 = 0. \tag{16}$$

Consequently these boundary conditions are characterised by the fact that the conditions on the functions and the derivatives of the functions at the origin are independently specified.

The associated scattering matrix has the form

$$S(k) = -\left[i\mathsf{F}_+^\dagger P^\perp + \mathsf{F}_{+,x}^\dagger P\right]\left[i\mathsf{F}_-^\dagger P^\perp + \mathsf{F}_{-,x}^\dagger P\right]^{-1}. \tag{17}$$

In the case of zero potential, the Jost solutions are then just the exponential functions we see that the scattering matrix

$$\begin{aligned} S(k) &= -\left[P^\perp - kP\right]\left[P^\perp + kP\right]^{-1} \\ &= -\left[P^\perp - kP\right]\left[P^\perp + \frac{1}{k}P\right]^{-1} \\ &= -P^\perp + P \\ &= -\mathbb{I} + 2P = U \end{aligned} \tag{18}$$

is constant. Therefore the scattering wave has no poles and there are no discrete eigenvalues.
In contrast, if U is not hermitian, we *will* have discrete eigenvalues, or alternatively resonances, when the potential is identically zero—a 'zero-range potential' at the origin. This is in analogy to the case of the Schrödinger operator on the line with zero potential but boundary conditions at the origin which correspond to a delta function; such an operator will clearly have either a discrete eigenvalue or resonance.

5 The Schrödinger Operator on Graphs with non-trivial Compact Part

Here we study an arbitrary 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 $H(\Gamma)$

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

The potentials q_i are continuous real functions which are integrable with finite first moment as in equation (1). The domain of $\mathcal{L}_0$ is defined as the set of smooth functions with compact suppport in the open intervals

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

It is easy to see that the deficiency indices of $\mathcal{L}_0$ are $(n+2p, n+2p)$. Consequently we may consider the self-adjoint extensions of $\mathcal{L}_0$ and indeed, using the results of the previous sections, parameterise these extensions by the unitary matrices $\mathsf{U}(n+2p)$. We will not discuss the details of the self-adjoint boundary conditions for an arbitrary graph Γ—the reader may find a discussion of this problem in [9]. Instead we just assume that we are given some $\mathcal{L}$ which satisfies self-adjoint boundary conditions at the vertices of $\mathcal{G}$.

In the above dicussion no mention was made of the precise structure of the graph Γ, ie. the structure of the compact graph Γ_c or points at which the n rays are attached to Γ_c. This assumes that we are free to specify boundary conditions between end-points of edges in an arbitrary way.
From a physical point of view however this is not acceptable. Rather, we are given the structure of Γ, ie. the way in which the end-points of edges are identified to form vertices is specified. Then in defining the self-adjoint boundary conditions we allow *only* boundary conditions between the end-points of edges which are identified at a vertex. Then we say that the self-adjoint operator $\mathcal{L}$ defined on Γ with such boundary conditions has *separated* boundary conditions. On the other hand, given a self-adjoint $\mathcal{L}$ we can always find an underlying graph Γ such that $\mathcal{L}$ has separated boundary conditions—we can always choose the graph with only one vertex.
In the case of separated boundary conditions the boundary conditions will not be parameterised by a unitary matrix from $\mathsf{U}(n+2p)$. Let us suppose that Γ has m vertices, with degrees $d(i)$ where $i = 1, \ldots, m$. Then the self-adjoint boundary conditions at vertex i are parameterised by a matrix from $\mathsf{U}(d(i))$. Consequently the set of all separated self-adjoint boundary conditions is parameterised by

$$\mathsf{U}(d(1)) \oplus \cdots \oplus \mathsf{U}(d(m)). \tag{19}$$

In any context where we are considering subgraphs of a given graph, for instance in the factorisation problem discussed in the following sections it is natural to assume that we have separated boundary conditions. For the other parts of this chapter, for instance in our discussion of the scattering matrix, it is not necessary to assume separated boundary conditions.

6 The Hermitian symplectic geometry of the asymptotic solutions

In this section, we construct a particular hermitian symplectic space which will be useful firstly in proving the unitarity of the scattering matrix and secondly in the factorisation problem. This construction follows an analogous construction by Novikov [12] for the discrete Schrödinger operator on graphs. Let us suppose that we are given a graph Γ and associated Hilbert space $H(\Gamma)$. In particular, we fix a representation of functions on the graph by $n+p$-dimensional vectors.

Definition 6.1 *The two-form $\langle \cdot, \cdot \rangle$, defined on (not necessarily square integrable) functions on the* rays *of the graph*

$$\langle \phi, \psi \rangle \equiv \sum_{i=1}^{n} \left[\bar{\phi}_i \psi_i' - \bar{\phi}_i' \psi_i \right] \Big|_{x_i \in [0,\infty)} \tag{20}$$

is a hermitian symplectic form. The evaluation is at an arbitrary point on each of the rays of the graph.

Let us consider the set of generalised eigenfunctions on the rays for spectral parameter λ

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

In particluar the functions from $H_{2n}(\Gamma, \mathcal{L}_0, \lambda)$ do not necessarily obey any boundary conditions at the vertices. Obviously $H_{2n}(\Gamma, \mathcal{L}_0, \lambda)$ is a $2n$-dimensional vector space (the Jost solutions or standard solutions on the rays form bases). The potentials on the rays $q_i(x_i)$ are given by the potentials of the operator $\mathcal{L}_0$. Often we assume that the graph Γ and the potentials, $\mathcal{L}_0$, are given and simply write $H_{2n}(\lambda)$ or H_{2n}.

Definition 6.2 *The vector space of generalised eigenfunctions on the rays $H_{2n}(\Gamma, \mathcal{L}_0, \lambda)$ for real λ equipped with the hermitian symplectic form of equation (20) is known as the asymptotic hermitian symplectic space.*

Our terminology is in analogy with the term—asymptotic symplectic space—used by Novikov [12].
To see that this is indeed a hermitian symplectic space we need only show that the form is nondegenerate. Not only is it nondegenerate but this space (as promised in remark 3.1) admits a canonical basis. To see this, consider the basis formed by the standard solutions $\{\theta_i, \phi_i\}^n$. These are the solutions which satisfy the boundary conditions

$$\begin{aligned} \theta_i|_0 &= 1, \quad & \theta_{i,x}|_0 &= 0 \\ \phi_i|_0 &= 0, \quad & \phi_{i,x}|_0 &= 1 \end{aligned}$$

on ray i and are zero on the other rays. It is not difficult to see that these form a canonical basis

$$\begin{aligned} \langle \theta_i, \phi_j \rangle = \delta_{ij} &= -\langle \phi_i, \theta_j \rangle \\ \langle \theta_i, \theta_j \rangle = 0 &= \langle \phi_i, \phi_j \rangle. \end{aligned}$$

In the case of the graph with trivial compact part this hermitian symplectic form is identical to the Wronskian

$$\langle \Phi, \Psi \rangle \equiv W\{\Phi^\dagger, \Psi\} = \Phi^\dagger \Psi_x - \Phi_x^\dagger \Psi$$

discussed above when we consider only positive λ. The main difference is that in the Wronskian of the previous subsection we apply the operation † to the first argument, instead of complex conjugation. We could define the asymptotic hermitian symplectic space in a similar manner and then we would be able to lift the assumption of real λ, however, as we are only interested in real λ here we will use the simlper definition.

The standard solutions are not a very useful basis 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 j-th where they coincide with the Jost solution

$$\lim_{x_i \to \infty} f_{\pm,j} = e^{\pm ikx_j}.$$

Again we use the notation $\lambda = k^2$. The fact that our two-form is defined using complex-conjugation (instead of †) complicates the hermitian symplectic form on the Jost solutions. We have

$$\begin{aligned} \langle f_{+,i}, f_{+,j} \rangle = 2ik\delta_{ij} = -\langle f_{-,i}, f_{-,j} \rangle \\ \langle f_{+,i}, f_{-,j} \rangle = 0 = \langle f_{-,i}, f_{+,j} \rangle \end{aligned} \tag{21}$$

but only for $\lambda > 0$ or $k \in \mathbb{R}$.
We can also construct a canonical basis using the Jost solutions, consider

$$\begin{aligned} \psi_{0,j} &= \frac{f_{+,j} + f_{-,j}}{2} \\ \chi_{0,j} &= \frac{f_{+,j} - f_{-,j}}{2ik} \end{aligned}$$

where $j = 1, \ldots, n$. The hermitian symplectic form on this basis gives

$$\begin{aligned} \langle \psi_{0,i}, \chi_{0,j} \rangle = \delta_{ij} = -\langle \chi_{0,i}, \psi_{0,j} \rangle \\ \langle \psi_{0,i}, \psi_{0,j} \rangle = 0 = \langle \chi_{0,i}, \chi_{0,j} \rangle \end{aligned}$$

so that it is a canonical basis. Note that these relations hold for all real λ, unlike the relations for the Jost solutions.

Now let us suppose that we have defined a self-adjoint $\mathcal{L}$ on the graph, an extension of $\mathcal{L}_0$. The generalised eigenfunctions of $\mathcal{L}$ are (not necessarily square integrable) solutions of the eigenvalue equation $\mathcal{L}\phi = \lambda\phi$. We also call the elements of $H_{2n}(\lambda)$ generalised eigenfunctions; the distinction is that the elements of $H_{2n}(\lambda)$ are only solutions on the rays and do not obey any self-adjoint boundary conditions at the vertices. It is clear that the generalised eigenfunctions of $\mathcal{L}$ at some real λ project onto elements of $H_{2n}(\lambda)$ and we will implicitly assume this projection in the sequel when we speak of the generalised eigenfunctions of $\mathcal{L}$ in $H_{2n}(\lambda)$.
It is the following observation by Novikov [12] which makes the asymptotic hermitian symplectic space useful for us:

Lemma 6.1 *Given the self adjoint extension $\mathcal{L}$, the generalised eigenspace of $\mathcal{L}$ at some real λ forms an isotropic subspace in $H_{2n}(\lambda)$.*

Proof: We formally[2] consider the boundary form of generalised eigenfunctions ϕ and ψ

$$(\mathcal{L}\phi,\psi)_\Gamma-(\phi,\mathcal{L}\psi)_\Gamma=\sum_{i=1}^{n}\left[\bar{\phi}_i\psi_i'-\bar{\phi}_i'\psi_i\right]\Big|_0-\sum_{j=1}^{l}\left[\bar{\phi}_{n+j}\psi_{n+j}'-\bar{\phi}_{n+j}'\psi_{n+j}\right]\Big|_0^{a_j}. \tag{22}$$

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

$$\sum_{i=1}^{n}\left[\bar{\phi}_i\psi_i'-\bar{\phi}_i'\psi_i\right]\Big|_0=\langle\phi,\psi\rangle=0. \tag{23}$$

This completes the proof. □

In Novikov's paper [12] the analogous statement is proved in theorem 3. Novikov shows that the eigenspaces form *Lagrange planes* for *any* complex value of λ. Here we are able to show that the generalised eigenspaces form Lagrange planes for any real λ.

Lemma 6.2 *Given the self-adjoint extension $\mathcal{L}$, the vector space of generalised eigenfunctions of $\mathcal{L}$ at real eigenvalue λ and with support on the rays of the graph is n-dimensional.*

We give the proof of this lemma in the Appendix as it depends on the results of the final section.

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

Corollary 6.1 *Given the self adjoint extension $\mathcal{L}$, the space of generalised 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 generalised eigenfunctions of the form

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

[2] As the generalised eigenfunctions are not square integrable.

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

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

where we have used equation (21) for real k. Hence, the scattering matrix is unitary for $\lambda > 0$ or real k.
The original idea for this proof is to be found in corollary 2 of Novikov's paper [12] where the author uses it to prove the *symmetry* of the scattering matrix (this again is due to the fact that he is using symplectic geometry).
Similarly we can find a condition for the symmetry of the scattering matrix. In the paper of Kostrykin and Schrader [9] the authors show that if the boundary conditions of an operator can be expressed using real matrices (in our notation $U \in \mathsf{O}(n)$) then the scattering matrix is symmetric. Suppose we have real boundary conditions, ie. $U \in \mathsf{O}(n)$, then this is equivalent to 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

$$\begin{aligned} 0 &= \langle \bar{\psi}_i, \psi_j \rangle \\ &= \langle f_{+,i} + \sum_l \bar{S}_{il} f_{-,l}, f_{-,j} + \sum_m S_{jm} f_{+,m} \rangle \\ &= 2ik [\sum_m S_{jm} \delta_{im} - \sum_l S_{il} \delta_{lj}] \end{aligned}$$

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 factorisation problem.

7 The scattering matrix as parameter of the Lagrange planes

We have shown that the space of generalised eigenfunctions corresponds to a Lagrange plane, and that the Lagrange planes are parameterised by a unitary matrix. It is not difficult to see that in this case this unitary matrix is in fact the scattering matrix when $\lambda > 0$. First we define some appropriate notation.

We emphasise that in the remainder we will assume that $\lambda > 0$ or $k \in \mathbb{R}_0 \equiv \mathbb{R}/\{0\}$. Now we define a new hermitian symplectic form simply by dividing the old form by k

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

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

$$\begin{aligned} \langle f_{+,i}, f_{+,j} \rangle = 2i\delta_{ij} = -\langle f_{-,i}, f_{-,j} \rangle \\ \langle f_{+,i}, f_{-,j} \rangle = 0 = \langle f_{-,i}, f_{+,j} \rangle . \end{aligned} \tag{24}$$

However, the canonical basis $\psi_{0,i}$, $\chi_{0,i}$ defined above is not canonical anymore. Instead we define the canonical basis

$$\begin{aligned} \psi_{0,j} &= \frac{f_{+,j} + f_{-,j}}{2} \\ \chi_{0,j} &= \frac{f_{+,j} - f_{-,j}}{2i} \end{aligned} \tag{25}$$

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

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

where $j = 1, \ldots, n$ to denote these basis vectors.
Now we recall corollary 3.2. Let us denote by $\Pi_{0,n}$ the Lagrange plane spanned by the first n vectors of the canonical basis $\{\xi_{0,i}\}_{i=1}^{2n}$. Then this corollary becomes:

Theorem 7.1 *The Lagrange plane Π_n corresponding to the generalised eigenspace of a self-adjoint $\mathcal{L}$ can be made to coincide with $\Pi_{0,n}$ by means of the hermitian symplectic transformation of the form*

$$g = W^\star \hat{g} W = W^\star \begin{pmatrix} S & 0 \\ 0 & \mathbb{I} \end{pmatrix} W = \frac{1}{2} \begin{pmatrix} S + \mathbb{I} & i(S - \mathbb{I}) \\ -i(S - \mathbb{I}) & S + \mathbb{I} \end{pmatrix} \tag{26}$$

where S is the scattering matrix.
In particular, the canonical basis $\{\xi_{0,i}\}_{i=1}^{2n}$ of equation (25) 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 get for $i = 1, \ldots, n$

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

which is the scattering wave solution. □

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

$$\chi_j = \xi_{j+n}$$

where again $j = 1, \ldots, n$, and it is easy to see that they have the form

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

Clearly this construction only works for $k \in \mathbb{R}_0$ when the scattering matrix is unitary. In the above sections the matrix U plays the rôle of a unitary 'parameter' which we were free to choose in order to select self-adjoint boundary conditions and hence a Lagrange plane. Here it is not at all clear how much freedom we have in selecting the unitary function $S(k)$—it depends in some complicated way on the potentials on the edges and the boundary conditions at the vertices.

8 The factorisation problem for the graph

Suppose that we are given two (or more) 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 link are outside of the support of the potential. The main idea in our approach is that of solutions which 'match' on the linking rays. Suppose we truncate ray $r' \in \Gamma'$ to length a' and likewise we truncate ray $r'' \in \Gamma''$ to length a'' and then join these rays end to end. We say that a solution on Γ' matches a solution on Γ'' on the newly formed edge if together they form a solution which is continuous with

continuous derivative at the point at which the rays join.
Then it is easy to see that any generalised eigenfunction of the operator $\mathcal{L}$ on the graph Γ can be represented by a generalised eigenfunction of $\mathcal{L}'$ on Γ' plus a generalised eigenfunction of $\mathcal{L}''$ on Γ'' such that these two generalised eigenfunctions match on *all* of the linking rays. This will give us a basis for the generalised eigenfunctions of $\mathcal{L}$ on Γ and hence the scattering matrix and the solution to the factorisation problem.
Sometimes this procedure gives us solutions with support only on the linking rays. These solutions have to be discarded as the Lagrange plane of generalised eigenfunctions consists of solutions with support on the rays.
We know that in terms of the asymptotic hermitian symplectic space the generalised eigenspaces form Lagrange planes. We will show that the set of solutions on the linking rays which 'match' is an isotropic subspace. Consequently the space of generalised eigenfunctions of the linked graph Γ is (modulo the isotropic subspace representing the matching solutions) the intersection of the Lagrange plane corresponding to the space of generalised eigenfunctions on the graphs Γ' and Γ'' with the orthogonal complement of this isotropic subspace. From the generalised eigenspace of Γ we can find the scattering matrix of $\mathcal{L}$ on Γ.

8.1 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; $\text{supp}(q_{r'}) \subset [0, a']$ and $\text{supp}(q_{r''}) \subset [0, a'']$, respectively. Then the edges $e' = [0, a']$ and $e'' = [0, a'']$ are formed by truncating the rays r' and r'' at a' and a'', respectively. We link the two graphs Γ' and Γ'' simply by joining these edges end to end thereby forming a new edge in the interior of Γ of length $a' + a''$.

Definition 8.1 *Given $\psi_{\Gamma'} \in H_{2m'}(\Gamma', \lambda)$ and $\psi_{\Gamma''} \in H_{2m''}(\Gamma'', \lambda)$ we say that these generalised eigenfunctions match on the edge formed by joining e' and e'' end to end if*

$$\begin{aligned} \psi_{\Gamma'}\Big|_{a'} &= \psi_{\Gamma''}\Big|_{a''} \\ \frac{d\psi_{\Gamma'}}{dx}\Big|_{a'} &= -\frac{d\psi_{\Gamma''}}{dx}\Big|_{a''} \end{aligned} \tag{27}$$

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.

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 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 8.1 *The element*

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

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

$$\begin{aligned} \langle \psi_{\Gamma'} \oplus \psi_{\Gamma''},\, \zeta f_{+,r'} \oplus f_{-,r''} \rangle &= 0 \\ \langle \psi_{\Gamma'} \oplus \psi_{\Gamma''},\, f_{-,r'} \oplus \zeta f_{+,r''} \rangle &= 0 \end{aligned} \tag{28}$$

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

$$\begin{aligned} \psi_{\Gamma'}\Big|_{r'} &= \alpha' f_{+,r'} + \beta' f_{-,r'} \\ \psi_{\Gamma''}\Big|_{r''} &= \alpha'' f_{+,r''} + \beta'' f_{-,r''} \end{aligned}$$

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

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

In order for equation (27) 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',

$$\bar{\zeta}\alpha' = \beta'', \quad \beta' = \bar{\zeta}\alpha''.$$

On the other hand, using equation (24), we have

$$\begin{aligned} 2i\bar{\alpha}' &= \langle \psi_{\Gamma'}, f_{+,r'} \rangle_{\Gamma'}, & -2i\bar{\beta}' &= \langle \psi_{\Gamma'}, f_{-,r'} \rangle_{\Gamma'} \\ 2i\bar{\alpha}'' &= \langle \psi_{\Gamma''}, f_{+,r''} \rangle_{\Gamma''} & -2i\bar{\beta}'' &= \langle \psi_{\Gamma''}, f_{-,r''} \rangle_{\Gamma''} \end{aligned}$$

so equation (27) becomes

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

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

Corollary 8.1 *The subspace of H_{2m} of elements with support confined to the rays r' and r'' and which match there 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 (28). Furthermore, the fact that these basis vectors satisfy equation (28) means that they are contained in their orthogonal complement, ie. 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 $m = m' + m''$, $n = n' + n''$ and, consequently, $m = n + 2p$.
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 generalisation of lemma 8.1, 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 8.1 the elements $\psi \in H_{2m}$ which match on each of the linking rays are just those elements $\psi \perp N$, ie. 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 8.2 *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 $\zeta_i = e^{-ika_i}$ 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.

8.2 Description of the Lagrange plane of generalised 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 linked graph Γ.
We recall that any generalised eigenfunction of $\mathcal{L}$ can be written as a generalised eigenfunction of $\mathcal{L}'$ on Γ' plus a generalised eigenfunction of $\mathcal{L}''$ on Γ'' such that these two functions match on all of the linking rays. This can be stated in the 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 generalised eigenfunctions on Γ' and Γ'') and $N^\perp$ (the solutions which match on the linking rays) gives us the generalised 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. This is linked to the fact that $\Pi_m \cap N^\perp$ is not generaly a Lagrange plane in H_{2m}. 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 $N^\perp/N$.

Lemma 8.2 *$N^\perp/N$ is a hermitian symplectic space of dimension $2n$*

Proof: Since the form is nondegenerate

$$\begin{aligned}\dim(N^\perp) &= \dim(H_{2m}) - \dim(N)\\ &= 2m - 2p\\ &= 2n + 2p\end{aligned}$$

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

$$\langle \phi + n_1, \psi + n_2 \rangle = \langle \phi, \psi \rangle \quad \phi, \psi \in N^\perp;\ n_1, n_2 \in N$$

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

$$\langle \phi, \psi \rangle = 0 \quad \forall \psi \in N^\perp$$

But this simply means that $\phi \in N$, ie. ϕ is in the coset containing zero. $\square$

The space $N^\perp/N$ has the correct dimension, moreover, it consists of solutions that match on all the linking rays. For this reason that 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 generalised 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 generalised eigenspace of $\mathcal{L}$ on Γ. Furthermore we show that this is a Lagrange plane.

Theorem 8.1 *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 only need to show that it has maximal dimension.

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

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

$$\begin{aligned} \dim(\Pi_m \cap N^\perp) &= \dim(H_{2m}) - \dim(\Pi_m + N) \\ &= 2m - \dim(\Pi_m + N) \end{aligned}$$

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

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

□

Corollary 8.3 *The Lagrange plane* $(\Pi_m \cap N^\perp)/N$ *in* $N^\perp/N$ *corresponds to the space of generalised eigenfunctions with support on the rays for the operator* $\mathcal{L}$ *on the graph* Γ.

It is easy to see that this description generalises 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.

In the next subsection, we find the explicit form of the scattering matrix for the linked graph.

8.3 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.

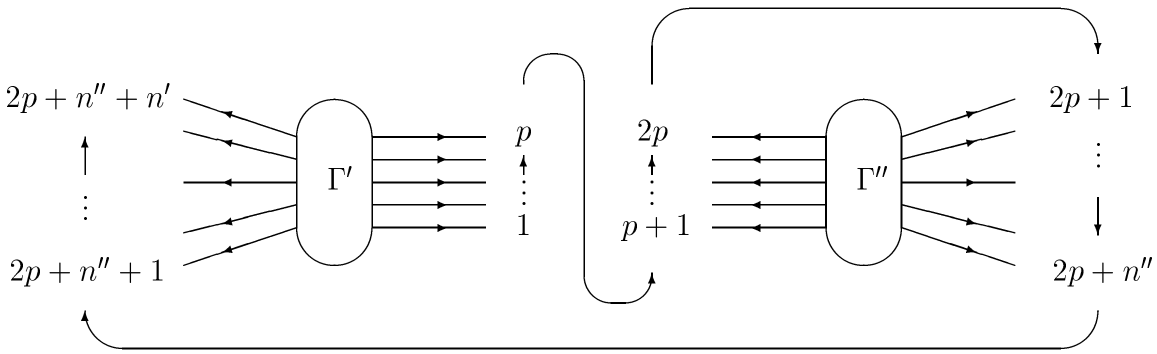

Figure 1: Labeling of the rays of the graphs

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:

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

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 (25), 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 7.1. 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 7.1, 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

$$S_{(m)} = \begin{pmatrix} S'_{(p)} & 0 & 0 & S'_{(p,n')} \\ 0 & S''_{(p)} & S''_{(p,n'')} & 0 \\ 0 & S''_{(n'',p)} & S''_{(n'')} & 0 \\ S'_{(n',p)} & 0 & 0 & S'_{(n')} \end{pmatrix}. \tag{29}$$

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 8.2, we see that the $2p$ elements defined by

$$\begin{aligned} \xi_{N,j} &= \frac{\zeta_j f_{+,j} + f_{-,p+j}}{2} \\ \xi_{N,j+p} &= \frac{\zeta_j f_{+,p+j} + f_{-,j}}{2} \end{aligned}$$

where $j = 1, \ldots, p$, $\zeta_j = e^{-ika_j}$ 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 $j = 2p+1, \ldots, m$. Then these elements span a Lagrange plane which, after theorem 7.1, has associated with it the 'scattering matrix'

$$T_{(m)} = \begin{pmatrix} \begin{matrix} 0 & \zeta_{(p)} \\ \zeta_{(p)} & 0 \end{matrix} & 0 \\ 0 & \mathbb{I}_{(n)} \end{pmatrix} \tag{30}$$

where $\zeta_{(p)}$ is a diagonal matrix with the entries on the diagonal being the 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 get the scattering matrix for the linked graph we first express the ξ_j in terms of the $\xi_{N,j}$. Since

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

and

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

we can write

$$\xi_i = \sum_{j,k=1}^{2m} g_{ij} g^\star_{N,jk} \xi_{N,k} = \sum_{j=1}^{2m} h_{ij} \xi_{N,j} \tag{31}$$

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 the $\{\xi_j\}_{j=1}^m$—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) i-th basis element of $(\Pi_m \cap N^\perp)/N$ is

$$\sum_{j=1}^{m} R_{ij} \xi_j = \sum_{j=1}^{m} \sum_{l=1}^{2m} R_{ij} h_{jl} \xi_{N,l} \tag{32}$$

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

I. We can write the matrix R in the form

$$R = \begin{pmatrix} \rho_{(n,2p)} & \mathbb{I}_{(n)} \end{pmatrix}. \tag{33}$$

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 7.1, there is a unitary matrix $S_{(n)}$ such that the i-th 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 $\{2p+1, \ldots, m\}$. But this is equivalent to equation (33). Really, the only way to ensure that the $f_{-,i}$ occur only 'on the diagonal' is to have $\mathbb{I}_{(n)}$ in R, as shown.

II. 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 (32) to be zero.

Let us express the matrix h in the following form:

$$h = \begin{pmatrix} A_{(m)} & B_{(m)} \\ -B_{(m)} & A_{(m)} \end{pmatrix} = \begin{pmatrix} A_{(2p)} & A_{(2p,n)} & B_{(2p)} & B_{(2p,n)} \\ A_{(n,2p)} & A_{(n)} & B_{(n,2p)} & B_{(n)} \\ -B_{(2p)} & -B_{(2p,n)} & A_{(2p)} & A_{(2p,n)} \\ -B_{(n,2p)} & -B_{(n)} & A_{(n,2p)} & A_{(n)} \end{pmatrix} \tag{34}$$

Using this representation, condition II can be expressed as

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

ie.

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

This gives us the matrix R so we can write

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

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 7.1, we see that

$$A = \frac{1}{2}(S_{(n)} + \mathbb{I}_{(n)}), \quad B = \frac{i}{2}(S_{(n)} - \mathbb{I}_{(n)})$$

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

$$\begin{aligned}
S_{(n)} &= A - iB \\
&= A_{(n)} - iB_{(n)} - B_{(n,2p)}B_{(2p)}^{-1}(A_{(2p,n)} - iB_{(2p,n)}) \\
&= \begin{pmatrix} S''_{(n'')} & 0 \\ 0 & S'_{(n')} \end{pmatrix} + \begin{pmatrix} S''_{(n'',p)}\bar{\zeta}_{(p)} & 0 \\ 0 & S'_{(n',p)}\bar{\zeta}_{(p)} \end{pmatrix} \times \\
&\quad \begin{pmatrix} \mathbb{I}p & -S'_{(p)}\bar{\zeta}_{(p)} \\ -S''_{(p)}\bar{\zeta}_{(p)} & \mathbb{I}p \end{pmatrix}^{-1} \begin{pmatrix} 0 & S'_{(p,n')} \\ S''_{(p,n'')} & 0 \end{pmatrix} \\
&= \begin{pmatrix} S''_{(n'')} & 0 \\ 0 & S'_{(n')} \end{pmatrix} + \begin{pmatrix} S''_{(n'',p)} & 0 \\ 0 & S'_{(n',p)} \end{pmatrix} \begin{pmatrix} \zeta_{(p)} & -S'_{(p)} \\ -S''_{(p)} & \zeta_{(p)} \end{pmatrix}^{-1} \times \\
&\quad \times \begin{pmatrix} 0 & S'_{(p,n')} \\ S''_{(p,n'')} & 0 \end{pmatrix}.
\end{aligned} \tag{35}$$

The inverse $B_{(2p)}^{-1}$ 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—ie. iff we can find solutions with no support on the external rays but support on the linking edges.

Lemma 8.3 *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 (31,34), we get

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

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 generalised eigenfunction for $\mathcal{L}$, since it is in $\Pi_m \cap N^\perp$. But then, by theorem 7.1, all the $\alpha_i = 0$. Another way to see this is that, since ψ is a generalised 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

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

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

Corollary 8.4 *Given a graph Γ with m vertices we split Γ up 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 i-th vertex of Γ. Then the zeroes 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 (35) for the scattering matrix is the same, in essence, as the equation given in the article by Kostrykin and Schrader [9]. In this article the authors consider how the scattering matrix for the Laplacean 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[3], 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 $B^{-1}_{(2p)}$) and refer to the condition of this inverse not existing as *Condition A*, although they do not give a characterisation in terms of embedded spectrum.

Example 8.1 *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.

[3] To be precise Kostrykin and Schrader do not present a derivation for their formula in the cited paper, nevertheless, their approach is based on the idea of a generalised star product—not hermitian symplectic geometry.

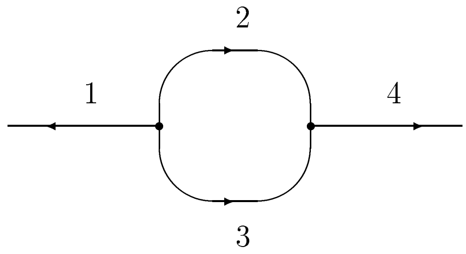

Figure 2: The graph from example 8.1

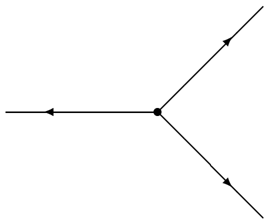

Figure 3: The 'Y' graph

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

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

So we get

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

and, furthermore,

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

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

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

Then from

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

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

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

Putting all of these into equation (35) 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.

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Appendix: The Multiplicity of the Continuous Spectrum on the Graph

Here we will use the results of the last section to prove lemma 6.2.

Lemma 6.2 *Given the self-adjoint extension $\mathcal{L}$, the vector space of generalised 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 of the graph Γ, equation (22). We know that this defines a hermitian symplectic form in the $2(n+2p)$-dimensional space of boundary values—from equation (22) we write it explicitly

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

Consequently, we may consider the space of boundary conditions as a hermitian symplectic space with this form (this construction is cosidered in detail in [9]), let us denote this space by $H_{2(n+2p)}$. It is clear that 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 the hermitian symplectic space of boundary conditions associated with our chosen self-adjoint $\mathcal{L}$. We emphasise that we are *not* considering the asymptotic hermitian symplectic space here, rather we consider the *hermitian symplectic space of boundary conditions* discussed in the first few sections.
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, and ϕ_i and θ_i are the standard solutions on edge i. It is clear that the boundary conditions on edge i match iff there is an eigenfunction on i whose boundary values at the ends of edge i are the same as the relevent 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 generalised eigenfunctions is constant. We note that this is an isotropic subspace for all real λ. The dimension of N is p.
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 used to generate a generalised eigenfunction of $\mathcal{L}$ on the graph Γ. Now we take $(P \cap N^{\perp})/N$, ie. we quotient out those boundary conditions (and hence eigenfunctions) with support confined to the interior edges and we obtain only those generalised eigenfunctions with *support on the rays.* But we know from theorem 8.1that $(P \cap N^{\perp})/N$ has dimension n and consequently the space of generalised eigenfunctions with support on the rays of the graph is n-dimensional. $\square$

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