PALINDROMIC CONTROL AND MIRROR SYMMETRIES IN
FINITE DIFFERENCE DISCRETIZATIONS OF 1-D
SCHRÖDINGER EQUATIONS

Katherine A. Kime

Department of Mathematics and Statistics
University of Nebraska Kearney
Kearney, Nebraska 68849, USA

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ABSTRACT. We consider discrete potentials as controls in systems of finite difference equations which are discretizations of a 1-D Schrödinger equation. We give examples of palindromic potentials which have corresponding steerable initial-terminal pairs which are not mirror-symmetric. For a set of palindromic potentials, we show that the corresponding steerable pairs that satisfy a localization property are mirror-symmetric. We express the initial and terminal states in these pairs explicitly as scalar multiples of vector-valued functions of a parameter in the control.

1. Introduction. In this section we give a synopsis of the paper. We consider discrete potentials as controls in systems of finite difference equations which are discretizations of 1-D Schrödinger equations with time-dependent rectangular potentials. The discretizations are an extension of the classic discretizations of Goldberg et al., [10].

A discrete initial state $Y_0$ is said to be steered to a discrete terminal state $Y_T$ by a discrete potential, in time $T$, if the unique solution of an initial value problem consisting of solving a system of finite difference equations with this potential, and with initial state $Y_0$, equals $Y_T$ at time $t = T$. If so, we say the initial-terminal pair is a steerable pair which corresponds to the discrete potential. The potential is real, and the initial and terminal states are complex vectors. If the last component(s) of the initial state and the first component(s) of the terminal state are equal to zero in a way to be further detailed, then the initial-terminal pair is said to be $\alpha$-localized.

A palindromic discrete potential is one that reads the same forward and backward, in space and time. If the sequence of absolute values of the components of the initial state and the sequence of absolute values of the components of the terminal state are mirror images, we say the initial-terminal pair is mirror-symmetric.

We give an example of a palindromic discrete potential and a corresponding steerable pair which is $\alpha$-localized and which has mirror-symmetry. We then give examples of palindromic potentials and corresponding steerable pairs which are not

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* Corresponding author: Katherine A. Kime.
α-localized and not mirror-symmetric. A palindromic potential does not always induce mirror-symmetry; palindromy $\neq$ mirror-symmetry.

We then prove a theorem which says that the solutions of homogeneous matrix equations, with matrices of a described form, are complex scalar multiples of complex vectors with a property that we call conjugate component symmetry. From this we conclude, for a set of palindromic discrete potentials, that if steerable pairs are required to be α-localized, then they are mirror-symmetric. Thus, for a certain class of discrete potentials, palindromy + α-localization $\Rightarrow$ mirror-symmetry. The proof of the theorem leads to explicit expressions for the pairs.

2. Background, motivation, outline of paper.

2.1. Control of the Schrödinger equation through the potential; bilinear, infinite-dimensional. A major problem in the control theory of ordinary or partial differential equations is the following: Given initial and terminal states in a specified state space, and a time $T > 0$, determine if there exists an admissible control function such that the unique solution of the initial value problem consisting of solving the equation in question with this control in place, (as a term in the equation or possibly in the boundary condition) and with the given initial state, equals the terminal state at time $t = T$. Such a control is said to “steer” the initial state to the terminal state.

If, for any choice of initial and terminal states, there is such a control, then the control system (or controlled equation) is said to be exactly controllable. Whether the system can be shown to be exactly controllable or not, it is of interest to characterize the initial-terminal pairs for which there does exist a control which steers the initial state to the terminal state in time $T$. The terminal state is thus an element of the set of states reachable from the initial state (the reachable set, from this initial state).

Here, we consider the 1-D Schrödinger equation with a time-dependent potential function $V(x,t)$ as control

$$\frac{\partial \psi}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + V(x,t)\psi, \quad 0 < x < L, \quad 0 < t < T,$$

and boundary conditions

$$\psi(0,t) = \psi(L,t) = 0,$$

where $L > 0, T > 0$ are given. The square of the absolute value of the wavefunction $\psi$, $|\psi|^2$, is taken to be a probability density. The control problem, as described above, for this system is infinite-dimensional, as the state space is a function space to be determined, and bilinear, as the control $V$ multiplies the solution $\psi$.

While much is known about infinite-dimensional control problems in which the control enters linearly or is a boundary term, such as those for the wave, heat and beam equations [14], [15], [19], less is known about infinite-dimensional bilinear control problems. In the case of control of the Schrödinger equation through the potential, important progress has been made in recent years by Beauchard, Coron, and co-workers, e.g. [2], [9], [16]. These works have treated the case in which the potential is a dipole potential, which models the interaction of an electromagnetic field with a quantum particle. The results are of local, approximate and exact controllability with Sobolev spaces as state spaces. Boscain and co-workers have studied related problems [4].
2.2. **Rectangular time-dependent barrier/wells as controls.** To our knowledge, the question of controllability has not been resolved for the system (1), (2) with the control a time-dependent rectangular potential barrier/well of the form

\[
V(x, t) = \begin{cases} 
0 & 0 \leq x < a \\
\nu(t) & a \leq x \leq b, \\
0 & b < x \leq L
\end{cases}, \quad 0 \leq t \leq T, \quad (3)
\]

where \(a, b\) are real numbers satisfying \(0 < a \leq b < L\) and \(\nu(t)\) is a real-valued function of \(t\). At times \(t\) at which \(\nu(t)\) is positive, we have a barrier, and at times \(t\) at which \(\nu(t)\) is negative, we have a well.

We are motivated to consider these barrier/wells by the fact that systems with static rectangular barriers and wells are the most basic examples beyond the case of the free particle (potential equaling zero), appearing early on in treatments such as [3], [20]. Less is known about time-dependent barriers, although they also have been a subject of interest, e.g. in relation to the tunneling time problem [6]. Mathematically, the rectangular barriers and wells are step functions, and could be used to approximate other functions serving as potentials.

2.3. **Discretizations and discrete control problem.** In this paper, we consider systems of finite difference equations which are discretizations of the controlled Schrödinger equation. As the Schrödinger equation cannot be solved exactly except in a very few cases, discretizations are widely used for approximating solutions of the Schrödinger equation even when control is not an issue. According to [5], the discretized (time-independent) Schrödinger equation is more physically reasonable than the continuous equation for modelling semiconductor quantum wells. Some form of numerical approximation will be needed for use in physical experiments of control, and the study of control of the discrete problem may contribute to understanding of the infinite dimensional problem. Discretization of control problems for other PDEs, e.g. semi-and full-discretization of boundary control problems for the wave equation, [21], is also a subject of study.

2.4. **Outline of the paper.** In Sec. 3, we specify the finite difference discretization method that we will use. In Sec. 4 we define discrete potential and pose a discrete initial value problem. We also pose a discrete control problem and indicate what is necessary for solving it for arbitrary discrete initial and terminal states, which is not yet possible.

The scope of the control problem may be reduced by looking for steerable pairs with a particular property. For the free-particle PDE system with a Gaussian initial state, \(|\psi|^2\) remains Gaussian but broadens in time [3], [20]. Generally the Gaussian is represented initially on the left of the space interval, broadening as it propagates to the right. This motivates us to consider discrete initial states which could be discretizations of continuous wavefunctions localized towards the left of the space interval, and similarly discrete terminal states towards the right, so as to model left-to-right propagation. In Sec. 5 we define side-localized vectors and the degree of restriction of such. We then define localized initial-terminal pairs and a particular type of these, \(\alpha\)-localized initial-terminal pairs.

To approach the identification of localized steerable pairs, we consider discrete potentials with a particular property. The potentials we consider are palindromic, as defined in Sec. 5. Our definition differs from that of Hof, Knill and Simon [11], who studied palindromic Schrödinger operators in a different context. In this section,
we also define mirror-symmetric initial-terminal pairs and conjugate component symmetry.

In Sec. 6, we give an example of a palindromic discrete potential and a corresponding $\alpha$-localized steerable pair which has mirror-symmetry. We then give another corresponding steerable pair for this potential which is not localized and is not mirror-symmetric. We also give an example of a different palindromic potential with a corresponding steerable pair in which the degrees of restriction of the initial and terminal states are equal, but the steerable pair is not $\alpha$-localized. This pair does not have mirror-symmetry.

Given a solution to an initial value problem with a palindromic discrete potential, the conjugate mirror image of the solution is the solution of an initial value problem with this same potential, which we call the conjugate mirror solution. We give details in Sec. 6. If one adds the original solution to its conjugate mirror solution, the sum is also a solution and has conjugate component symmetry. This process of superposition generates a mirror-symmetric initial-terminal pair that corresponds to the palindromic potential. However, in the superposition, the nature of localization may change.

In Sec. 7, we write the system of finite difference equations in the form of a homogeneous matrix equation in which the matrix is a block matrix that we call a stackmatrix. We then write a homogeneous matrix equation for a matrix formed by deleting columns from the stackmatrix. This deleted stackmatrix is associated with solutions of the system with localized initial-terminal pairs with equal degree of restriction. In Sec. 8, we define a set $\Lambda$ of palindromic discrete potentials, and form deleted stackmatrices which are associated with solutions with $\alpha$-localized initial-terminal pairs. We prove in Theorem 8.1 that solutions of the homogeneous equations for the deleted stackmatrices are complex scalar multiples of complex vectors which have conjugate component symmetry. In Sec. 9, we use Theorem 8.1 to show that the $\alpha$-localized steerable pairs corresponding to elements of $\Lambda$ are mirror-symmetric and give explicit expressions for them.

3. Finite difference methods. We now discuss finite difference methods for (1), (2), (3). Let $L > 0$, $T > 0$ be given. Let $J, N$ be positive integers. We form a grid on $[0, L] \times [0, T]$ as follows. The step size in space, $\Delta x$, is defined by $\Delta x = \frac{L}{J+1}$, and we define $x_j = j \Delta x$, $j = 0, \ldots, J+1$. The step size in time, $\Delta t$, is $\Delta t = \frac{T}{N}$, and we define $t_n = n \Delta t$, $n = 0, \ldots, N$, and $t_{n+\frac{1}{2}} = t_n + \frac{\Delta t}{2}$. Thus there are $J$ internal grid points and $J + 1$ intervals in space, $N-1$ internal gridpoints and $N$ intervals in time.

3.1. Method of Goldberg et al., [10], for the time-independent potential. A classic paper of Goldberg et al., [10], gives a finite difference discretization method for the 1-D Schrödinger equation with time-independent potential barriers and wells, which may be shown to be the Crank-Nicolson scheme, although it is motivated by the Cayley transform. Striking representations of the impingement of a wavefunction with Gaussian initial data on barriers and wells are given, showing transmission and reflection (also see [20]). Due to the visualizations generated and the extensive use made of this work, we will use a discretization method for (1), (2), with a rectangular potential of the form (3) that extends the scheme of [10].

We discuss the method of [10]. Consider the 1-D Schrödinger equation with $V(x)$ a time-independent potential barrier or well.
\[ \frac{i}{\partial t} \psi = -\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi. \] (4)

As the physical system is viewed as being situated in a “box” and the wavefunction must vanish at the “walls”, it is required that \( \psi(0, t) = \psi(L, t) = 0 \) for all \( t \), where the box extends from 0 to \( L \) : \( 0 \leq x \leq L \). The system of finite difference equations for \( \Psi^n_j \), where \( \Psi^n_j \) approximates \( \psi(x_j, t_n) \) and \( V(x_j) = V_j \) is

\[
\begin{align*}
\Psi^{n+1}_{j+1} + \left( i \frac{2(\Delta x)^2}{\Delta t} - (\Delta x)^2 V_j - 2 \right) \Psi^{n+1}_j + \Psi^{n+1}_{j-1} \\
= -\Psi^n_{j+1} + \left( i \frac{2(\Delta x)^2}{\Delta t} + (\Delta x)^2 V_j + 2 \right) \Psi^n_j - \Psi^n_{j-1},
\end{align*}
\]

(5)

with boundary conditions \( \Psi^n_0 = \Psi^n_{N+1} = 0 \) for all \( n \). The initial state considered in [10] is Gaussian and localized on the left side of the barrier, and the propagation is as described above.

3.2. Method for the time-dependent potential. We will extend [10] to the case of the time-dependent potential by using an approach of Burden and Faires, [7] for the heat equation. Our method will also discretize the potential as is done in in [1], which we now review. Other treatments of finite difference schemes for the Schrödinger equation include [8], [17].

Akrivis and Dougalis, [1], studied finite difference discretizations with variable mesh in a variable domain. They considered the problem

\[
\begin{align*}
&u_t = u_{xx} + \beta(x, t)u, \quad 0 \leq t \leq T, \quad 0 \leq x \leq s(t), \\
&u(0, t) = u(x(t), t) = 0, \quad 0 \leq t \leq T, \\
&u(x, 0) = u_0(x), \quad 0 \leq x \leq s(0) = 1.
\end{align*}
\]

(6)

It is assumed that (6) has a unique solution which is smooth enough for numerical approximation. We consider the rectangular domain with \( s(t) = 1 \) on \([0, T]\), thus \( 0 \leq x \leq 1 \) for all \( t \), and with constant step size.

In [1], approximations \( U^0_j \) to the values \( u(x_j, t_n) \) are given. For \( n = 0 \), \( U^0_j = u_0(x_j) \), and for \( 0 \leq n \leq N - 1 \) the approximations are given by

\[
\begin{align*}
U^{n+1}_{j+1} + \left( i \frac{2(\Delta x)^2}{\alpha \Delta t} - 2 \right) U^{n+1}_j + \frac{\Delta x^2}{\alpha} \beta(x_j, t_{n+1/2}) U^{n+1}_{j-1} \\
= -U^n_{j+1} + \left( i \frac{2(\Delta x)^2}{\alpha \Delta t} + 2 \right) U^n_j - U^n_{j-1} - \frac{\Delta x^2}{\alpha} \beta(x_j, t_{n+1/2}) U^n_{j-1}.
\end{align*}
\]

(7)

As the mesh size is uniform, this is the Crank-Nicolson scheme. In [1], stability, consistency and an optimal \( l_2 \) order estimate are proved.

In [7], the Crank-Nicolson method for the heat equation is obtained by averaging the Forward Difference method at the \( n \)th step in \( t \) and the Backward Difference method at the \((n + 1)\)st step in \( t \). Such averaging was used in [13] for a 1-D Schrödinger equation with the potential in the forward method evaluated at the \( nth \) step and the potential in the backward method evaluated at the \((n + 1)\)st step. In [12], the approach of [13] was extended to a nonlinear Schrödinger equation.

We now use the averaging approach of [7] to discretize (1), (2), (3), with initial condition

\[ \psi(x, 0) = \psi_0(x), \]

(8)

where \( \psi_0(x) \) is a given initial state. The potential will be evaluated at the midpoints in time, \( t_{n+\frac{1}{2}} \), as in [1] (see (7)). This is also computationally convenient and is
amenable to comparison with semi-discretization. In the following $\Psi^n_j$ approximates $\psi(x_j, t_n)$. We average each equation in the forward method at the $n$th step in $t$

$$
\frac{(\Psi_j^{n+1} - \Psi_j^n)}{\Delta t} + \frac{(\Psi_j^{n+1} - 2\Psi_j^n + \Psi_j^{n-1})}{(\Delta x)^2} - V(x_j, t_n + \frac{\Delta t}{2})\Psi_j^n = 0
$$

(9)

and its corresponding equation in the backward method at the $(n+1)$st step in $t$

$$
\frac{(\Psi_j^{n+1} - \Psi_j^n)}{\Delta t} + \frac{(\Psi_j^{n+1} - 2\Psi_j^{n+1} + \Psi_j^{n+1})}{(\Delta x)^2} - V(x_j, t_{n+\frac{\Delta t}{2}})\Psi_j^{n+1} = 0
$$

(10)

obtaining, after simplification, the system of equations

$$
\Psi_{j+1}^{n+1} + \left(2\frac{(\Delta x)^2}{\Delta t} - 2\right)\Psi_j^{n+1} + \Psi_{j-1}^{n+1} - (\Delta x)^2 V(x_j, t_{n+\frac{\Delta t}{2}})\Psi_j^{n+1}
$$

$$
= - \Psi_j^{n+1} + \left(2\frac{(\Delta x)^2}{\Delta t} + 2\right)\Psi_j^n - \Psi_{j-1}^{n+1} + (\Delta x)^2 V(x_j, t_{n+\frac{\Delta t}{2}})\Psi_j^n,
$$

(11)

$j = 1, ..., J, \quad n = 0, ..., N - 1.$

The discrete boundary condition is

$$
\Psi_0^n = \Psi_J^{n+1} = 0 \quad n = 0, ..., N.
$$

(12)

The discrete initial condition is

$$
\Psi_j^0 = \psi_0(x_j) \quad j = 1, ..., J.
$$

(13)

One sees that (11) reduces to (5) if $V$ is time-independent, i.e. $V(x_j, t_{n+\frac{\Delta t}{2}}) = V(x_j) = V_j$. Thus (11) is an extension of the method of [10], and is the method that we will use. Also, (11) is of the form (7) when $\alpha = 1, \beta(x, t) = -V(x, t)$ and $L = 1$.

Remark 1. We do not assert at this point that solutions of (1), (2), with a rectangular potential of the form (3), and (8) are sufficiently smooth for the conclusions of [1] to hold here.

For each rectangular potential $V$ of the form (3), and for each choice of $J$ and $N$, we have a system (11), which, with (12), will be called the discretization of (1), (2) generated by $V$ at grid level $(J + 1, N)$.

4. Discrete potential, initial value problem and control problem. In this section we define discrete potential, systems of difference equations $S$ and pose a discrete initial value problem and control problem. From now on, $[\gamma_1 \cdots \gamma_n]^T$ denotes the transpose of the row vector $[\gamma_1 \cdots \gamma_n]$.

4.1. Discrete potential.

Definition 4.1. Let $J, N$ be positive integers, and let $j_L, j_R$ be positive integers with $0 < j_L \leq j_R < J + 1$. Let $\{\xi_n\}_{n=0, ..., N-1}$ be a sequence of real numbers. For $j = 1, ..., J, \quad n = 0, ..., N - 1$ let

$$
P^n_j = \begin{cases} 
0 & 1 \leq j < j_L \\
\xi_n & j_L \leq j \leq j_R \\
0 & j_R < j \leq J.
\end{cases}
$$

(14)

The doubly indexed sequence $\{P^n_j\}_{j=1, ..., J}$ is called a discrete potential of dimensions $J \times N$.
4.1.1. Relationship between rectangular potential and discrete potential. First, suppose \( V \) is a rectangular potential of the form (3). Then, for any choice of \( J, N \), with a grid as above, we may use \( V \) to define a discrete potential \( \{ P^n_j \} \) of dimensions \( J \times N \) by \( P^n_j = V(x_j, t_{n+\frac{1}{2}}), \ j = 1, ..., J, \ n = 0, ..., N - 1 \). Then \( \xi_n = \nu(t_{n+\frac{1}{2}}) \).

Second, suppose \( \{ P^n_j \} \) is a discrete potential of dimensions \( J \times N \). Let \( L > 0, T > 0 \) be given. We may define the values of a function \( V \) at the points \((x_j, t_{n+\frac{1}{2}})\), by \( V(x_j, t_{n+\frac{1}{2}}) = P^n_j \). There are then infinitely many ways to choose the values of \( V \) at the remaining points, so that the form (3) results (which means choosing the values \( \nu(t) \) for \( t \neq t_{n+\frac{1}{2}} \)). Thus there are infinitely many \( V \)s which correspond to a choice of \( L, T \) and discrete potential \( \{ P^n_j \} \). This lack of uniqueness motivated the definition of \( \{ P^n_j \} \).

4.2. System \( S \). In the remainder of the paper, we will assume \( \Delta x = 1, \Delta t = 2 \). Thus, a choice of \( J, N \) determines \( L, T \).

**Definition 4.2.** Let \( J, N \) be positive integers and let \( \{ P^n_j \} \) be a discrete potential of dimensions \( J \times N \). The system of difference equations

\[
\Psi_j^{n+1} + (-2 + i) \Psi_j^{n+1} + \Psi_{j-1}^{n+1} - P^n_j \Psi_j^{n+1} = -\Psi_{j+1}^{n+1} + (2 + i) \Psi_{j-1}^{n+1} + P^n_j \Psi_j^{n+1}, \quad j = 1, ..., J, \quad n = 0, ..., N - 1,
\]

with \( \Psi_0^0 = \Psi_{J+1}^0 = 0 \) for \( n = 0, ..., N \), is called a system \( S \) at grid level \((J+1, N)\) corresponding to \( \{ P^n_j \} \).

4.2.1. Relationship between discretizations and systems \( S \). First, if \( V \) is a potential of the form (3), then the discretization generated by \( V \) at grid-level \((J+1, N)\) is a system \( S \) at grid-level \((J+1, N)\) in which the discrete potential \( \{ P^n_j \} \) is given by \( P^n_j = V(x_j, t_{n+1/2}) \). Second, if we start with a discrete potential \( \{ P^n_j \} \) of dimension \( J \times N \), and form the corresponding system \( S \), this system is a discretization which is generated by infinitely many \( V \)s.

4.3. Discrete initial value problem. Let \( J, N \) be positive integers and let \( \{ P^n_j \} \) be a discrete potential of dimensions \( J \times N \). Let \( Y_0 \) be a complex \( J \) vector, \( Y_0 = [Y_{0,1} \cdots Y_{0,J}]^T \). Solve the system \( S \), (15), with \( \{ P^n_j \} \) and with the initial condition \( \Psi_j^0 = Y_{0,j}, \ j = 1, ..., J \).

This is a system of \( NJ \) equations in the \( NJ \) variables \( \Psi_1^1, ..., \Psi_J^1, ..., \Psi_1^N, ..., \Psi_J^N \). If \( \Psi = [\Psi_1^1 \cdots \Psi_J^0 \cdots \Psi_1^N \cdots \Psi_J^N]^T \) is a solution of the initial value problem, then the vector \( \Psi_t^a = [\Psi_1^a \cdots \Psi_J^a]^T \) will be called the state at time \( t_n = n\Delta t = 2n, n = 0, ..., N \). The pair \( (\Psi_0^0, \Psi_N^N) \) is the initial-terminal pair of this solution and corresponds to \( \{ P_j^n \} \).

Let \( A \) be the \( J \times J \) matrix defined by

\[
A = \begin{bmatrix}
-2 + i & 1 & 0 & \cdots & 0 \\
1 & -2 + i & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 1 & -2 + i & 1 \\
0 & \cdots & 0 & 1 & -2 + i 
\end{bmatrix}.
\]
For \( n = 0, ..., N - 1 \), let \( \hat{P}^n \) be the \( J \times J \) diagonal matrix defined by

\[
\hat{P}^n = \begin{bmatrix}
P_1^n & 0 & 0 & \cdots & 0 \\
0 & P_2^n & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & 0 & P_{J-1}^n & 0 \\
0 & \cdots & 0 & 0 & P_J^n
\end{bmatrix}.
\] (17)

Let \( A^* \) be the conjugate transpose of \( A \). For each \( n, n = 0, ..., N - 1 \), the corresponding subsystem of (15), can be written in matrix form as

\[
(A - \hat{P}^n) \begin{bmatrix}
\Psi_1^{n+1} \\
\vdots \\
\Psi_J^{n+1}
\end{bmatrix} = (-A^* + \hat{P}^n) \begin{bmatrix}
\Psi_1^n \\
\vdots \\
\Psi_J^n
\end{bmatrix}.
\] (18)

If \( (A - \hat{P}^n) \) is invertible for \( n = 0, 1, ..., N - 1 \), then one may solve the initial value problem with arbitrary initial data \( Y_0 \) by starting with \( n = 0 \) in (18), setting \( \Psi^0 = Y_0 \), and solving for \( \Psi^1 \). Then, using \( \Psi^1 \) in the subsystem for \( n = 1 \), one solves for \( \Psi^2 \), and continues this process up to \( n = N - 1 \). At each stage, the solution to the matrix equation exists and is unique, and thus the solution to the initial value problem \( \Psi \) exists and is unique.

4.4. Discrete control problem. Let \( J, N \) be positive integers. Let complex \( J \) vectors \( Y_0, Y_T \) be given. Find a discrete potential \( \{P^n_j\} \) of dimensions \( J \times N \) such that

a) the matrices \( (A - \hat{P}^n) \) are invertible for \( n = 0, 1, ..., N - 1 \)

b) the unique solution of the initial value problem consisting of solving the system \( S \) with \( \{P^n_j\} \) and initial condition \( \Psi^0 = Y_0 \) also satisfies \( \Psi^N = Y_T \).

If such a discrete potential exists, it is said to steer \( Y_0 \) to \( Y_T \) in time \( T = N\Delta t = 2N \), and the initial-terminal pair \((Y_0, Y_T) = (\Psi^0, \Psi^N)\) is said to be steerable. A steerable pair \((Y_0, Y_T)\) corresponding to \( \{P^n_j\} \) is thus a pair which serves as the initial and terminal states in the unique solution of system \( S \) with \( \{P^n_j\} \) and initial condition \( \Psi^0 = Y_0 \).

With \((Y_0, Y_T)\) specified, any system \( S \) has \( NJ \) equations with the \((N - 1)J \) variables, \( \Psi_1^1, ..., \Psi_1^{N-1}, ..., \Psi_J^1, ..., \Psi_J^{N-1} \). The discrete potential has up to \( N \) variables. Thus to solve the control problem, one must solve \( NJ \) equations in at most \((N - 1)J + N = NJ + (N - J) \) variables. These equations are nonlinear in the variables. To our knowledge these equations cannot be solved for arbitrary initial and terminal states at this time, although the limits of computer algebra systems such as Maple remain to be determined.

5. Localized initial-terminal pair, palindromic discrete potential and mirror-symmetric initial-terminal pairs.

5.1. Localization. Let \( J \) be a positive integer and \( k \) be an integer with \( 1 \leq k < J \). A complex \( J \)-vector of the form \([\gamma_1 \cdots \gamma_k 0 \cdots 0]^T\) with \( \gamma_k \neq 0 \), or of the form \([0 \cdots 0 \gamma_{J-k+1} \cdots \gamma_J]^T\) with \( \gamma_{J-k+1} \neq 0 \), is called side-localized with degree of restriction \( J - k \). The former is called side-localized towards the left, the latter side-localized towards the right.

An initial-terminal pair in which the initial state is side-localized towards the left and the terminal state is side-localized towards the right is called localized. If the
degree of restriction is the same for the initial state and terminal state and equals \( J - k \), the initial-terminal pair is localized with equal degree of restriction \( J - k \).

**Definition 5.1.** Let \( J \) be odd and let \( k = \frac{J+1}{2} \). An initial-terminal pair which is localized with equal degree of restriction \( J - k = J - \frac{J+1}{2} = \frac{J-1}{2} \) is called \( \alpha \)-localized.

5.2. **Palindromic potentials.** Rosen, [18], defines a palindrome as a string (finite sequence) which reads the same forwards and backwards. Our next definition is a small modification of this.

**Definition 5.2.** A finite sequence of real numbers which reads the same forward and backward is called a palindromic sequence.

A discrete potential is said to be palindromic in time if the sequence \( \{\xi_n\}_{n=0,\ldots,N-1} \) appearing in (14) is a palindromic sequence. A discrete potential is said to be palindromic in space if, for each \( n \), the sequence \( P_n^1, \ldots, P_n^J \) is a palindromic sequence. This is equivalent to the barrier/well being centered in the space interval.

**Definition 5.3.** A discrete potential which is palindromic in space and palindromic in time is called palindromic.

5.3. **Mirror-symmetric initial-terminal pairs, conjugate component symmetry.**

**Definition 5.4.** Let \((\Psi^0, \Psi^N)\) be an initial-terminal pair of a solution of an initial value problem. If

\[
|\Psi^0_j| = |\Psi^N_{J+1-j}|, \quad j = 1, \ldots, J,
\]

then the initial-terminal pair is called mirror-symmetric.

**Definition 5.5.** A vector \( \zeta \in \mathbb{C}^m \) is said to have conjugate component symmetry, or CCS, if

\[
\bar{\zeta}_\ell = \zeta_{m+1-\ell},
\]

\( \ell = 1, \ldots, m/2 \) for \( m \) even, \( \ell = 1, \ldots, (m - 1)/2 \) for \( m \) odd.

If \( \zeta \) has CCS, then the sequence of absolute values of the components of \( \zeta \) is palindromic, and this also holds for any complex scalar multiple of \( \zeta \). Thus if a solution of a discrete initial value problem has CCS or is a complex scalar multiple of a vector which has CCS, then its initial-terminal pair is mirror-symmetric.

6. **Examples.** The solutions in Examples 1 and 3 were found by using Maple to solve the homogeneous matrix equation, (34), in Sec. 7. In all examples, the process described at the end of Sec. (4.3) was used to check or find (Ex. 2) the solution. Inverses of the matrices \((A - \bar{P}^n)\) were found and checked by Maple.

6.1. **Example 1.** \( \alpha \)-localized, mirror-symmetric. Let \( J = 3, N = 3 \). Let \( \xi_0 = -2, \xi_1 = 4, \) and \( \xi_2 = -2 \). Then \( \{\xi_n\}_{n=0,1,2} \) is a palindromic sequence of length 3. Taking \( j_L = 1 \) and \( j_R = 3 \), we define the palindromic potential

\[
P^n_j = \begin{cases} 
\xi_n & j = 1 \\
\xi_n & j = 2 \\
\xi_n & j = 3 
\end{cases}
\]

for \( n = 0,1,2 \). Thus, for each \( n \), the discrete potential “extends” from \( j = 1 \) to \( j = 3 \), with heights varying as -2, 4, -2. The second dimension of this discrete
potential is the smallest possible for which a palindromic discrete potential could be non-constant in time.

Let

\[ \Psi_0 = \begin{bmatrix}
\frac{5}{2} - \frac{5}{12}i \\
-(305/1848) - (215/308)i \\
0
\end{bmatrix}. \]  

(20)

Solving (18) with \( n = 0 \) for \( \Psi^1 \),

\[
\begin{bmatrix}
i & 1 & 0 \\
1 & i & 1 \\
0 & 1 & i
\end{bmatrix}
\begin{bmatrix}
\Psi_1^1 \\
\Psi_2^1 \\
\Psi_3^1
\end{bmatrix} =
\begin{bmatrix}
i & -1 & 0 \\
-1 & i & -1 \\
0 & -1 & i
\end{bmatrix}
\begin{bmatrix}
\frac{5}{2} - \frac{5}{12}i \\
-(305/1848) - (215/308)i \\
0
\end{bmatrix},
\]

(21)

we obtain

\[ \Psi_1^1 = \begin{bmatrix}
100/77 - (115/462)i \\
205/616 + (585/308)i \\
-185/154 + (155/924)i
\end{bmatrix}. \]

Then, in the next step, with \( n = 1 \), solving

\[
\begin{bmatrix}
-6 + i & 1 & 0 \\
1 & -6 + i & 1 \\
0 & 1 & -6 + i
\end{bmatrix}
\begin{bmatrix}
\Psi_1^2 \\
\Psi_2^2 \\
\Psi_3^2
\end{bmatrix} =
\begin{bmatrix}
i & -1 & 0 \\
-1 & 6 + i & -1 \\
0 & -1 & 6 + i
\end{bmatrix}
\begin{bmatrix}
100/77 - (115/462)i \\
205/616 + (585/308)i \\
-185/154 + (155/924)i
\end{bmatrix},
\]

(22)

we obtain

\[ \Psi_2^2 = \begin{bmatrix}
-185/154 - (155/924)i \\
205/616 - (585/308)i \\
100/77 + (115/462)i
\end{bmatrix}. \]

Finally, with \( n = 2 \), solve (21), with \( \Psi_2^2 \) in place of \( \Psi_0 \) and \( \Psi_3^2 \) in place of \( \Psi_1 \), obtaining the terminal state

\[ \Psi_3^3 = \begin{bmatrix}
0 \\
-(305/1848) + (215/308)i \\
5/2 + (5/12)i
\end{bmatrix}. \]

The initial-terminal pair \((\Psi_0, \Psi_3^3)\) has equal degree of restriction \( 3 - 2 = 1 \), is \( \alpha \)-localized, and mirror-symmetric. The solution \( \Psi \) has CCS. See Figure 1. As the square of the absolute value of the solution of the Schrödinger equation is a probability density, we plot \((j, |\Psi_n|^2)\) at times \( t_n = n \Delta t = 2n \), for \( n = 0, 1, 2, 3 \). The plotted points are connected with lines in a graph generated by MATLAB. If \( \nu \) is defined by

\[ \nu(t) = \begin{cases}
3t - 5 & 0 \leq t \leq 3 \\
-3t + 13 & 3 < t \leq 6
\end{cases}, \]  

(23)

and \( V \) is defined as in (3), using \( \nu \), with \( a = 1, b = 3 \), then \( P_j^n = V(x_j, t_{n+1/2}) \). Thus \( V \) is one of the infinitely many rectangular potentials which correspond to the discrete potential \( P_j^n \) (see Sec. 4.1.1). In each subplot, \( n = 0, 1, 2, 3 \), we also plot \( V(x, t_n) \) and draw vertical lines to show the “sides” of the rectangular potential.
6.2. Not $\alpha$-Localized, not mirror-symmetric.

6.2.1. Example 2. Initial-terminal pair not localized. Here we use the same discrete potential as in Example 1. Let

$$\Psi^0 = \begin{bmatrix} 1 + i \\ 2 + i \\ 0 \end{bmatrix}. \quad (24)$$

Solving (18) successively as above, we obtain

$$\Psi^1 = \frac{1}{3} \begin{bmatrix} -1 + 5i \\ -4 + i \\ -4 + 2i \end{bmatrix}, \quad \Psi^2 = \frac{1}{45621} \begin{bmatrix} 39193 - 62331i \\ 66378 + 12617i \\ 67552 - 4380i \end{bmatrix},$$

$$\Psi^3 = \frac{1}{136863} \begin{bmatrix} -121145 + 79185i \\ 67044 + 200873i \\ -36068 + 253038i \end{bmatrix}. \quad (25)$$

See Figure 2.

6.2.2. Example 3. Initial-terminal pair localized with equal degree of restriction equal to 1, not $\alpha$-Localized. Let $J = 5$, $N = 3$. Let $\xi_0 = 1$, $\xi_1 = -3$, and $\xi_2 = 1$. We define a palindromic potential using this sequence, as in Example 1. Let

$$\Psi^0 = \frac{1}{69022825} \begin{bmatrix} -74429454 + 2068978i \\ 22936437 - 11778984i \\ 58094370 + 40721760i \\ 56930282 + 102795874i \\ 0 \end{bmatrix}. \quad (25)$$
Solving (18) successively as above, we obtain

\[
\Psi_1 = \frac{1}{69022825} \begin{bmatrix}
61757860 + 43983480i \\
-19036717 + 13749044i \\
-8195588 - 38890884i \\
123114264 - 32983348i \\
12873942 + 27562156i
\end{bmatrix},
\]

\[
\Psi_2 = \frac{1}{69022825} \begin{bmatrix}
-1667302 + 17628414i \\
-67408907 - 11935776i \\
865834 + 23837912i \\
25389910 + 29161630i \\
-99903384 + 89036888i
\end{bmatrix},
\]

\[
\Psi_3 = \begin{bmatrix}
0 \\
(44778587/69022825) + (63153716/69022825)i \\
0 \\
0 \\
2
\end{bmatrix}.
\]

If \( \nu \) is defined by

\[
\nu(t) = \begin{cases} 
-2t + 3 & 0 \leq t \leq 3 \\
2t - 9 & 3 < t \leq 6
\end{cases},
\]

and \( V \) is defined as in (3), using \( \nu \), with \( a = 1, b = 3 \), then \( P_j^n = V(x_j, t_{n+1/2}) \). See Figure 3.

6.3. Superposition of solution and conjugate mirror solution. In this and following sections, the complex conjugate of a complex number \( \gamma \) will be denoted by \( \overline{\gamma} \). Let \( \Psi = [\Psi_1^0 \cdots \Psi_j \cdots \Psi_j^0 \cdots \Psi_j^N]^T \) be the solution of an initial value problem.
Figure 3. Example 3. Localized with Equal Degree of Restriction Equal to 1, Not $\alpha$-Localized, Not Mirror-Symmetric

Consider (18). As the $j$th row of $A - \hat{P}^n$ is the mirror image of the $(J + 1 - j)$th row of $A - \hat{P}^n$, and similarly for $-A^* + \hat{P}^n$, we may write
\[
(A - \hat{P}^n) \begin{bmatrix} \Psi_j^{n+1} \\ \vdots \\ \Psi_1^n \end{bmatrix} = (-A^* + \hat{P}^n) \begin{bmatrix} \Psi_j^n \\ \vdots \\ \Psi_1^n \end{bmatrix}.
\] (27)

If we take conjugates of both sides and rearrange, we obtain
\[
(A - \hat{P}^n) \begin{bmatrix} \Psi_j^n \\ \vdots \\ \Psi_1^n \end{bmatrix} = (-A^* + \hat{P}^n) \begin{bmatrix} \Psi_j^{n+1} \\ \vdots \\ \Psi_1^{n+1} \end{bmatrix}.
\] (28)

Observe that, if the discrete potential is palindromic, then, in the case of $N$ odd $\hat{P}^0 = \hat{P}^{N-1}$, ..., $\hat{P}^{N-2} = \hat{P}^{N+2}$, with $\hat{P}^{N-2}$ unpaired. If $N$ is even, then $\hat{P}^0 = \hat{P}^{N-1}$, ..., $\hat{P}^{N/2 - 1} = \hat{P}^{N/2}$. Starting with $n = N - 1$, write
\[
(A - \hat{P}^{N-1}) \begin{bmatrix} \Psi_j^{N-1} \\ \vdots \\ \Psi_1^{N-1} \end{bmatrix} = (-A^* + \hat{P}^{N-1}) \begin{bmatrix} \Psi_j^N \\ \vdots \\ \Psi_1^N \end{bmatrix}
\]
as
\[
(A - \hat{P}^0) \begin{bmatrix} \Psi_j^{N-1} \\ \vdots \\ \Psi_1^{N-1} \end{bmatrix} = (-A^* + \hat{P}^0) \begin{bmatrix} \Psi_j^N \\ \vdots \\ \Psi_1^N \end{bmatrix}.
\] (29)
Continuing in this way, until \( n = 0 \), we find that
\[
[\Psi_N \ldots \Psi_1 \Psi_{N-1} \ldots \Psi_J \ldots \Psi_1^T]
\]
is the solution of an initial value problem with the same discrete potential and initial data \([\Psi_N \ldots \Psi_1]^T\). This is the conjugate mirror solution of the original solution. Adding these two solutions gives a solution which has conjugate component symmetry, and thus the initial-terminal pair is mirror-symmetric. However, if the initial-terminal pair of the superposition is localized, it will be localized with equal degree of restriction even if this was not the case for the original solution.

7. Matrix equations with stack matrix \( M \), deleted stack matrix \( B \).

7.1. Stack matrix \( M \). Let \( J, N \) be positive integers and let \( \{ P^n \} \) be a discrete potential of dimensions \( J \times N \). We will now write the corresponding system \( S \) as a single matrix equation.

Equation (18) can be written as
\[
\begin{bmatrix}
A^* - \hat{P}^n & A - \hat{P}^n \\
0 & A^* - \hat{P}^1 & \cdots \\
0 & \cdots & \cdots & \cdots \\
0 & \cdots & \cdots & A^* - \hat{P}^{N-1} & A - \hat{P}^{N-1}
\end{bmatrix}
\begin{bmatrix}
\Psi_1^0 \\
\vdots \\
\Psi_j^0 \\
\Psi_{N-1}^0 \\
\vdots \\
\Psi_J^0
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{bmatrix}. 
\] (30)

We appropriately “stack” the small block matrices in equation (30), for \( n = 0, \ldots, N - 1 \), to form a large block matrix which we call a stack matrix and denote by \( M \):
\[
M = 
\begin{bmatrix}
A^* - \hat{P}^0 & A - \hat{P}^0 \\
0 & A^* - \hat{P}^1 & A - \hat{P}^1 \\
0 & \cdots & \cdots & \cdots \\
0 & \cdots & \cdots & A^* - \hat{P}^{N-1} & A - \hat{P}^{N-1}
\end{bmatrix}
\] (31)

Here 0 denotes the \( J \times J \) zero matrix. \( M \) has \( N \) rows of \( N + 1 \) blocks, each of size \( J \times J \). Thus \( M \) is an \( NJ \times (N + 1)J \) matrix. The matrix equation corresponding to the total system (15) of \( NJ \) equations in \( (N + 1)J \) variables is
\[
M\Psi = 0. 
\] (32)

The vector \( \Psi = [\Psi_1^0 \ldots \Psi_j^0 \ldots \Psi_{N-1}^0 \ldots \Psi_J^0]^T \) is a solution of an initial value problem for system \( S \) with \( \{ P^n \} \) and initial state \( \Psi^0 \), if and only if \( \Psi \) is a solution of (32).

If, further, the matrices \( A - \hat{P}^n \) are invertible, then \( (\Psi^0, \Psi^N) \) is a steerable pair corresponding to \( \{ P^n \} \). If \( \Psi \) is of the form
\[
\Psi = [\Psi_1^0 \ldots \Psi_k^0 0 \ldots 0 \Psi_{J-k}^1 \ldots \Psi_{J-1}^{N-1} \ldots \Psi_J^{N-1} 0 \ldots 0 \Psi_{J-k+1}^N \ldots \Psi_{J-1}^N]^T, 
\] (33)
with \( \Psi_k^0 \neq 0, \Psi_{J-k+1}^N \neq 0 \), then \( (\Psi^0, \Psi^N) \) is localized with equal degree of restriction \( J - k \).
7.2. Deleted stackmatrix $B$. Let $M$ be a stackmatrix, (31). Let $k$ be an integer with $1 < k < J$. Let $B$ denote the submatrix of $M$ obtained by deleting columns $k+1$ to $J$ and columns $(NJ+1)$ to $(NJ+J-k)$ from $M$. The submatrix $B$ is an $NJ \times ((N-1)J+2k)$ matrix, which we call a deleted stackmatrix.

We may describe $B$ as follows. Let $F = A^* - \tilde{P}^0$. Let $F_j$ be the $j$th column of $F$, $j = 1, \ldots, J$, and let $\tilde{F}_k = [F_1 \cdots F_k]$. Let $G = A - \tilde{P}^{N-1}$. Let $G_j$ be the $j$th column of $G$, $j = 1, \ldots, J$, and let $\tilde{G}_k = [G_{J-k+1} \cdots G_J]$. Then

$$B = \begin{bmatrix} F_k & A - \tilde{P}^0 & 0_j & \cdots & 0_{J\times k} \\ 0_{J\times k} & A^* - \tilde{P}^1 & A - \tilde{P}^1 & \cdots & 0_{J\times k} \\ 0_{J\times k} & \cdots & \cdots & \cdots & 0_J \\ 0_{J\times k} & 0_j & A^* - \tilde{P}^{N-1} & \tilde{G}_k \end{bmatrix}.$$  

Here $0_{J\times k}$ denotes the $J \times k$ zero matrix and $0_J$ denotes the $J \times J$ zero matrix.

Consider the matrix equation

$$Bw = 0. \quad (34)$$

First, if $\Psi$ is a solution of (32) of the form (33), then the subvector of $\Psi$, obtained by “deleting zeros”,

$$[\Psi^0 \cdots \Psi^0_k \Psi^1_k \cdots \Psi^j_k \cdots \Psi^{N-1}_k \Psi^{N-1}_j \Psi^N_{J-k+1} \cdots \Psi^N_{J}]^T, \quad (35)$$

is a solution of (34). This is due to the fact that in (32), the entries in columns $k+1$ to $J$ and columns $(NJ+1)$ to $(NJ+J-k)$ of $M$ are multiplied by the zeros in $\Psi$, (of form (33)), and thus the system of equations corresponding to (32) is reduced to the system of equations corresponding to (34).

Second, if $w$ is any solution of (34), then a solution $\Psi$ of (32) of the form (33) may be constructed from $w$ by the insertion of $J-k$ zeros after $w_k$ and $J-k$ zeros after $w_{(N-1)J+k}$, obtaining

$$\Psi = [w_1 \cdots w_k 0 \cdots 0 w_{k+1} \cdots w_{(N-1)J+k} 0 \cdots 0 w_{(N-1)J+k+1} \cdots w_{(N-1)J+2k}]^T. \quad (36)$$

8. Set $\Lambda$ and Theorem 8.1. Let $J = 3$, $N = 2$, and let $j_L = j_R = 2$. Let $v$ be any real number. Define a sequence $\{\xi_n\}_{n=0,1}$ by $\xi_0 = \xi_1 = v$. Note that the only sequences $\{\xi_n\}_{n=0,1}$ that are palindromic are constant. Then define

$$P^n_j \begin{cases} 0 & j = 1 \\ \xi_n(= v) & j = 2 \\ 0 & j = 3 \end{cases} \quad n = 0, 1. \quad (37)$$

The set $\Lambda$ will be the set of all such discrete potentials (as $v$ runs over the real numbers).

The matrices $A - \tilde{P}^0$, $A - \tilde{P}^1$ are both equal to

$$\begin{bmatrix} -2 + i & 1 & 0 \\ 1 & -2 + i - v & 1 \\ 0 & 1 & -2 + i \end{bmatrix}, \quad (38)$$

which is invertible, with inverse

$$\frac{1}{2 - 3v + (9 + 4v)i} \begin{bmatrix} 2 + 2v - (4 + v)i & 2 - i & 1 \\ 2 - i & 3 - 4i & 2 - i \\ 1 & 2 - i & 2 + 2v - (4 + v)i \end{bmatrix}.$$  

It is not the case that every steerable pair corresponding to an element of $\Lambda$ is mirror-symmetric. One example is that of the initial state in Example 1 propagated
by the potential in $\Lambda$ with $v = 4$, which can be computed as the earlier examples. The initial-terminal pair is not $\alpha$-localized.

Let $q = -2 + i$. For any discrete potential in $\Lambda$, we may form the corresponding system $S$, and then stackmatrix $M$

$$M = \begin{bmatrix}
\bar{q} & 1 & 0 & q & 1 & 0 & 0 & 0 & 0 \\
1 & \bar{q} - v & 1 & 1 & q - v & 1 & 0 & 0 & 0 \\
0 & 1 & \bar{q} & 0 & 1 & q & 0 & 0 & 0 \\
0 & 0 & 0 & \bar{q} & 1 & 0 & q & 1 & 0 \\
0 & 0 & 0 & 1 & \bar{q} - v & 1 & 1 & q - v & 1 \\
0 & 0 & 0 & 0 & 1 & \bar{q} & 0 & 1 & q
\end{bmatrix}.$$  \hfill (39)

With $k = \frac{j + 1}{2} = 2$, the deleted stackmatrix $B$ is

$$B = \begin{bmatrix}
\bar{q} & 1 & q & 1 & 0 & 0 & 0 \\
1 & \bar{q} - v & 1 & q - v & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & q & 0 & 0 \\
0 & 0 & \bar{q} & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & \bar{q} - v & 1 & q - v & 1 \\
0 & 0 & 0 & 1 & \bar{q} & 1 & q
\end{bmatrix}.$$  \hfill (40)

The set of all matrices of the form (40) is denoted by $B$.

**Theorem 8.1.** Let $q = -2 + i$ and let

$$B = \left\{ \begin{bmatrix}
\bar{q} & 1 & q & 1 & 0 & 0 & 0 \\
1 & \bar{q} - v & 1 & q - v & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & q & 0 & 0 \\
0 & 0 & \bar{q} & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & \bar{q} - v & 1 & q - v & 1 \\
0 & 0 & 0 & 1 & \bar{q} & 1 & q
\end{bmatrix} : v \in \mathbb{R} \right\}.$$  \hfill (41)

Let $B \in B$. Then $B$ is of full rank, and if $w$ is any solution of

$$Bw = 0,$$  \hfill (42)

then $w$ is a complex scalar multiple of a vector $\zeta$ which satisfies

$$\zeta_1 = \zeta_7, \quad \zeta_2 = \zeta_6, \quad \zeta_3 = \zeta_5,$$  \hfill (43)

i.e., $w$ is a complex scalar multiple of a vector $\zeta$ which has conjugate component symmetry, CCS.

**Proof.** Let $B \in B$. We consider the augmented matrix $[B : 0]$. The augmented matrix will be reduced to a row echelon form, in three main steps. The $i$th row of the matrix in question will be denoted by $R_i$.

**Step 1. Inward Pass.** Adding $-(1/\bar{q})R_1$ to $R_2$ in $[B : 0]$, then adding $-(1/q)R_6$ to $R_5$ in $[B : 0]$ gives
\[
\begin{bmatrix}
\bar{q} & 1 & q & 1 & 0 & 0 & 0 & : & 0 \\
0 & c_1 & -\frac{2i}{\bar{q}} & c_2 & 1 & 0 & 0 & : & 0 \\
0 & 1 & 0 & 1 & q & 0 & 0 & : & 0 \\
0 & 0 & \bar{q} & 1 & 0 & 1 & 0 & : & 0 \\
0 & 0 & 1 & \bar{c}_2 & \frac{2i}{q} & \bar{c}_3 & 0 & : & 0 \\
0 & 0 & 0 & 1 & \bar{q} & 1 & q & : & 0
\end{bmatrix},
\]
(44)

where \(c_1 = \bar{q} - v - 1/\bar{q}\) and \(c_2 = q - v - 1/\bar{q}\). One may check that \(c_1 = -(8/5 + v) - (6/5)i\) and \(c_2 = -(8/5 + v) + (4/5)i\). We see that \(c_1\) and \(c_2\) are never zero.

We interchange \(R_2\) and \(R_3\), interchange \(R_4\) and \(R_5\), then add \(-c_1 R_2\) to \(R_3\) and add \(-\bar{c}_1 R_5\) to \(R_4\), obtaining

\[
\begin{bmatrix}
\bar{q} & 1 & q & 1 & 0 & 0 & 0 & : & 0 \\
0 & 1 & 0 & 1 & q & 0 & 0 & : & 0 \\
0 & 0 & -\frac{2i}{\bar{q}} & 2i & c_3 & 0 & 0 & : & 0 \\
0 & 0 & \bar{c}_3 & -2i & \frac{2i}{q} & 0 & 0 & : & 0 \\
0 & 0 & \bar{q} & 1 & 0 & 1 & 0 & : & 0 \\
0 & 0 & 0 & 1 & \bar{q} & 1 & q & : & 0
\end{bmatrix},
\]
(45)

where \(c_3 = 1 - c_1 q\). One may check that \(c_3 = -(17/5 + 2v) + (-4/5 + v)i\); \(c_3\) is never zero.

**Step 2. Central Block.** Now consider the central block of the previous matrix, consisting of rows three and four, and columns three through five:

\[
\begin{bmatrix}
-\frac{2i}{\bar{q}} & 2i & c_3 \\
\bar{c}_3 & -2i & \frac{2i}{q}
\end{bmatrix}.
\]
(46)

We perform row operations on this block (the zeros in columns one, two, six, and seven are unaffected) as follows. We multiply \(R_3\) by \(-\bar{q}/(2i)\), then add \(-\bar{c}_3 R_3\) to \(R_4\), obtaining

\[
\begin{bmatrix}
1 & -\bar{q} & -\frac{c_3 q}{c_4} \\
0 & -2i + \bar{c}3q & \frac{c_4 q}{c_4}
\end{bmatrix},
\]
(47)

where

\[
c_4 = |q|^2|c_3|^2 - 4 = 5 \left( \left( \frac{17}{5} + 2v \right)^2 + \left( -\frac{4}{5} + v \right)^2 \right) - 4 = 25v^2 + 60v + 57. \quad (48)
\]

The roots of \(c_4\) are \(-\frac{8}{5} \pm \frac{\sqrt{21}}{5}i\), and thus \(c_4\) is never zero. We multiply \(R_4\) by \((2i q)/c_4\), and then add \((c_3 q/2i) R_4\) to \(R_3\), obtaining

\[
\begin{bmatrix}
1 & -\bar{q} + c_3 |q|^2(-2i + \bar{c}_3 q)/c_4 & 0 \\
0 & 2i q(-2i + \bar{c}_3 q)/c_4 & 1
\end{bmatrix}.
\]
(49)
We consider the \((3, 4)\) entry:
\[
-\frac{c_3 |q|^2 (-2i + c_5 \bar{q})}{c_4} = -\frac{\bar{q} c_4 + c_3 |q|^2 (-2i + c_5 \bar{q})}{c_4} = \frac{-\bar{q} (|q|^2 |c_3|^2 - 4) + c_3 |q|^2 (-2i + c_5 \bar{q})}{c_4} = \frac{47 - 2i |q|^2 c_3}{c_4}.
\]

We denote the numerator \(47 - 2i |q|^2 c_3\) by \(c_5\). We have
\[
c_5 = 4(-2 - i) - 10i(-17/5 + 2v) + (-4/5 + v)i = -16 + 10v + (30 + 20v)i,
\]
and \(c_5\) is never zero. The numerator of the \((4, 4)\) entry is \(4q + 2i c_3 |q|^2 = c_5\). Thus we have obtained (recall \(c_4\) is real)
\[
\begin{bmatrix}
\bar{q} & 1 & q & 1 & 0 & 0 & 0 & : & 0 \\
0 & 1 & 0 & 1 & q & 0 & 0 & : & 0 \\
0 & 0 & 1 & c_5/c_4 & 0 & 0 & 0 & : & 0 \\
0 & 0 & 0 & c_5/c_4 & 1 & 0 & 0 & : & 0 \\
0 & 0 & \bar{q} & 1 & 0 & 1 & 0 & : & 0 \\
0 & 0 & 0 & 1 & \bar{q} & 1 & q & : & 0
\end{bmatrix}.
\]

**Step 3. Outward Pass.** Adding \(-qR_4\) to \(R_2\) and \(-\bar{q}R_3\) to \(R_5\) gives
\[
\begin{bmatrix}
\bar{q} & 1 & q & 1 & 0 & 0 & 0 & : & 0 \\
0 & 1 & 0 & c_6/c_4 & 0 & 0 & 0 & : & 0 \\
0 & 0 & 1 & c_5/c_4 & 0 & 0 & 0 & : & 0 \\
0 & 0 & 0 & c_5/c_4 & 1 & 0 & 0 & : & 0 \\
0 & 0 & 0 & c_5/c_4 & 0 & 1 & 0 & : & 0 \\
0 & 0 & 0 & 1 & \bar{q} & 1 & q & : & 0
\end{bmatrix},
\]

where
\[
c_6 = c_4 - qc_5 = 25v^2 + 60v + 57 - (-2 + i)(-16 + 10v - (30 + 20v)i)
\] -\(25v^2 + 60v - 5 - 2(22 + 25v)i.\)

The roots of \(25v^2 + 60v - 5\) are \(-6/5 \pm \sqrt{11}/5\); \(c_6\) is never zero. Consider the block consisting of the first three rows and first four columns:
\[
\begin{bmatrix}
\bar{q} & 1 & q & 1 \\
0 & 1 & 0 & c_6/c_4 \\
0 & 0 & 1 & c_5/c_4
\end{bmatrix}.
\]

Adding \(-(c_6/c_5)R_3\) to \(R_2\), and \(-(c_4/c_5)R_3\) to \(R_1\) gives
\[
\begin{bmatrix}
\bar{q} & 1 & c_7/c_5 & 0 \\
0 & 1 & -c_6/c_5 & 0 \\
0 & 0 & 1 & c_5/c_4
\end{bmatrix}.
\]
where
\[
c_7 = q c_5 - c_4 = (-2 + i)(-16 + 10v + (30 + 20v)i) - (25v^2 + 60v + 57) = -(5(5v^2 + 20v + 11) + (76 + 30v)i).
\] (56)

The roots of \(5v^2 + 20v + 11\) are \(-2 \pm 3\sqrt{5}/5\); \(c_7\) is never zero. We add \((c_7/c_6)R_2\) to \(R_1\), obtaining
\[
\begin{bmatrix}
q & (c_6 + c_7)/c_6 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -c_6/c_5 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & c_5/c_4 & 0 & 0 & 0 \\
0 & 0 & 0 & \sqrt{5}/c_4 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & -\sqrt{5}/\sqrt{5} & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & (\sqrt{5} + \sqrt{5})/\sqrt{5} & q & 0 \\
\end{bmatrix}.
\] (57)

We have
\[
c_6 + c_7 = c_4 - q\sqrt{5} + q c_5 - c_4 = q(c_5 - \sqrt{5}) = -20(3 + 2v + 2(3 + 2v)i).
\]

The \((1, 2)\) entry equals zero when \(v = -3/2\), however there are no further row reduction steps that could be affected. We perform the conjugate operations on corresponding rows in the block of (45) consisting of the rows four through six and columns four through seven, finally obtaining the following row echelon form:
\[
\begin{bmatrix}
q & (c_6 + c_7)/c_6 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -c_6/c_5 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & c_5/c_4 & 0 & 0 & 0 \\
0 & 0 & 0 & \sqrt{5}/c_4 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & -\sqrt{5}/\sqrt{5} & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & (\sqrt{5} + \sqrt{5})/\sqrt{5} & q & 0 \\
\end{bmatrix}.
\] (58)

We see that \(B\) is of full rank, and thus the nullspace of \(B\) is of dimension one. Let \(w\) be any solution of \(Bw = 0\). We examine the components of \(w\), starting with \(w_3\) and \(w_5\), writing them in terms of \(w_4\). From the third row and the fourth row,
\[
w_3 = -\frac{c_5}{c_4} w_4 \quad \text{and} \quad w_5 = -\frac{c_5}{c_4} w_4.
\] (59)

From the second row and the fifth row,
\[
w_2 = \frac{c_6}{c_5} w_3 = -\frac{c_6}{c_4} w_4 \quad \text{and} \quad w_6 = \frac{c_6}{c_5} w_5 = -\frac{c_6}{c_4} w_4.
\] (60)

From the first row,
\[
w_1 = -\frac{1}{q} \left( \frac{c_6 + c_7}{c_6} \right) w_2 = \frac{1}{q} \left( \frac{c_6 + c_7}{c_4} \right) w_4,
\]
and from the sixth row,
\[
w_7 = -\frac{1}{q} \left( \frac{\sqrt{5} + \sqrt{5}}{\sqrt{5}} \right) w_6 = \frac{1}{q} \left( \frac{\sqrt{5} + \sqrt{5}}{c_4} \right) w_4.
\]
Thus we have written every component of \( w \) in terms of \( w_4 \), which may be chosen to be any complex number. Writing \( r \) for \( w_4 \), we see that

\[
w = \frac{r}{c_4} \begin{bmatrix} (c_6 + c_7)/q \\ -c_6 \\ -c_5 \\ c_4 \\ -c_5 \\ (c_6 + c_7)/q \end{bmatrix}
\]

\[
= \frac{r}{25v^2 + 60v + 57} \begin{bmatrix} -20(3 + 2v)(1 + 2i)/(−2 − i) \\ -2v^2 + 60v − 5 − 2(22 + 25v)i \\ -(−16 + 10v + (30 + 20v)i \\ 25v^2 + 60v + 57 \\ -(−16 + 10v − (30 + 20v)i \\ -2v^2 + 60v − 5 + 2(22 + 25v)i \\ -20(3 + 2v)(1 − 2i)/(−2 + i) \end{bmatrix}
\]  

(61)

Let \( ζ \) be \( 1/c_4 \) times the vector on the right-hand side of the first equation in (61) (subsequently expressed in terms of \( v \)). Recall \( v \) is real and fixed for given \( B \). We see that \( ζ \) satisfies (43) and thus has CCS, \( r \) is a complex number and \( w \) is a complex scalar multiple of \( ζ \).

\[ \square \]

**Remark 2.** Maple has been used to double-check steps, with the RowOperation and other commands.

### 9. Steerable pairs.

Let \( \{P^n_j\} \) be a discrete potential in \( Λ \). Recall that the matrices \( A − \hat{P}^0, A − \hat{P}^1 \) are invertible.

First, if \( w \) is a solution of \( Bw = 0 \), then we may insert zeros as in (36), to obtain

\[ Ψ = [w_1 \ w_2 \ 0 \ w_3 \ w_4 \ w_5 \ 0 \ w_6 \ w_7]^T \]  

(62)

Then, via the stackmatrix (39), \( Ψ \) is the unique solution of the initial value problem for system \( S \) with \( \{P^n\} \) and initial state \( Ψ^0 = [w_1 \ w_2 \ 0]^T \), and has terminal state \( Ψ^2 = [0 \ w_6 \ w_7]^T \). Thus \( (Ψ^0, Ψ^2) \) is an \( α \)-localized steerable pair corresponding to \( \{P^n_j\} \) and is mirror-symmetric; note \( w_2 ≠ 0, w_6 ≠ 0 \).

Second, if \( (Ψ^0, Ψ^2) \) is a steerable pair corresponding to \( \{P^n\} \) which is \( α \)-localized, then \( (Ψ^0, Ψ^2) \) serves as the initial and terminal states in the unique solution \( Ψ \) of system \( S \) with \( \{P^n\} \) and initial state \( Ψ^0 \), and \( Ψ \) is of the form (33). The subvector of \( Ψ \) formed by deleting zeros as in (35) is a solution of \( Bw = 0 \) where \( B \) is an element of \( B \). Theorem 8.1 tells us that this subvector is a complex scalar multiple of the vector \( ξ \) above. Thus, we see \( (Ψ^0, Ψ^2) \) is mirror-symmetric (and \( Ψ \) itself is a complex scalar multiple of a vector with CCS).

Using elements of \( Λ \) as controls (which could be considered admissible controls), the \( α \)-localized steerable pairs are of the form \( (Ψ^0, Ψ^2) \), where

\[ Ψ^0 = \frac{r}{25v^2 + 60v + 57} \begin{bmatrix} -20(3 + 2v)(1 + 2i)/(−2 − i) \\ -2v^2 + 60v − 5 − 2(22 + 25v)i \\ 0 \end{bmatrix} \equiv r \hat{f}_1(v), \]

\[ Ψ^2 = \frac{r}{25v^2 + 60v + 57} \begin{bmatrix} 0 \\ -2v^2 + 60v − 5 + 2(22 + 25v)i \\ -20(3 + 2v)(1 − 2i)/(−2 + i) \end{bmatrix} \equiv r \hat{f}_2(v), \]
for \( r \in \mathbb{C} \) and \( v \in \mathbb{R} \). Determination of the ranges of \( \vec{f}_1, \vec{f}_2 \) remains for future study.

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**REFERENCES**

[1] G. D. Akrivis and V. A. Dougalis, Finite difference discretization with variable mesh of the Schrödinger equation in a variable domain, *Bulletin Greek Mathematical Society*, 31 (1990), 19–28.

[2] K. Beauchard, *Local controllability of a 1-D Schrödinger equation*, *J. Math. Pures Appl.*, 84 (2005), 851–956.

[3] D. Bohm, *Quantum Theory*, Dover Publications Inc., New York, 1989.

[4] U. Boscain, J.-P. Gauthier, F. Rossi and M. Sigalotti, Approximate controllability, exact controllability and conical eigenvalue intersections for quantum mechanical systems, *Comm. Math. Phys.*, 333 (2015), 1225–1239.

[5] T. Boykin and G. Klimel, The discretized Schrödinger equation and simple models for semiconductor quantum wells, *Eur. J. Phys.*, 25 (2004), 503–514.

[6] M. Buttiker and R. Landauer, Traversal time for tunneling, *Advances in Solid State Physics*, 25 (2007), 711–717.

[7] R. Burden and J. Faires, *Numerical Analysis*, 5th edition, PWS, Boston, 1993.

[8] T. Chan and L. Shen, Stability analysis of difference schemes for variable coefficient Schrödinger type equations, *SIAM. J. Numer. Anal.*, 24 (1987), 336–349.

[9] K. Beauchard and J.-M. Coron, Controllability of a quantum particle in a moving potential well, *Journal of Functional Analysis*, 232 (2006), 328–389.

[10] A. Goldberg, H. Schey and J. Schwartz, Computer-generated motion pictures of one-dimensional quantum-mechanical transmission and reflection phenomena, *American Journal of Physics*, 35 (1967), 177–186.

[11] A. Hof, O. Kuil and B. Simon, Singular continuous spectrum for palindromic Schrödinger operators, *Communications in Mathematical Physics*, 174 (1995), 149–159.

[12] A. Kacar and O. Terzioglu, Symbolic computation of the potential in a nonlinear Schrödinger Equation, *Numer. Methods Partial Differential Equations*, 23 (2007), 475–483.

[13] K. Kime, Finite difference approximation of control via the potential in a 1-D Schrodinger equation, *Archives of Computational Methods in Engineering*, 12 (2005), 173–199.

[14] I. Lasiecka and R. Triggiani, Exact controllability of the Euler-Bernoulli equation with boundary controls for displacement and moment, *J. Math. Anal. Appl.*, 146 (1990), 1–33.

[15] J. L. Lions, Exact controllability, stabilization and perturbations for distributed systems, *SIAM Review*, 30 (1988), 1–68.

[16] M. Morancey and V. Nersesyan, Simultaneous global exact controllability of an arbitrary number of 1D bilinear Schrödinger equations, *J. Math. Pures Appl.*, 103 (2015), 228–254.

[17] A. Nissen, G. Kreiss and M. Gerritsen, High order stable finite difference methods for the Schrödinger equation, *J. Sci. Comput.*, 55 (2013), 173–199.

[18] K. H. Rosen, *Discrete Mathematics and Its Applications*, 6th edition, McGraw Hill, New York, 2007.

[19] D. L. Russell, A unified boundary controllability theory for hyperbolic and parabolic partial differential equations, *Studies in Applied Mathematics*, 52 (1973), 189–211.

[20] L. I. Schiff, *Quantum Mechanics*, McGraw Hill, New York, 1968.

[21] E. Zuazua, Propagation, observation, and control of waves approximated by finite difference methods, *SIAM Review*, 47 (2005), 197–243.

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E-mail address: kimek@unk.edu