Implementation of Numerical Approximations of Control of the Schrodinger Equation with MATLAB

Katherine Kime

Abstract— **This paper considers the use of MATLAB to numerically implement the propagation in time of a quantum wavepacket in the presence of static or moving potential barriers. Time-dependent barriers are of interest as controls. We show the results of propagation with trigonometrically oscillating barriers at different frequencies. We give an example of steering localized initial data to localized terminal data.**

Keywords— **MATLAB, Schrodinger, potential**

I. Introduction

EFFORTS to control atomic and molecular systems have probably been made, at least informally, since interest in these systems began. In recent years, with such striking technological advances as the development of fast (picosecond) lasers and the construction of quantum dots and other nanometer-scale devices, the problem of control of quantum-mechanical systems has received heightened stimulus, e.g. [1], [2]. Each system is associated with an appropriate Schrodinger equation,

$$i\frac{\partial \Psi}{\partial t} = -H\Psi + V\Psi.$$

Solutions Ψ of the equation are called wavefunctions or state functions and are used to describe the behavior of the system. In particular, the product of the wavefunction and its complex conjugate is considered to be a probability density for position. Here H is the Hamiltonian of the system and V is the potential, assumed real.

Experimentally, control is generally exercised by choice of the potential, e.g. corresponding to choice of laser radiation. Mathematically this gives a bilinear control problem, as the potential multiplies the state. There is a developed theory for controllability of finite dimensional bilinear systems (ODEs), using differential geometry and Lie theory. Great progress has been made in treating controllability problems for infinite dimensional systems such as the wave, heat and rod equations, in which control enters linearly or through the boundary. However, less is known about controllability of infinite dimensional bilinear systems, such as the Schrodinger equation with the potential as control. Further, the Schrodinger equation can be solved exactly only in a few elementary cases, and otherwise solutions must be approximated numerically.

Here, we will consider the one-dimensional Schrodinger equation,

$$i\frac{\partial \Psi}{\partial t} = -\frac{\partial^2 \Psi}{\partial x^2} + V(x,t)\Psi, \qquad 0 < x < 1, t > 0, \quad (1)$$

K. Kime is with the Dept. of Mathematics and Statistics,University of Nebraska at Kearney, Kearney, NE 68849 U.S.A. E-mail: kimek@unk.edu

with an oscillating square potential barrier,

$$V(x,t) = \begin{cases} 0 & 0 \le x < a \\ \widehat{V}(t) & a \le x \le b \\ 0 & b < x \le 1. \end{cases}$$

Technically, when $\widehat{V}(t)$ is positive we have a barrier and when negative a well, but we will use the word barrier whether $\widehat{V}(t)$ is negative or positive. Such potentials are simpler than the dipole potential associated with laser radiation and may be a precursor to treating the dipole and other more complicated potentials. The initial condition is

$$\Psi(x,0) = \Psi^0(x),$$

where $\Psi^0(x)$ is a complex function, and the boundary conditions are

$$\Psi(0,t) = \Psi(1,t) = 0.$$

We approximate numerically using the Crank-Nicolson (C-N) method, [3], with h the space step and k the time step, obtaining the difference equations

$$\frac{-i}{2h^2}\Psi_{j+1}^{n+1} + \left(\frac{1}{k} + \frac{i}{h^2} + \frac{iV_j^{n+1}}{2}\right)\Psi_j^{n+1} - \frac{i}{2h^2}\Psi_{j-1}^{n+1} = \frac{i}{2h^2}\Psi_{j+1}^{n} + \left(\frac{1}{k} - \frac{i}{h^2} - \frac{iV_j^{n}}{2}\right)\Psi_j^{n} + \frac{i}{2h^2}\Psi_{j-1}^{n}, \quad j = 1 \dots J-1. \quad (2)$$

Here, Ψ_j^n approximates $\Psi(x_j, t_n)$, $j = 1..J-1$, $n > 0$, where $x_j = jh, t_n = nk$, and V_j^n approximates $V(x_j, t_n)$. We take $\Psi_0^n = \Psi_J^n = 0$ for all n and $\Psi_j^0 = \Psi^0(x_j), j = 1..J-1$.

II. Time-independent potentials

In the case of time-independent potential barriers ($\widehat{V}(t) \equiv c$), the C-N method is equivalent to that obtained from the Cayley form and is used in the classic work of Goldberg et al, [4], as well as subsequent works, e.g. [5]. The propagation (snapshots in time) of a wavefunction with Gaussian initial data, with impingement on a barrier and consequent transmission and reflection, is shown in [4].

The C-N method may be implemented in MATLAB. It may be shown analytically that when no barrier or well is present (free propagation) a wavepacket with Gaussian initial data remains Gaussian and spreads in time, in concurrence with the Heisenberg Uncertainty Principle.

In Fig. 1, we show free propagation of a wavepacket with Gaussian initial data and observe the spread in time. In Fig. 2 we show propagation of the same initial data in the presence of a time-independent (static) barrier.

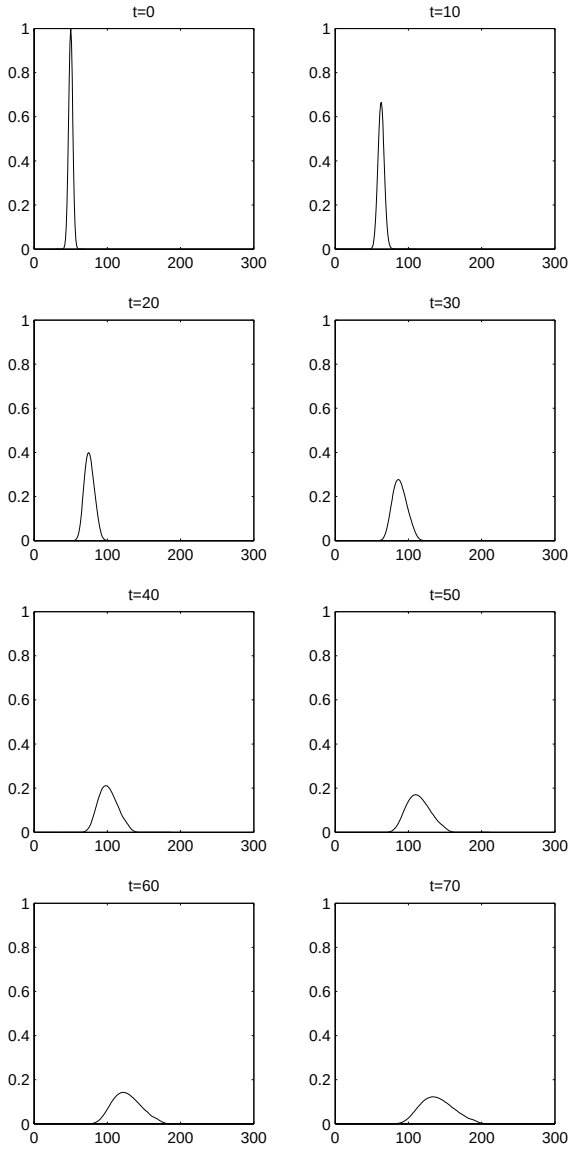

Fig. 1. Free propagation of Gaussian initial data, 70 time steps

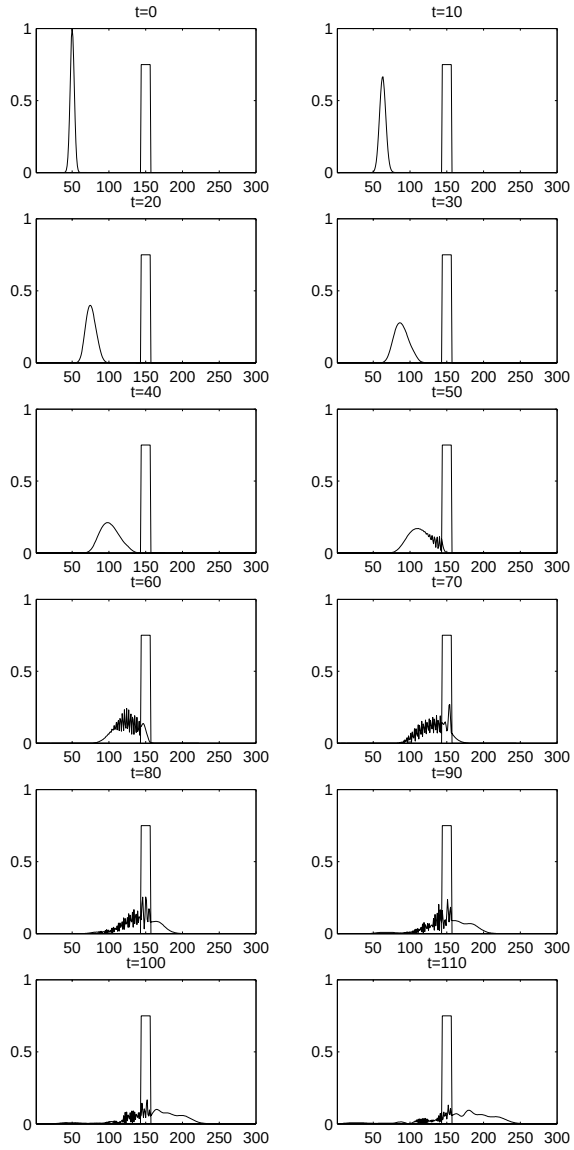

Fig. 2. Propagation of Gaussian initial data in the presence of a static barrier, $V_j^n = 0.75, j = 144..156$, 110 time steps

III. Time-dependent potentials and control

The C-N method with a time-dependent potential was used in [6] to treat a discretized control problem, with small numbers of space and time steps. We wish to study the problem with a larger number of space and time steps, which is needed for physical interpretations. We consider the question: Given a discretized initial state, a discretized terminal state and a time $T = Nk$, is there a discretized time-dependent potential which steers the initial state to the terminal state by time T? That is, given $\{x_j\}, j = 1..J-1$, and $\{y_j\}, j = 1..J-1$, does there exist a sequence $\{z_j^n\}, j = 1..J-1, n = 0..N$, such that the solution of the system of difference equations with $\{\Psi_j^0\} = \{x_j\}$ and $\{V_j^n\} = \{z_j^n\}$ satisfies $\{\Psi_j^N\} = \{y_j\}$? This discretized time-dependent potential is then the desired control.

Several issues arise. First, one would like to have some examples of the behavior of a wavepacket with a known time-dependent potential, using a sufficiently large number of space and time steps. This aids with visualization and suggests what one might expect from control. Propagation of an initial Gaussian with a time-independent vs. a time-dependent potential may be examined. To our knowledge, closed form solutions of the Schrodinger equation

with time-dependent barrier/wells have not been found, although there are abstract existence results.

The C-N method with time-dependent potentials may be implemented in MATLAB. In Fig. 3 and Fig. 4, we show the propagation of the same initial data as in Fig. 1 and 2, now in the presence of cosinusoidally oscillating barriers.

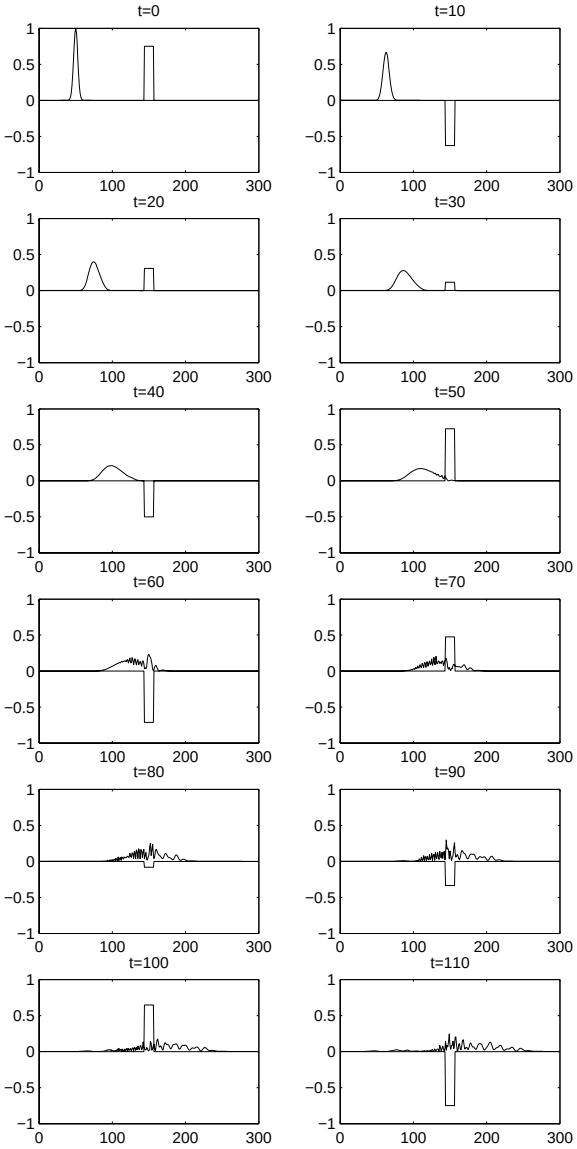

Fig. 3. Propagation of Gaussian initial data in the presence of a time-dependent barrier, $V_j^n = (0.75)cos(n), j = 144..156$, 110 time steps

Comparing Fig. 2 with Fig. 3 and Fig. 4, we see there is marked contrast between the propagation of Gaussian initial data with a time-independent potential and propagation with trigonometrically oscillating potentials. The higher frequency of oscillation of the barrier in Fig. 4 gives rise to spikes at t=80,90,100 and 110 which are not present in the other cases. The wavefunctions with oscillating barriers have complicated forms, indicating that characterization of pairs of initial/terminal data, for which a desired "steering" control exists, will not be simple.

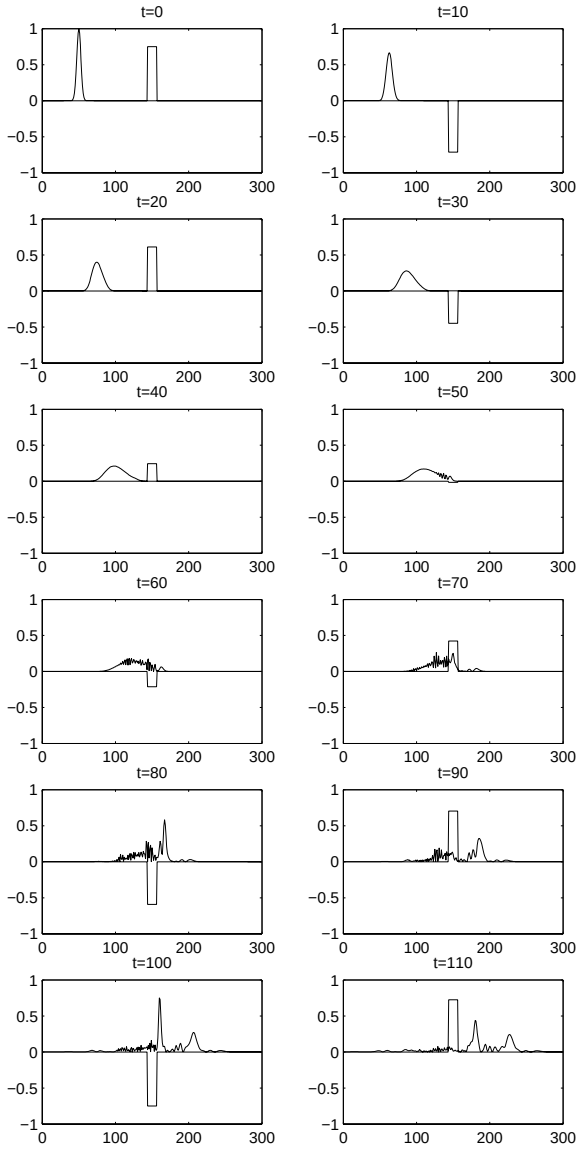

Fig. 4. Propagation of Gaussian initial data in the presence of a time-dependent barrier, $V_j^n = (0.75)cos(6n), j = 144..156$, 110 time steps

In Fig. 5 we show the propagation of centered Gaussian initial data in the presence of a static barrier. The wavefunction splits; one bunch of peaks approaches the boundary on the left and another the boundary on the right. In Fig. 6 we show the propagation of the same initial data in the presence of a cosinusoidally oscillating barrier. The

wavefunction is gradually flattened and spread and the side bunches of peaks do not arise in the same time interval. In Fig. 7 we show the propagation of the same initial data with a barrier oscillating at five times the frequency as that in Fig. 6. Now two bunches of peaks form on each side of the barrier.

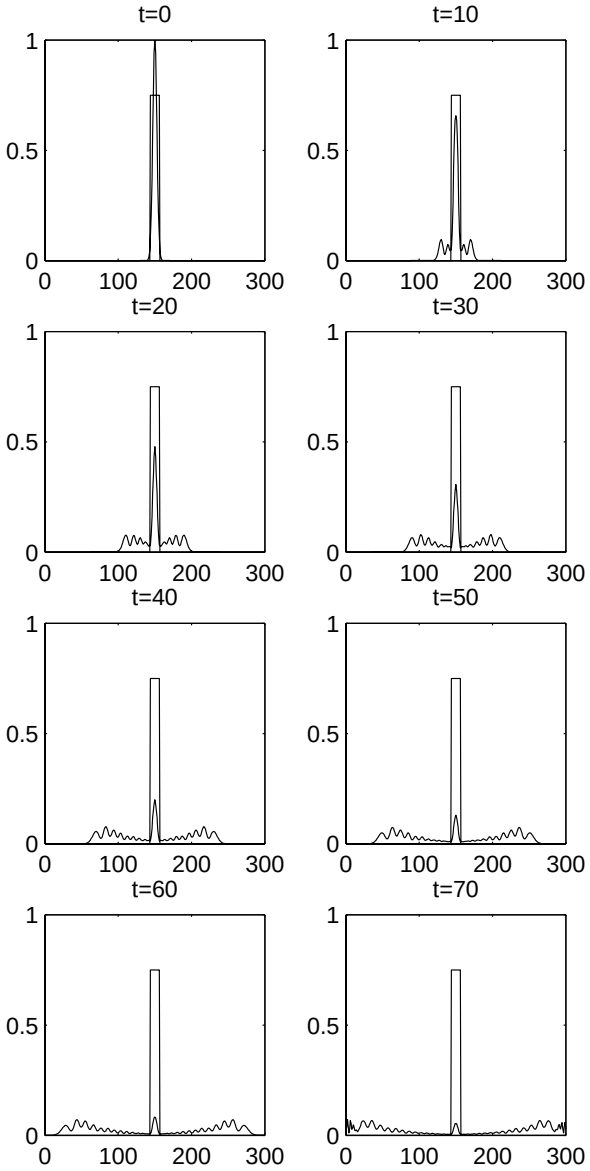

Fig. 5. Propagation of centered Gaussian initial data in the presence of a static barrier,$V_j^n = 0.75, j = 144..156$, 70 time steps

Second, attempting to find a desired sequence $\{z_j^n\}, j = 1..J-1, n = 0..N$, for a given pair of initial/terminal data is a symbolic problem. It may be approached using the computer algebra system Maple, but increasing the number of space and time steps pushes Maple's computational

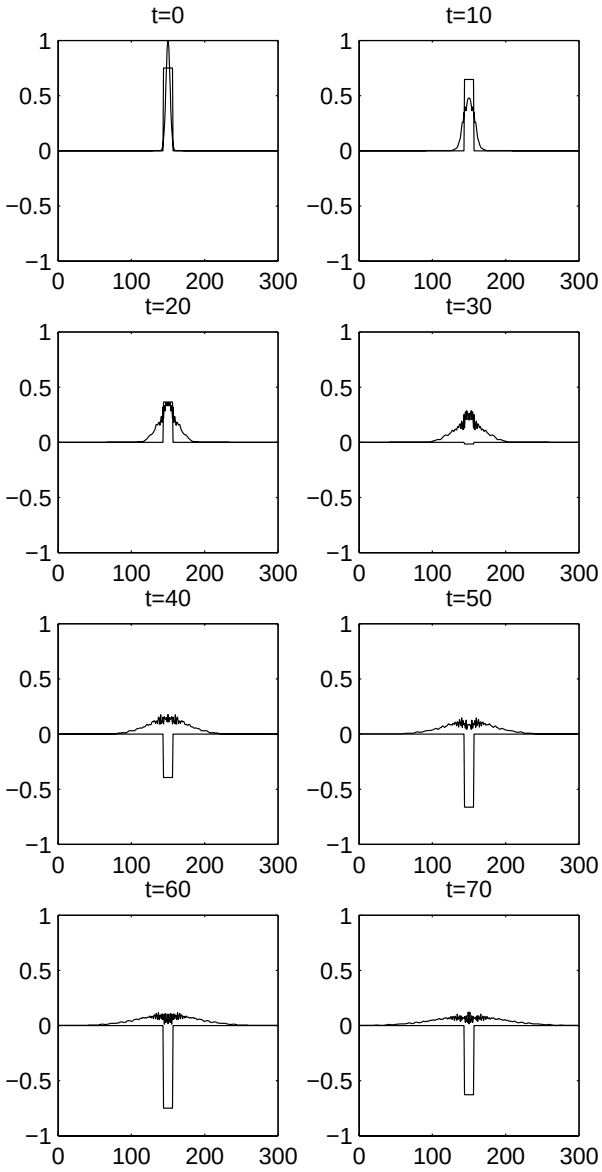

Fig. 6. Propagation of centered Gaussian initial data in the presence of a time-dependent barrier, $V_j^n = (0.75)cos(10n), j = 144..156$, 70 time steps

limits. As in [6], taking $h = 1$ and $k = 2$, we may write (2) in matrix form as follows:

$$\left(\begin{bmatrix} i-2 & 1 & 0 & \cdots & 0 \\ 1 & i-2 & 1 & \cdots & 0 \\ 0 & 1 & i-2 & \cdots & 0 \\ \ddots & & \ddots & & 1 \\ 0 & & & 1 & i-2 \end{bmatrix} \right.$$

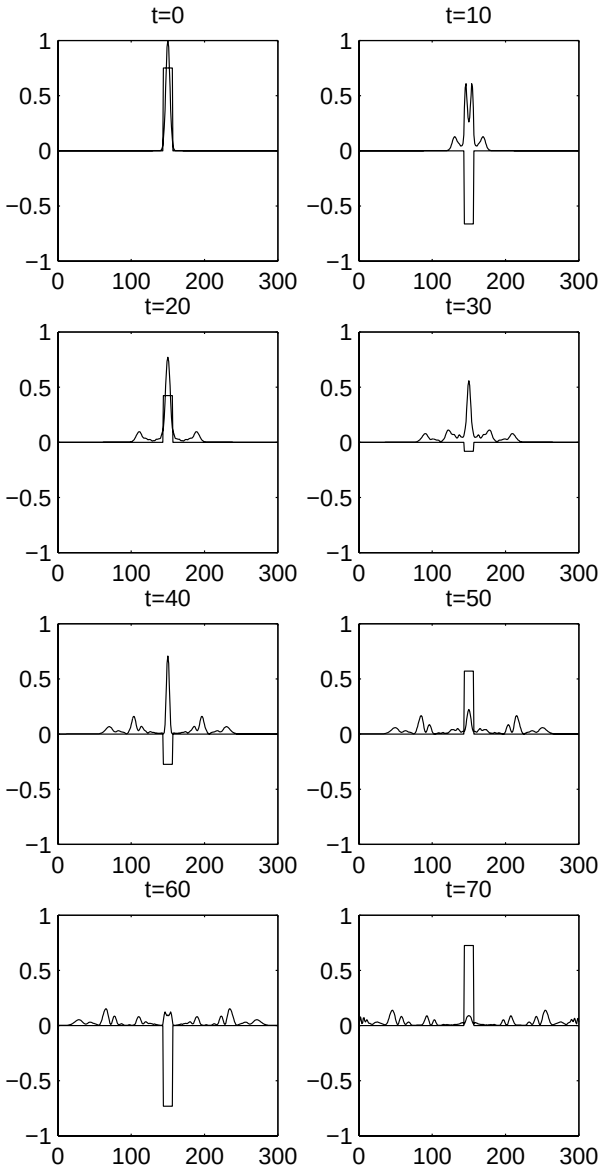

Fig. 7. Propagation of centered Gaussian initial data in the presence of a time-dependent barrier, $V_j^n = (0.75)cos(50n), j = 144..156$, 70 time steps

$$= \left(\begin{bmatrix} i+2 & -1 & 0 & \cdots & 0 \\ -1 & i+2 & -1 & \cdots & 0 \\ 0 & -1 & i+2 & \cdots & 0 \\ \ddots & & \ddots & & 1 \\ 0 & & & -1 & i+2 \end{bmatrix} + \begin{bmatrix} V_1^n & 0 & & & \\ 0 & \ddots & 0 & & \\ & & & \ddots & 0 \\ & & & 0 & V_{J-1}^n \end{bmatrix} \right) \begin{bmatrix} \Psi_1^n \\ \vdots \\ \\ \vdots \\ \Psi_{J-1}^n \end{bmatrix}. \quad (3)$$

Separating real and imaginary parts, with $\Psi_j^n = R_j^n + iM_j^n$,

$$A = \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \\ \ddots & \ddots & & & \\ & & & 1 & -2 \end{bmatrix},$$

and

$$\widehat{V^n} = \begin{bmatrix} V_1^n & 0 & & & \\ 0 & \ddots & 0 & & \\ & & & \ddots & 0 \\ & & & 0 & V_{J-1}^n \end{bmatrix},$$

we have

$$\left(\begin{bmatrix} A & -I \\ I & A \end{bmatrix} - \begin{bmatrix} \widehat{V^{n+1}} & 0 \\ 0 & \widehat{V^{n+1}} \end{bmatrix} \right) \begin{bmatrix} R_1^{n+1} \\ \vdots \\ R_{J-1}^{n+1} \\ M_1^{n+1} \\ \vdots \\ M_{J-1}^{n+1} \end{bmatrix}$$

$$= \left(\begin{bmatrix} -A & -I \\ I & -A \end{bmatrix} + \begin{bmatrix} \widehat{V^n} & 0 \\ 0 & \widehat{V^n} \end{bmatrix} \right) \begin{bmatrix} R_1^n \\ \vdots \\ R_{J-1}^n \\ M_1^n \\ \vdots \\ M_{J-1}^n \end{bmatrix}. \quad (4)$$

$$- \left(\begin{bmatrix} V_1^{n+1} & 0 & & & \\ 0 & \ddots & 0 & & \\ & & & \ddots & 0 \\ & & & 0 & V_{J-1}^{n+1} \end{bmatrix} \right) \begin{bmatrix} \Psi_1^{n+1} \\ \vdots \\ \\ \vdots \\ \Psi_{J-1}^{n+1} \end{bmatrix}$$

We may specify initial values R_j^0, M_j^0, $j = 1..J-1$ and terminal values $R_j^N, M_j^N, j = 1..J-1$, write (4) for $n = 0..N-1$, and form the resulting system of equations. Thus, if we let S^n be the matrix in parentheses on the left side of (4), and T^n be the matrix on the right side of (4), for 3 time steps we would form

$$\begin{bmatrix} T^0 & -S^1 & 0 & 0 \\ 0 & T^1 & -S^2 & 0 \\ 0 & 0 & T^2 & -S^3 \end{bmatrix} \begin{bmatrix} R_1^0 \\ \vdots \\ R_1^1 \\ \vdots \\ R_1^2 \\ \vdots \\ R_1^3 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 0 \end{bmatrix}.$$

We then ask, for which values of V_j^n are there non-trivial solutions of the system? These solutions will be R_j^n, M_j^n, $j = 1..J-1, n = 1..N-1$, the intermediate states between the initial and terminal data. When there are solutions, we may also obtain the values of the control. Clearly this becomes very complex as more space and time steps are taken. Within its limits, Maple will perform row reduction on such systems, resulting in equations for the V_j^n. Computations for examples obtained thus far may involve polynomials in the V_j^n with some coefficients of the order of 10^{14}.

One can consider specifying properties of initial/terminal pairs to be studied, such as the degree to which they are localized and the amount of contact with the barrier. Examples suggest that the simple choice of a trigonometrically oscillating barrier as control will not serve to steer localized initial data to localized terminal data. The tendency of the wavefunction to spread remains important.

In one example with 12 space steps, we have shown that it is possible to steer initial data fully localized on the left(zero on the right half of the space interval) to terminal data fully localized on the right(zero on the left half of the space interval) in 3 time steps. Both the initial data and the terminal data have contact with the barrier.

In Fig. 8, we show free propagation of the localized initial data. At t=3, the wavefunction is non-zero at each space step, although of small magnitude for the first five steps. In Fig. 9 we show the propagation of the localized initial data with a time-dependent barrier which is centered and one-sixth the width of the interval. The time-dependence is not trigonometric. Now the wavefunction is zero for the first 6 space steps. Comparing t=2 in Fig. 8 and Fig. 9, we see that a large peak was created at that time in the case of the time-dependent barrier. This raises the question of "trade-offs" that may result if one wishes to control to localized terminal data.

This numerical approach has the advantage of allowing, when possible, explicit construction of the desired controls for initial/terminal data pairs. Remaining subjects

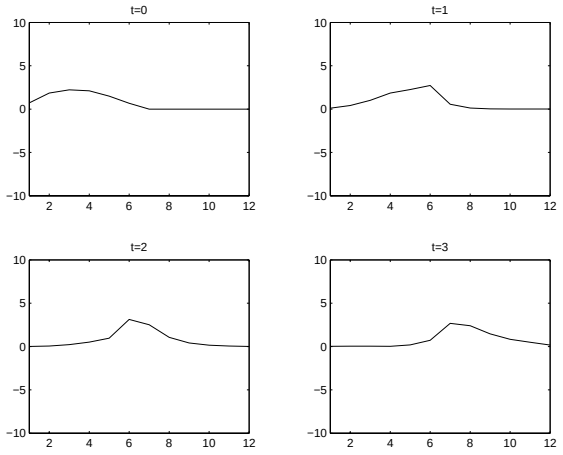

Fig. 8. Free propagation of localized initial data, t=0..3

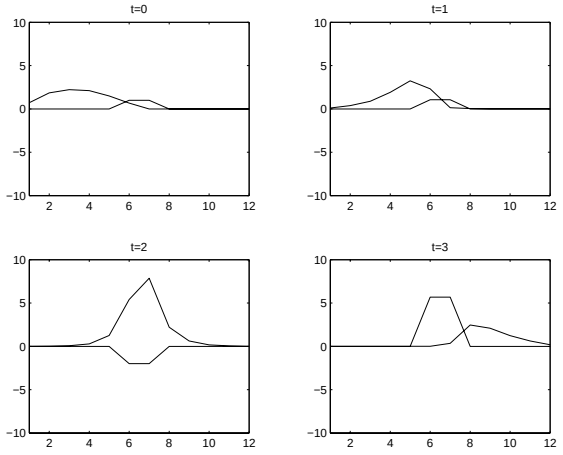

Fig. 9. Propagation of localized initial data, moving barrier, t=0..3

of study include determining the size of systems such as those above that Maple can treat successfully, characterizing properties of "steerable" initial/terminal pairs with various sizes of barriers, and determining the degree to which the full infinite dimensional problem is approximated with Crank-Nicolson and other numerical methods.

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