Hermitian Symplectic Spaces, von Neumann's Extension Theory, and Scattering on Quantum Graphs

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Abstract. We begin with the definition of a skew-Hermitian form and the corresponding Hermitian symplectic group. We motivate these definitions with a discussion of their relevance to self-adjoint extensions of Hamiltonian operators. In doing so, we introduce the basics of von Neumann's extension theory. Next, we develop the necessary tools from Hermitian symplectic linear algebra to study self-adjoint extensions of Hamiltonian operators on simple one-dimensional regions. We apply these concepts to the scattering problem on non-compact quantum star graphs. Further, we suggest an experiment to determine the particular self-adjoint extension at play. Throughout the discussion, we make explicit note of the appearance of the unitary group $U(n)$, as it parametrizes the set of self-adjoint extensions, the Lagrangian Grassmannian and the possible scattering matrices for a non-compact quantum star graph.

*This material is based upon work supported by the National Science Foundation under agreement No. DMS-1055897. Any opinions, findings and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

1 Introduction

With the high demand for ever smaller electronic devices, nanowire as well as molecular and atomic wires have become a topic of great interest [1]. Current technology is capable of creating wires with the width of a single atom [2]. We may model these systems with ideal one-dimensional wires. The microstructure at a junction of two or more wires is crucial for understanding the dynamics of such a system. At this subatomic scale, quantum mechanics is necessary, and we must pay careful attention to the mathematical details in order to study the junctions. Scattering on these systems is of particular interest, as scattering experiments may be performed to probe a connection between wires. In this paper we will establish a clear correspondence between the boundary conditions near a junction and scattering theory.

More precisely, we examine the relationship between Hermitian symplectic spaces, von Neumann's extension theory and scattering on quantum graphs. The unitary group $U(n)$ will provide us with an explicit link between these three ideas. Therefore, we will make special note of it as it appears in our discussion. The general outline is as follows. As Hermitian symplectic spaces are fundamental to our discussion, we will start off with the definition of a Hermitian symplectic space. Immediately afterwards, we will give a physical context to Hermitian symplectic spaces. That is, we relate Hermitian symplectic spaces to finding self-adjoint extensions of a Hamiltonian operator. Next, we introduce von Neumann's extension theory. After covering a bit of Hermitian symplectic linear algebra, we will be able to find a concrete relationship between von Neumann's extension theory and the Lagrangian Grassmannian of a Hermitian symplectic space. Finally, we analyze scattering on a non-compact quantum star graph. We will see that there is an explicit connection between the scattering problem and the problem of finding self-adjoint extensions of a Hamiltonian operator. We will also propose an experimental method for determining the boundary conditions on a non-compact quantum star graph from scattering information.

2 Hermitian Symplectic Spaces

Definition. A Hermitian symplectic space is a complex vector space S with a two form $[\cdot : \cdot]^1 : S \times S \to \mathbb{C}$ satisfying the following properties for $\psi, \phi, \xi \in S$ and $\alpha, \beta \in \mathbb{C}$

i) $[\cdot : \cdot]$ is linear in its first entry. For example, $[\alpha\psi + \beta\xi : \phi] = \alpha[\psi : \phi] + \beta[\xi : \phi]$.

ii) $[\cdot : \cdot]$ is skew-hermitian. That is, $[\psi : \phi] = -\overline{[\phi : \psi]}$, where the bar denotes complex conjugation.

[1] The dot "$\cdot$" is a placeholder for the vector entry.

iii) $[\cdot : \cdot]$ is nondegenerate. Meaning, if $[\psi, \phi] = 0$, $\forall \phi \in S$, then $\psi = 0$.

Notice $[\psi : \alpha\phi + \beta\xi] = \bar{\alpha}[\psi : \phi] + \bar{\beta}[\psi : \xi]$ follows immediately from properties (i) and (ii). We will often refer to $[\cdot : \cdot]$ as the Hermitian symplectic product, and $[\psi : \phi]$ as the Hermitian symplectic product of ψ and ϕ. Therefore, one might say the Hermitian symplectic product is skew-linear in the second entry.

For now, we will only give the definition of a Hermitian symplectic space. We will give a more thorough discussion of Hermitian symplectic spaces after it has been properly motivated. We also take this moment to briefly introduce the Hermitian symplectic group, which will be the focus of our attention in later discussion.

Definition. Let S_1 and S_2 be Hermitian symplectic spaces with Hermitian symplectic products $[\cdot : \cdot]_1$ and $[\cdot : \cdot]_2$, respectively. We say S_1 and S_2 are isomorphic if there exists a bijective, linear function $G : S_1 \to S_2$ such that

$$[\psi : \phi]_1 = [G\psi : G\phi]_2$$

$\forall \psi, \phi \in S_1$. If $S_1 = S_2$, then G is a Hermitian symplectic automorphism.

Definition. Let S be a Hermitian symplectic space. The set of Hermitian symplectic automorphisms on S is called the Hermitian symplectic group.

For the remainder of this paper, we will restrict our discussion of the Hermitian symplectic group to the case in which S is finite dimensional. It is possible to naturally identify a finite dimensional Hermitian symplectic space with the complex vector space $\mathbb{C}^m$ with appropriate Hermitian symplectic structure. We will discuss this point further later in the text. For the moment, however, our goal is to understand the role of the Hermitian symplectic group in the following physical context.

3 Physical Motivation for Studying Hermitian Symplectic Spaces

Introductory textbooks on quantum mechanics often analyze the problem of a particle stuck in a one dimensional infinite potential well [3, 4]. This problem entails solving the time-independent Schrödinger equation

$$E\psi(x) = \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}$$

on a finite interval with appropriate boundary conditions. Typically, textbook authors assume Dirichlet boundary conditions, that is, $\psi(x)$ evaluated at the boundary equals zero. However, the mathematical foundations of quantum mechanics suggest that this need not be the case. In assuming Dirichlet boundary conditions, subtle mathematics are overlooked. The natural question is, what are allowable boundary conditions? The restriction on our choice of boundary conditions comes from the fact that the Hamiltonian operator must be self-adjoint. We will now spend some time discussing exactly what all of this means.

First, we describe the Hamiltonian operator. We may write the Schrödinger equation $E\psi(x) = \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}$ as $E\psi = H\psi$. H is the so called Hamiltonian operator. We must not forget to specify the domain of H. The Hamiltonian operator acts on a subset of the L_2 Hilbert space, where

$$L_2(\Omega) = \{\psi : \Omega \to \mathbb{C} : \|\psi\|^2 := \int_\Omega |\psi(\mathbf{x})|^2 d\mathbf{x} < +\infty\}.$$

The particular subspace of L_2 is chosen such that the Hamiltonian operator is self-adjoint. We give a precise definition of self-adjoint shortly. But first, why might it be necessary that the Hamiltonian operator is self-adjoint? The Schrödinger equation tells us about the time-evolution of a quantum mechanical system. Without going into too much detail, the requirement that the Hamiltonian operator is self-adjoint guarantees that probability is conserved. For the problem of a particle stuck in an infinite potential well, this implies that there is no net flux of particles into or out of the well. In addition, the eigenvalues of a self-adjoint Hamiltonian operator are strictly real. The physical interpretation of this is that when we make a measurement of a quantum system we are guaranteed to get a real result. For a more complete explanation of the importance of a self-adjoint Hamiltonian operator, one might consult [5]. We now provide a proper definition of self-adjoint.

Definition. Let V be a complex vector space with Hermitian inner product $\langle\cdot,\cdot\rangle$ and H a linear operator with dense domain $D(H)$. The adjoint H^* of an operator H on V is the unique operator satisfying

$$\langle\phi, H\psi\rangle = \langle H^*\phi, \psi\rangle, \text{ for all } \psi \in D(H),\ \phi \in D(H^*).^2$$

$D(H^*)$ above is the set of $\phi \in V$ such that there exists a $\tilde{\phi} \in V$ for which $\langle\phi, H\psi\rangle = \langle\tilde{\phi}, \psi\rangle,\ \forall\psi \in D(H)$.

Definition. A linear operator H on a complex vector space V is a Hermitian operator if H is equal to its adjoint on $D(H)$. More formally, H is a Hermitian operator if $\langle\phi, H\psi\rangle = \langle H\phi, \psi\rangle,\ \forall\phi, \psi \in D(H)$.

Definition. A linear operator H is self-adjoint if it is a Hermitian operator and $D(H) = D(H^*)$.

Let's say we have a physical system and a candidate for the Hamiltonian operator describing the system. We would like to check whether the Hamiltonian operator H is self-adjoint. We must first demonstrate that H is a Hermitian operator. To do so, we may study the expression $\langle H\phi, \psi\rangle - \langle\phi, H\psi\rangle$. If

[2] Recall that a Hermitian inner product is one that satisfies $\langle\phi, \psi\rangle = \overline{\langle\psi, \phi\rangle}$.

$\langle H\phi, \psi\rangle - \langle \phi, H\psi\rangle$ is zero for all $\phi, \psi \in D(H)$, then H is a Hermitian operator. Notice that the two form $[\phi : \psi]_H := \langle H\phi, \psi\rangle - \langle \phi, H\psi\rangle$ satisfies properties (i) and (ii) of the definition of a Hermitian symplectic product. Therefore, it is a skew-Hermitian sesquilinear form. In our search for a self-adjoint Hamiltonian operator we have stumbled across something similar to a Hermitian symplectic product. In this way, Hermitian symplectic products arise naturally out of quantum theory. To be a Hermitian symplectic product, however, it must be nondegenerate (property (iii) above). Thus, we can simply find a complex vector space on which $[\cdot : \cdot]_H$ is nondegenerate and we have found ourselves a Hermitian symplectic product.

Here is how we may find an acceptable complex vector space on which our two form is a Hermitian symplectic product. Let H_1 be a linear operator on a complex vector space V. We will consider the two form $[\phi : \psi]_{H_1} := \langle H_1\phi, \psi\rangle - \langle \phi, H_1\psi\rangle$. Next, we let H_0 be defined as follows.

$$D(H_0) := \{\psi \in D(H_1) : [\phi : \psi]_{H_1} = 0 \text{ for all } \phi \in D(H_1)\}$$

and

$$H_0\psi = H_1\psi \text{ on } D(H_0).$$

We also assume that $H_0^* = H_1$. H_0 defined in this way is called the initial Hermitian operator. Notice, by the definition of $D(H_0)$, $D(H_0) \subseteq D(H_1)$. Next, we show that under the assumption $H_0^* = H_1$, the quotient space $D(H_1)/D(H_0)$ with two form $[\cdot : \cdot]_{H_1}$ is a Hermitian symplectic space. An element $\boldsymbol{\phi}$ of $D(H_1)/D(H_0)$ is a coset of $\phi \in D(H_1)$ such that $\boldsymbol{\phi} = \{\phi + D(H_0)\}$. By the definition of $D(H_0)$, $[\cdot : \cdot]_{H_1}$ is well defined on $D(H_1)/D(H_0)$.

Proposition. Let H_1 and H_0 be as defined above. Let $S = D(H_1)/D(H_0)$ with the skew-Hermitian sesquilinear form $[\cdot : \cdot]_{H_1}$ given above. S is a Hermitian symplectic space.

Proof. As we have noticed previously, $[\cdot : \cdot]_{H_1}$ satisfies properties (i) and (ii) given in the definition of a Hermitian symplectic space. All that is left to show is that $[\cdot : \cdot]_{H_1}$ is nondegenerate. Suppose $[\boldsymbol{\phi} : \boldsymbol{\psi}]_{H_1} = 0$, $\forall \boldsymbol{\phi} \in S$, then it must be that $\psi \in D(H_0)$ (by the definition of $D(H_0)$). As $\psi \in D(H_0)$ implies $\boldsymbol{\psi} = 0$ in S, $[\cdot : \cdot]_{H_1}$ is nondegenerate. □

Our construction of this Hermitian symplectic space may seem a bit contrived, but we will see that it provides us with a very geometric means of identifying self-adjoint Hamiltonian operators. In order to appreciate this construction, however, we will need to discuss von Neumann's extension theory. von Neumann's extension theory applies most readily to operators acting on finite dimensional vector spaces. As it stands, S is infinite dimensional. Fortunately, there is a quick simplification we can make so that for simple one dimensional systems (like those shown in the Figure 1 below) our Hermitian symplectic space of interest is finite dimensional.

Using integration by parts, we will find a Hermitian symplectic product that acts on the so called boundary value space (BVS). Recall that the inner

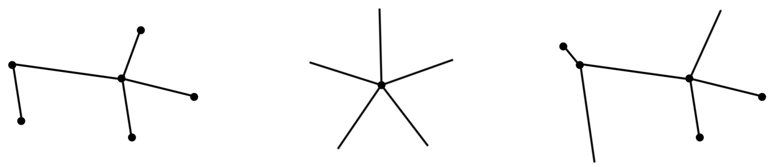

Figure 1: Examples of one-dimensional regions with a finite number of boundary points.

product on an L_2 Hilbert space is an integral over the whole region of interest. Also note that the Hamiltonian operator for a free particle is simply a constant multiple of the Laplace operator. Therefore, integration by parts twice gives us an equivalent Hermitian symplectic product dependent upon the value of the function and its derivative evaluated on the boundary. We will now work out an example of this technique for a one-dimensional system with n boundary points. Let Ω be a one-dimensional region with n boundary points. Let $H_1 = H_0^*$ be the hamiltonian operator for a free particle on Ω. Suppose H_0 is as defined above. Then for $\psi, \phi \in D(H_0^*)$ we have [3]

$$\begin{aligned}
\langle \psi, H_0^* \phi \rangle &= \int_\Omega \overline{\psi}(x) H_0^* \phi(x) dx \\
&= \int_\Omega \overline{\psi}(x) \Big(-\frac{\partial^2 \phi}{\partial x^2}(x) \Big) dx \\
&= -\overline{\psi}(x) \Big|_{\partial\Omega} \frac{\partial \phi}{\partial x}(x) \Big|_{\partial\Omega} + \int_\Omega \frac{\partial \overline{\psi}}{\partial x}(x) \frac{\partial \phi}{\partial x}(x) dx \\
&= -\overline{\psi}(x) \Big|_{\partial\Omega} \frac{\partial \phi}{\partial x}(x) \Big|_{\partial\Omega} + \frac{\partial \overline{\psi}}{\partial x}(x) \Big|_{\partial\Omega} \phi(x) \Big|_{\partial\Omega} + \langle H_0^* \psi, \phi \rangle
\end{aligned}$$

Therefore,

$$\begin{aligned}
[\psi : \phi]_{H_0^*} &= \langle H_0^* \psi, \phi \rangle - \langle \psi, H_0^* \phi \rangle \\
&= \overline{\psi}(x) \Big|_{\partial\Omega} \frac{\partial \phi}{\partial x}(x) \Big|_{\partial\Omega} - \frac{\partial \overline{\psi}}{\partial x}(x) \Big|_{\partial\Omega} \phi(x) \Big|_{\partial\Omega} \\
&= \sum_{j=1}^{n} (\overline{\psi_j} \phi_{xj} - \overline{\psi_{xj}} \phi_j)
\end{aligned}$$

where ϕ_j is $\phi(x)$ evaluated at the j^{th} boundary point and ϕ_{xj} is $\frac{\partial \phi}{\partial x}(x)$ evaluated at the j^{th} boundary point.[4] For simple one-dimensional systems, we are now

[3] $\partial\Omega$ is the boundary of Ω.

[4] The x coordinate is measured from the boundary point.

able to think of $[\cdot:\cdot]_{H_0^*}$ as acting on a $2n$ dimensional complex vector space of boundary values, or BVS. We will elaborate on this point later. In any event, this is a dramatic simplification and now allows us to gain insight from von Neumann's extension theory, which we discuss next.

4 von Neumann's Extension Theory

The exposition of von Neumann's extension theory that follows is by no means rigorous or comprehensive. For a more thorough description of extension theory one could refer to [6] or [7]. In any event, we hope to get across the main results of von Neumann's extension theory.

Let H_0 be a Hermitian operator on a complex vector space V with inner product $\langle \cdot, \cdot \rangle$. Then the domain of the adjoint $D(H_0^*)$ is given by

$$D(H_0^*) = D(H_0) + \aleph_{+i} + \aleph_{-i}$$

where $\aleph_{+i}$ and $\aleph_{-i}$ are the deficiency subspaces. $D(H_0)$, $\aleph_{+i}$, and $\aleph_{-i}$ are linearly independent. The deficiency subspaces are defined by

$$\aleph_{\pm i} = \ker(H_0^* \pm i).$$

The dimensions of the deficiency subspaces $\dim(\aleph_{\pm i}) = n_{\pm}$ are called the deficiency indices, and are essential for determining when a self-adjoint extension of a Hermitian operator is possible. A self-adjoint extension is possible if and only if $n_+ = n_- = n$.[5] According to von Neumann, the set of self-adjoint extensions of H_0 is parametrized by the group of unitary matrices $U(n)$ on an n-dimensional space, where n is the deficiency index.[6] Essentially the argument goes as follows. We would like to extend the Hermitian operator H_0. We can do this by enlarging its domain up until it is equal to the domain of its adjoint. We may add functions from the deficiency subspaces to $D(H_0)$, but the rule is if we add a function from $\aleph_{+i}$ we must add a function of equivalent norm from $\aleph_{-i}$. Hence, each self-adjoint extension of H_0 corresponds to a unitary map from $\aleph_{+i}$ to $\aleph_{-i}$.

Now, once we have developed some Hermitian symplectic linear algebra, we will be able to make an explicit connection between the Hermitian symplectic space we developed in the previous section and von Neumann's extension theory.

5 Hermitian Symplectic Linear Algebra

Our goal is to construct a set of mathematical objects which is in bijective correspondence with $U(n)$. In doing so, we will have constructed a collection of

[5] Note that we have previously used n to refer to the number of boundary points in a simple one-dimensional region. In fact, the value n, of the number of boundary points coincides with n, the deficiency index. This can be seen from the definition of the BVS and $D(H_0^*)$.

[6] As a reminder, $U(n)$ is the set of matrices with complex entries such that if $U \in U(n)$ then $U^*U = I$.

objects which parametrizes the set of self-adjoint extensions of a Hermitian operator with deficiency indices equal to n (by von Neumann's extension theory). This correspondence will not just be an isomorphism in terms of cardinality. We will also obtain the domain of the operator in terms of boundary conditions. The mathematical structure that will fulfill these requirements is the Lagrangian Grassmannian. We will now provide the definition of the Lagrangian Grassmannian and present the relevant Hermitian symplectic linear algebra in order to show that it is in bijective correspondence with $U(n)$.

Definition. Let S be a Hermitian symplectic space with Hermitian symplectic form $[\cdot : \cdot]$. We call two vectors $\psi, \phi \in S$ skew-orthogonal if $[\psi : \phi] = 0$. Furthermore, we call two subspaces $P, Q \subset S$ skew-orthogonal, written as $[P : Q] = 0$, if $\forall \psi \in P$ and $\forall \phi \in Q$, $[\psi : \phi] = 0$.

Definition. For a Hermitian symplectic space S of dimension $2n$ with symplectic form $[\cdot : \cdot]$, a complete Lagrangian L is an n-dimensional subspace of S which is skew-orthogonal to itself $[L : L] = 0$ and complete in the following sense. If $[\psi : \phi] = 0 \; \forall \psi \in L$, then $\phi \in L$.

Definition. A Lagrangian Grassmannian Λ_n is the set of all complete Lagrangians for a given Hermitian symplectic space of dimension $2n$.

Now we develop a few further concepts with the aim of showing that Λ_n is isomorphic to $U(n)$ in terms of cardinality, where $2n$ is the dimension of the Hermitian symplectic space. Along the way we will showcase the role of the Hermitian symplectic group.

Definition. Let S be a Hermitian symplectic space of dimension $2n$ with Hermitian symplectic product $[\cdot : \cdot]$. Recall that S may be identified with the complex vector space $\mathbb{C}^{2n}$ with a suitable Hermitian symplectic structure. We say that S is a canonical Hermitian symplectic space if it admits a basis $\{\xi_i\}_{i=1}^n \cup \{\xi'_j\}_{j=1}^n$ such that

$$[\xi_i : \xi'_j] = \delta_{ij}, \; [\xi'_j : \xi_i] = -\delta_{ij}, \text{ and } [\xi_k : \xi_\ell] = [\xi'_k : \xi'_\ell] = 0$$

and $\{\xi_i\}_{i=1}^n \cup \{\xi'_j\}_{j=1}^n$ is orthonormal with respect to the standard Hermitian inner product of $\mathbb{C}^{2n}$. $\{\xi_i\}_{i=1}^n \cup \{\xi'_j\}_{j=1}^n$ is called a canonical basis.

Notice that the span of $\{\xi_i\}_{i=1}^n$ and the span of $\{\xi'_j\}_{j=1}^n$ are both complete Lagrangians. We state the next Lemma without proof. The proof may be found in [8].

Lemma. A Hermitian symplectic space of dimension $2n$ is a canonical Hermitian symplectic space if and only if it has a complete Lagrangian subspace.

The proof in one direction is immediate. A canonical Hermitian symplectic space naturally contains a complete Lagrangian, as the span of the first n or last n basis vectors is a complete Lagrangian. This proposition allows us to use a canonical basis when talking about Hermitian symplectic spaces containing a complete Lagrangian.

We will show now that the Hermitian symplectic product $[\cdot : \cdot]$ for a canonical Hermitian symplectic space S of dimension $2n$ can be written using a Hermitian inner product. Suppose we would like to find $[\psi : \phi]$. As S is a canonical Hermitian symplectic space we may find a basis $\{\xi_i\}_{i=1}^n \cup \{\xi_j'\}_{j=1}^n$ satisfying the properties in the previous definition. Therefore, we may write ψ and ϕ as

$$\psi = \sum_{i=1}^n \alpha_i \xi_i + \sum_{j=1}^n \alpha_j' \xi_j', \text{ and } \phi = \sum_{i=1}^n \beta_i \xi_i + \sum_{j=1}^n \beta_j' \xi_j'.$$

Hence, the Hermitian symplectic product of ψ with ϕ is

$$[\psi : \phi] = \sum_{k=1}^n (\overline{\alpha}_k \beta_k' - \overline{\alpha'}_k \beta_k).$$

One should note the similarity between this evaluation of $[\psi, \phi]$ and the evaluation of $[\psi, \phi]_{H_0^*}$ at the end of section 3. The Hermitian symplectic product $[\cdot : \cdot]$ on S is equivalent to $\langle \cdot, J \cdot \rangle$ on $\mathbb{C}^{2n}$, where again, the angled brackets denote the Hermitian inner product. J is the canonical symplectic structure and

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

where I is the $n \times n$ identity matrix. Now, let's explicitly evaluate $\langle \psi, J\phi \rangle$, where ψ and ϕ are the same as before.

$$J\phi = \sum_{j=1}^n \beta_j' \xi_j - \sum_{i=1}^n \beta_i \xi_i'$$

Thus,

$$\langle \psi, J\phi \rangle = \sum_{k=1}^n (\overline{\alpha}_k \beta_k' - \overline{\alpha'}_k \beta_k).$$

This shows that the canonical Hermitian symplectic space S of dimension $2n$ with Hermitian symplectic product $[\cdot : \cdot]$ is equivalent to $\langle \cdot, J \cdot \rangle$ on $\mathbb{C}^{2n}$.

This gives us a nice way of characterizing an element of the Hermitian symplectic group for a canonical Hermitian symplectic space of dimension $2n$. Let S be a $2n$-dimensional canonical Hermitian symplectic group with Hermitian symplectic product $[\cdot : \cdot]$. By identifying S with $\mathbb{C}^{2n}$ we may write the Hermitian symplectic product as $\langle \cdot, J \cdot \rangle$. A member G of the Hermitian symplectic group preserves the Hermitian symplectic product. This means, $\forall \psi, \phi \in \mathbb{C}^{2n}$,

$$\langle \psi, J\phi \rangle = \langle G\psi, JG\phi \rangle = \langle \psi, G^* JG\phi \rangle.^7$$

[7] Here the * denotes the complex conjugate transpose. For a matrix, it's adjoint is exactly its complex conjugate transpose.

Therefore, all elements of the Hermitian symplectic group satisfy $G^*JG = J$. The converse of this statement is true as well. If G satisfies $G^*JG = J$, then G is in the Hermitian symplectic group. In this context, G maps complete Lagrangians to complete Lagrangians. We will see in a moment that an element of the Hermitian symplectic group gives us a map from any complete Lagrangian to any other complete Lagrangian. Before we get to that, let's make a few observations about the structure of an element of the Hermitian symplectic group. Suppose G is in the Hermitian symplectic group and G takes on the block form

$$G = \begin{pmatrix} A & B \\ C & D \end{pmatrix}.$$

Then the condition that $G^*JG = J$ implies

$$\begin{pmatrix} CA^* - C^*A & A^*D - C^*B \\ B^*C - D^*A & B^*D - D^*B \end{pmatrix} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

This gives us the four following conditions

$$\begin{aligned} CA^* - C^*A &= 0 \\ B^*D - D^*B &= 0 \\ A^*D - C^*B &= I \\ B^*C - D^*A &= -I. \end{aligned}$$

We will use these findings in the next proposition.

Lemma. Let S be a $2n$-dimensional canonical Hermitian symplectic space. Let L_0 and L be two complete Lagrangians contained in S. Let $\{\xi_i\}_{i=1}^n \cup \{\xi_j'\}_{j=1}^n$ be a basis for S such that L_0 is the span of $\{\xi_i\}_{i=1}^n$. There exists an element G of the Hermitian symplectic group of S such that G can be used to map L to L_0.

Proof. We identify S with $\mathbb{C}^{2n}$. Suppose the canonical basis $\{\eta_i\}_{i=1}^n \cup \{\eta_j'\}_{j=1}^n$ for S is such that $\{\eta_i\}_{i=1}^n$ spans L. We will show that the map G for which

$$\eta_i = \sum_{j=1}^n G_{ij}\xi_j + \sum_{j=1}^n G_{i(n+j)}\xi_j', \text{ for } i = 1, 2, ..., n$$

is in the Hermitian symplectic group for S. In the $\{\xi_i\}_{i=1}^n \cup \{\xi_j'\}_{j=1}^n$ basis, G is the matrix of row vectors

$$G = \begin{pmatrix} \eta_1 & \eta_2 & \dots & \eta_n & \eta_1' & \eta_2' & \dots & \eta_n' \end{pmatrix}^T$$

where ^{T} is the transpose operation. Let us divide up G into the block form

$$G = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

where A,B,C, and D are $n \times n$ matrices. Since the vectors in $\{\eta_i\}_{i=1}^n \cup \{\eta'_j\}_{j=1}^n$ are orthonormal, we obtain

$$\begin{aligned} A^*A + B^*B &= I \\ C^*C + D^*D &= I \\ A^*C + B^*D &= 0 \\ C^*A + D^*B &= 0. \end{aligned}$$

As $\{\eta_i\}_{i=1}^n \cup \{\eta'_j\}_{j=1}^n$ is a canonical basis, $\langle \eta_k, J\eta'_k \rangle = 1$. This tells us that $J\eta'_k = \eta_k$. Therefore, $A = D$ and $C = -B$. Altogether we have

$$G = \begin{pmatrix} A & B \\ -B & A \end{pmatrix}$$

with the conditions that $A^*A + B^*B = I$ and $A^*B - B^*A = 0$. Referring to the four conditions stated before the proposition, we see that G is an element of the Hermitian symplectic group. □

We are finally in a position to demonstrate the correspondence between Λ_n and $U(n)$. A transformation G from the proof of the last Lemma takes one complete Lagrangian to another complete Lagrangian. However, G may keep the complete Lagrangian fixed. Let's define the subgroup of the Hermitian symplectic group

$$\mathcal{G} = \left\{ G = \begin{pmatrix} A & B \\ -B & A \end{pmatrix} : G \in U(2n) \right\}.$$

By requiring that $G \in U(2n)$ we incorporate the conditions $A^*A + B^*B = I$ and $A^*B - B^*A = 0$ from before. Therefore, $\mathcal{G}$ gives us the set of transformations arising in the previous proof. We would like to mod out the matrices which send a complete Lagrangian to itself. That way, we can identify elements of $\mathcal{G}$ with complete Lagrangians. The subset of $\mathcal{G}$ that keeps complete Lagrangians fixed is

$$\mathcal{F} = \left\{ F = \begin{pmatrix} K & 0 \\ 0 & K \end{pmatrix} : F \in U(2n) \right\}.$$

This can be seen by how $G \in \mathcal{G}$ maps one canonical basis to another in the proof of the Lemma above. Therefore, there is a one to one correspondence between Λ_n and $\mathcal{G}/\mathcal{F}$. $\mathcal{G}/\mathcal{F}$ is in one to one correspondence with $U(n)$ by the following theorem.

Theorem. Λ_n is in one to one correspondence with $U(n)$.

Proof. It will suffice to show that $\mathcal{G}/\mathcal{F}$ is in one to one correspondence with $U(n)$. Consider the $2n \times 2n$ unitary matrix

$$W = \frac{1}{\sqrt{2}} \begin{pmatrix} I & iI \\ iI & I \end{pmatrix}.$$

W block diagonalizes the elements of $\mathcal{G}$. For $G \in \mathcal{G}$ with

$$G = \begin{pmatrix} A & B \\ -B & A \end{pmatrix}$$

we have

$$WGW^* = \begin{pmatrix} A - iB & 0 \\ 0 & A + iB \end{pmatrix}.$$

Thus, $\mathcal{G}$ is unitarily equivalent to

$$\tilde{\mathcal{G}} := \left\{ \tilde{G} = \begin{pmatrix} M & 0 \\ 0 & N \end{pmatrix} : \tilde{G} \in U(2n) \right\}.$$

The matrices in $\mathcal{F}$ are already block diagonal, so $\tilde{F} := W\mathcal{F}W^* = \mathcal{F}$. Each coset of $\tilde{\mathcal{G}}/\tilde{\mathcal{F}}$ can be represented by a unique matrix of the form

$$\begin{pmatrix} U & 0 \\ 0 & I \end{pmatrix}.$$

This is because

$$\begin{aligned} \begin{pmatrix} M & 0 \\ 0 & N \end{pmatrix} \tilde{\mathcal{F}} &= \begin{pmatrix} M & 0 \\ 0 & N \end{pmatrix} \begin{pmatrix} N^{-1} & 0 \\ 0 & N^{-1} \end{pmatrix} \tilde{\mathcal{F}} \\ &= \begin{pmatrix} MN^{-1} & 0 \\ 0 & I \end{pmatrix} \tilde{\mathcal{F}} \\ &= \begin{pmatrix} U & 0 \\ 0 & I \end{pmatrix} \tilde{\mathcal{F}}. \end{aligned}$$

We now have the desired result. $\mathcal{G}/\mathcal{F}$ is in one to one correspondence with $U(n)$. □

Let's go one step further and develop a labeling system for our complete Lagrangians. That is, given a complete Lagrangian spanned by the first n elements of a canonical basis $\{\eta_i\}_{i=1}^n \cup \{\eta'_j\}_{j=1}^n$ we'd like to assign a member of $U(n)$ to this complete Lagrangian. Here is one way we can go about doing this. Let $\{\xi_i\}_{i=1}^n \cup \{\xi'_j\}_{j=1}^n$ be a canonical basis for a Hermitian symplectic space S identified with $\mathbb{C}^{2n}$. Then, let $\{\eta_i\}_{i=1}^n \cup \{\eta'_j\}_{j=1}^n$ be another canonical basis for S. As before, we define G as the matrix satisfying

$$\eta_i = \sum_{j=1}^{n} G_{ij}\xi_j + \sum_{j=1}^{n} G_{i(n+j)}\xi'_j, \text{ for } i = 1, 2, ..., n.$$

Again, we break up G into the block matrix form with $n \times n$ matrices.

$$G = \begin{pmatrix} A & B \\ -B & A \end{pmatrix}$$

with A and B satisfying $A^*A + B^*B = I$ and $B^* - A^*B = 0$. From previous calculations we know that G is unitarily equivalent to

$$\tilde{G} := \begin{pmatrix} A - iB & 0 \\ 0 & A + iB \end{pmatrix}.$$

From our earlier findings we know that the coset of $\tilde{\mathcal{G}}/\tilde{\mathcal{F}}$ (as defined above) containing $\tilde{G}$ can be represented by a matrix of the form

$$\begin{pmatrix} MN^{-1} & 0 \\ 0 & I \end{pmatrix}$$

where $M = (A - iB)$ and $N = (A + iB)$. We will show that $(A \pm iB)$ is unitary which shows that $(A - iB)(A + iB)^{-1}$ is unitary.

$$\begin{aligned} (A \pm iB)^*(A \pm iB) &= (A^* \mp iB^*)(A \pm iB) \\ &= (AA^* + B^*B) \mp i(B^*A - A^*B) \\ &= I \end{aligned}$$

Therefore, we can assign $(A-iB)(A+iB)^{-1} \in U(n)$ to the complete Lagrangian spanned by the first n basis vectors of the canonical basis $\{\eta_i\}_{i=1}^n \cup \{\eta'_j\}_{j=1}^n$.

Conversely, given an element of $U(n)$ we would like to be able to identify, up to ordering of the elements, the corresponding canonical basis vectors which span a complete Lagrangian. Let S be a Hermitian symplectic space with canonical basis $\{\xi_i\}_{i=1}^n \cup \{\xi'_j\}_{j=1}^n$. Suppose we are given $U \in U(n)$. Using the same notation as developed above, we have that we can represent a coset of $\tilde{\mathcal{G}}/\tilde{\mathcal{F}}$ with

$$\begin{pmatrix} U & 0 \\ 0 & I \end{pmatrix}.$$

There is an element $G \in \mathcal{G}$ that is unitarily equivalent to this matrix. That is,

$$WGW^* = \begin{pmatrix} U & 0 \\ 0 & I \end{pmatrix}.$$

This means that

$$\begin{aligned} G &= \frac{1}{2} \begin{pmatrix} I & -iI \\ -iI & I \end{pmatrix} \begin{pmatrix} U & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & iI \\ iI & I \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} U + I & i(U - I) \\ -i(U - I) & U + I \end{pmatrix}. \end{aligned}$$

This G encodes the necessary information for a transformation from $\{\xi_i\}_{i=1}^n \cup \{\xi'_j\}_{j=1}^n$ to another canonical basis $\{\eta_i\}_{i=1}^n \cup \{\eta'_j\}_{j=1}^n$. We will define the first n vectors of $\{\eta_i\}_{i=1}^n \cup \{\eta'_j\}_{j=1}^n$ by

$$\eta_i = \sum_{j=1}^n G_{ij}\xi_j + \sum_{j=1}^n G_{i(n+j)}\xi'_j, \text{ for } i = 1, 2, ..., n.$$

Thus, the span of $\{\eta_i\}_{i=1}^n$ is given by

$$\mathrm{im}\begin{pmatrix} U+I \\ i(U-I) \end{pmatrix}$$

where "im" stands for image.

We now have an explicit connection between complete Lagrangians and members of $U(n)$. Let's apply the Hermitian symplectic linear algebra that we have just developed to the aforementioned physically relevant problem of finding self-adjoint extensions of a Hermitian operator.

This means that we have a concrete connection between complete Lagran

6 Physical Implications

In this section, we will begin by recalling the boundary value space (BVS) for a Hermitian operator H_0 introduced at the end of section 3. Then we will show that the BVS admits a canonical basis. Hence, the $2n$-dimensional BVS contains complete Lagrangians. As we have just discovered, the set of these complete Lagrangians is parametrized by $U(n)$. By von Neumann's extension theory, this tells us that there is a self-adjoint extension of H_0 for each complete Lagrangian and vice-versa. We will be able to determine the boundary conditions for the particular self-adjoint extension using the complete Lagrangian.

Let us get started by reviewing the concept of a BVS. We begin with an initial Hermitian Hamiltonian operator H_0. For convenience, we may take the domain of H_0 to be the set of functions in $L_2(\Omega)$ whose second derivative is in $L_2(\Omega)$ and the value of the function and its first derivative are zero when evaluated at the boundaries. This make checking that H_0 is Hermitian simple, as the boundary terms go away. Then, from von Neumann's extension theory, we have

$$D(H_0^*) = D(H_0) + \aleph_{+i} + \aleph_{-i}.$$

If Ω is a simple one dimensional region, we may consider the space $D(H_0^*)/D(H_0)$ with Hermitian symplectic product $[\cdot : \cdot]_{H_0^*}$ defined by

$$[\psi : \phi]_{H_0^*} = \sum_{j=1}^{n} (\overline{\psi_j}\phi_{xj} - \overline{\psi_{xj}}\phi_j).$$

We can think of $[\cdot : \cdot]_{H_0^*}$ as acting on a $2n$-dimensional space ($n = \dim \aleph_{+i} = \dim \aleph_{-i}$). We define this $2n$-dimensional space as the boundary value space of H_0.

We will now construct a canonical basis for the BVS of the initial Hermitian operator H_0 with deficiency indices equal to n. That is, say we have n boundary points so that the BVS of H_0 has dimension $2n$. The first n basis vectors will be $\{\xi_i\}_{i=1}^n$. These are the functions that are zero at every boundary point except for the i^{th} boundary point at which $\xi_i = 1$. Also, the first derivative of the functions in $\{\xi_i\}_{i=1}^n$ is zero at each boundary point. We let the last n of our basis be the functions $\{\xi'_j\}_{j=1}^n$. We define these to be the functions that are zero at the boundary and have first derivative evaluated at the boundary equal to zero except for at the j^{th} boundary point at which $\xi'_{xj} = 1$. If we identify the BVS with $\mathbb{C}^{2n}$, we see that our basis is just the standard basis of $\mathbb{C}^{2n}$, so it is orthonormal. Using the Hermitian symplectic product that we derived earlier for the BVS, we will show that this indeed forms a canonical basis. In the following calculations, $(\xi_i)_{xk}$ is the derivative of the function ξ_i evaluated at the k^{th} boundary point. Therefore, we have

$$[\xi_i : \xi_j] = \sum_{k=1}^{n} \left(\overline{(\xi_i)}_k (\xi_j)_{xk} - \overline{(\xi_i)_{xk}} (\xi_j)_k \right) = 0$$

as $\xi_{ix} = 0$ at all boundary points. We also have

$$[\xi'_i : \xi'_j] = \sum_{k=1}^{n} \left(\overline{(\xi'_i)}_k (\xi'_j)_{xk} - \overline{(\xi'_i)_{xk}} (\xi'_j)_k \right) = 0$$

because $\xi'_{ix} = 0$ at all boundary points. Next, we observe that

$$[\xi_i : \xi'_j] = \sum_{k=1}^{n} \left(\overline{(\xi_i)}_k (\xi'_j)_{xk} - \overline{(\xi_i)_{xk}} (\xi'_j)_k \right) = \delta_{ij}.$$

Switching ξ_i and ξ'_j in the Hermitian symplectic form will of course give us $-\delta_{ij}$. Thus, $\{\xi_i\}_{i=1}^n \cup \{\xi'_j\}_{j=1}^n$ as we have defined it, is a canonical basis for the BVS of a given initial Hermitian operator with deficiency indices equal to n.

Now that we have a canonical basis for the BVS of H_0, we can talk about complete Lagrangian subspaces of the BVS. Again, we are able to identify each complete Lagrangian with an element of $U(n)$. von Neumann's extension theory then says that we are identifying each complete Lagrangian with a particular self-adjoint extension of H_0. In von Neumann's extension theory, the choice of $U(n)$ tells us which elements we are adding from the deficiency subspaces to the domain of H_0. Therefore, given a $U \in U(n)$ we can determine the boundary values of the functions we are adding into the domain of H_0 by using the corresponding complete Lagrangian. Let us now verify that the complete Lagrangians of boundary value space specify the domain of a self-adjoint extension of H_0.

Proposition. Let $S = D(H_0^*)/D(H_0)$ be the BVS for the initial Hermitian Hamiltonian operator H_0. Let H be a self-adjoint extension of H_0. Then, $L := D(H)/D(H_0)$ is a complete Lagrangian subspace of S.

Proof. First we demonstrate that L is skew-orthogonal to itself. Then we show that L is complete. Let $\psi, \phi \in D(H)$. Then $\boldsymbol{\psi} = \{\psi + D(H_0)\}$ and $\boldsymbol{\phi} = \{\phi + D(H_0)\}$ are in S. Now note that

$$[\boldsymbol{\psi} : \boldsymbol{\phi}]_{H_0^*} = [\psi : \phi]_{H_0^*} = \langle H_0^* \psi, \phi \rangle - \langle \psi, H_0^* \phi \rangle = \langle H\psi, \phi \rangle - \langle \psi, H\phi \rangle = 0.$$

The last equality holds because H is Hermitian. We now see that L is skew-orthogonal to itself but we must still show that L is complete. Suppose $\varphi \in D(H_0^*)$ is such that $[\boldsymbol{\varphi} : L]_{H_0^*} = 0$. That is, $[\boldsymbol{\varphi} : \psi]_{H_0^*} = 0$, $\forall \psi \in D(H)$. Then

$$\langle H_0^* \varphi, \psi \rangle = \langle \varphi, H_0^* \psi \rangle = \langle \varphi, H\psi \rangle, \forall \psi \in D(H).$$

Therefore, $\varphi \in D(H^*) = D(H)$, so $\boldsymbol{\varphi} \in L$. Thus, L is complete. $\square$

We may now use the complete Lagrangians of the BVS to specify the domain of the self-adjoint extensions. Choose a unitary matrix $U \in U(n)$. As we found earlier, the corresponding complete Lagrangian for this choice of U is

$$\operatorname{im} \begin{pmatrix} U + I \\ i(U - I) \end{pmatrix}.$$

This is just

$$\ker \begin{pmatrix} i(U^* - I) & U^* + I \end{pmatrix}.$$

This can be checked by direct computation and by noticing that the matrices are of rank n. Hence, the complete Lagrangian is spanned by functions ψ satisfying

$$i(U^* - I)\psi\big|_{\partial\Omega} + (U^* + I)\psi'\big|_{\partial\Omega} = 0$$

where

$$\psi\big|_{\partial\Omega} = \begin{pmatrix} \psi_1 & \psi_2 & \dots & \psi_n \end{pmatrix}^T \text{ and } \psi'\big|_{\partial\Omega} = \begin{pmatrix} \psi'_1 & \psi'_2 & \dots & \psi'_n \end{pmatrix}^T$$

in the $\{\xi_i\}_{i=1}^n \cup \{\xi'_j\}_{j=1}^n$ basis described above. This gives us the self-adjoint extension corresponding to U in terms of boundary conditions. The unitary matrix corresponding to Dirichlet boundary conditions ($\psi\big|_{\partial\Omega} = 0$) is $-I$. The unitary matrix corresponding to Neumann boundary conditions ($\psi'\big|_{\partial\Omega} = 0$) is I. In this next section we will show that this unitary matrix $U \in U(n)$ is not just a tool to help us get from self-adjoint extensions to boundary conditions, but it also has physical meaning in the context of scattering on a quantum graph.

7 Scattering on Quantum Graphs

Naturally, one might wonder about the "correct" self-adjoint extension or in the case of simple one dimensional problems the "correct" boundary conditions. As far as the author is aware and according to recent publications, [9] for example, this is still an open question. If there is a correct self-adjoint extension, one may have to impose further conditions in order to determine it. One might consider time-reversal invariant or parity preserving Hamiltonian operators the most physical options. One technique for assessing the legitimacy of a particular self-adjoint extension is to analyze the behavior of the quantum mechanical system under the classical limit. If in the classical limit a particular self-adjoint extension gives rise to bizarre classical behavior, one might be able to rule out that self-adjoint extension as being unphysical, see [10] for an example.

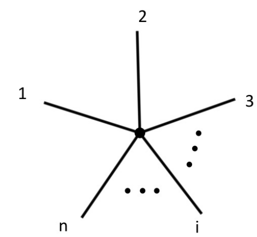

Figure 2: A non-compact star graph with n branches.

Here we suggest an experiment. Suppose we have a nice one-dimensional region such as a star graph pictured in Figure 2. Say we shoot a particle down the first branch of the graph, labeled 1. We expect the particle to hit the vertex and scatter. Quantum mechanics tells us this is a probabilistic event. It is possible that the particle hits the vertex and then continues traveling down the third branch. There might also be a chance that the particle reflects or goes down any of the other branches. We can continue to shoot particles down the first branch and record where they end up after being scattered. After, a sufficient number of scatterings we can obtain an estimate of the probability that the particle goes down the i^{th} branch. We might also be curious to see the probabilities if we instead shoot the particle down the i^{th} branch. After we have performed the experiment on each branch, we can tabulate our results. This is the concept behind a scattering matrix. We claim that given the scattering matrix, we can determine the specific self-adjoint extension at play. But first, we will give a definition of a quantum star graph and a more precise explanation of a scattering matrix.

Most generally, a graph is a set of vertices $V = \{v_i\}$ along with a set of edges $E = \{e_j\}$ that connect the vertices. For our purposes, a metric graph is a graph in which each edge is assigned a non-negative length and a direction. Further, there is a coordinate x_{e_j} on each edge which increases in the direction of the edge. A quantum graph, then, is a metric graph Γ along with a Hamiltonian operator defined on a subspace of $L_2(\Gamma) = \bigoplus_{e \in E} L_2(e)$.

A quantum star graph is a quantum graph with one vertex and n edges. We will focus our attention on the non-compact quantum star graph Γ_n which is a quantum star graph with each edge having infinite length and identified with the interval $[0, \infty)$. Therefore, a Hamiltonian operator for the non-compact quantum star graph acts on a subspace of $L_2(\Gamma_n) = \bigoplus_{i=1}^{n} L_2\big([0, \infty)\big)$. The initial Hermitian Hamiltonian operator is then defined on $\bigoplus_{i=1}^{n} C_0^{\infty}\big([0, \infty)\big)$. Star graphs are amenable to study because they are relatively simple and in some sense, they are fundamental. At any vertex, a metric graph looks locally like a star graph.

On an edge, the Schrödinger equation takes the form

$$-\frac{d^2\psi(x)}{dx^2} = k^2\psi(x).$$

The solutions of this equation are linear combinations of e^{-iix} and e^{iix}. e^{-ikx} is interpreted as a left traveling wave and e^{iix} is interpreted as a right traveling wave (positive direction). We have solved the time-independent Schrödinger equation, so these waves are really static in time. Nonetheless, it is useful to think of them as a constant stream of particles with momentum $\hbar k$.

We will define the scattering matrix $\sigma(k)$ on a non-compact quantum star graph with n edges as follows. We want the $\sigma_{e_i,e_j}(k)$ entry to be the scattering coefficient from edge e_j to edge e_i. When $i = j$ the entry is the reflection coefficient. Say we shoot a stream of particles down edge e_i with momentum $\hbar k$. The solution in this scenario then looks like

$$\psi_i(x) = \begin{cases} \psi_{e_i}(x_{e_i}) & = e^{-ikx_{e_i}} + \sigma_{e_i,e_i}(k)e^{ikx_{e_i}} \\ \psi_{e_j}(x_{e_j}) & = \sigma_{e_j,e_i}(k)e^{ikx_{e_j}} \text{ for } i \neq j \end{cases}$$

with $\psi(x)$ satisfying the boundary condition.

We would like to know the relationship between the scattering matrix and the boundary conditions. Well, for a stream of particles with momentum $\hbar k$ being sent down the edge e_i, we can analyze the vector Ψ_{e_i} of values of the solution at the boundary and the vector Ψ'_{e_i} of values of the derivative at the boundary. By looking at the solution above, we see that the j^{th} entry of Ψ_{e_i} is $\delta_{e_i,e_j} + \sigma_{e_j,e_i}$ and the j^{th} entry of Ψ'_{e_i} is $ik(-\delta_{e_i,e_j} + \sigma_{e_j,e_i})$. These should satisfy the equation for the boundary conditions. In fact, Ψ_{e_i} and Ψ'_{e_i} satisfy the equation for the boundary conditions for all $i = 1, ..., n$. Therefore, we may construct the following two $n \times n$ matrices, which together solve the equation for the boundary conditions. The first, Ψ is the matrix whose i^{th} column is the vector Ψ_{e_i}. The second, Ψ', is the matrix whose i^{th} column is the vector Ψ'_{e_i}. Hence, the i,j element of Ψ is $\Psi_{ij} = \delta_{e_i,e_j} + \sigma_{e_j,e_i}$, so $\Psi = I + \sigma$. The i,j element of Ψ' is $\Psi'_{ij} = ik(-\delta_{e_i,e_j} + \sigma_{e_j,e_i})$, so $\Psi' = ik(\sigma - I)$. These matrices should satisfy the boundary condition equation

$$i(U^* - I)\Psi + (U^* + I)\Psi' = 0.$$

Thus,

$$i(U^* - I)(I + \sigma) + ik(U^* + I)(-I + \sigma) = 0$$

and solving for σ we obtain

$$\sigma(k) = \left[(k+1)U^* + (k-1)\right]^{-1}\left[(k-1)U^* + (k+1)\right]$$

assuming that $\left[(k+1)U^* + (k-1)\right]$ is invertible. This is the scattering matrix in terms of the unitary matrix U corresponding to a particular self-adjoint extension of H_0. In this example, U tells us about the properties of the system. U specifies how a particle will scatter at a vertex. This suggests that it is possible to determine the boundary conditions from a scattering matrix. We have a means of potentially determining the "correct" boundary conditions, as one can use scattering data to recover the boundary conditions.

Let us examine a few special cases. First, when $k = -1$ we see that $\sigma(-1) = U^*$. This isn't terribly interesting, however, because we have assumed that $k > 0$. Next, when we have Dirichlet boundary conditions ($U = -I$) the scattering matrix is $\sigma(k) = -I$. This is in accord with our classical expectations. $\sigma(k) = -I$ says that the incoming wave is completely reflected and the amplitude switches sign. In the analogous classical system, if one were to tie a string to a solid wall and shake the string, the wave inverts upon reflection. For Neumann boundary conditions, $U = I$, and the scattering matrix is $\sigma(k) = I$. Again, this agrees with the classical picture of a string with a free end. The reflected wave is of the same sign as the incident wave.

Suppose that we want the stream of particles to scatter in a particular way. Is it possible to determine the boundary conditions that give us this scattering behavior? That is, given a scattering matrix, we would like to put the boundary conditions in terms of the scattering matrix. We can solve for U^* as a function of k and σ.

$$\sigma(k) = \big[(k+1)U^* + (k-1)\big]^{-1}\big[(k-1)U^* + (k+1)\big]$$

so assuming the invertibility of $\big[(k+1)\sigma - (k-1)\big]$ we have

$$U^* = \big[(k+1) - (k-1)\sigma\big]\big[(k+1)\sigma - (k-1)\big]^{-1}.$$

From here, we can write the equation for the boundary conditions in terms of k and σ. This goes to show that we can obtain the desired scattering by imposing the appropriate boundary conditions.

Altogether we now have a means of potentially determining the "correct" boundary conditions, as one can use scattering data to recover the boundary conditions. We have also shown that create a system with predetermined boundary conditions to obtain the desired scattering.

8 Acknowledgements

The author would like to give a special thanks to Professor Renato Feres for his patience and guidance throughout this project. He would also like to extend his sincere gratitude to the ARTU administration for their part in making this research possible.

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