

Finite difference approximation of control via the potential in a 1-D Schrodinger equation *

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Abstract

We consider the problem of steering given initial data to given terminal data via a time-dependent potential, the control, in a 1-D Schrodinger equation. We determine a condition for existence of a transferring potential within our approximation. Using Maple, we give equations for the control and also examples in which the potential is restricted to be centralized and to be a step potential.

1 Introduction

In this paper we allow time-dependence of the potential, considered to be a control, in a numerical approximation of a 1-D Schrodinger equation obtained from the Crank-Nicolson method [1]. Our purpose is to examine the following question: Given a discretized initial state and a discretized final state, is there a discretized time-varying potential which steers the initial state to the terminal state? We consider an example in which the potential is restricted to be "centralized", thus having the nature of a barrier, and one in which it is restricted to be a step potential.

Square potential barriers and wells are basic examples in quantum physics and arise in many physical models, among them nanostructures [11]. Potential barriers which oscillate in time have been studied in several scientific works [2, 5, 6, 14, 13, 17], although apparently have had less attention per se in the area of numerical analysis. There is interest in the question of how quantum wells may be driven or controlled [4] involving various formulations. Here we focus on a simple set-up with a time-dependent potential which may be a precursor to understanding more complicated situations. Our results indicate that approaching the control problem described above would have been prohibitively complicated until the recent advent of computer algebra systems such as Maple.

In Sec. 2 we consider the Crank-Nicolson method as in [1] and apply it to the Schrodinger equation with a time-dependent potential. The difference equations that result reduce, in the case of a time-independent potential, to those obtained

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in a classic numerical approximation [3] (see [15]), which we discuss. That this should be so is indicated in [8], although we are unaware of whether or not the correspondence that we find appears in the literature. Crank-Nicolson methods are considered one of the main types of methods used for the time-dependent Schrodinger equation [12, 16, 18].

In Sec. 3, we write the system of difference equations in the form of a matrix equation and determine a condition on the components of an initial-terminal pair under which we have existence of a potential which steers the initial data at time step $n = 0$ to the terminal data at time step $n = 1$. Under this condition we may obtain equations for the potential in question in terms of the initial and terminal data, thereby allowing construction of the desired control. However these equations grow increasingly complicated as the number of space steps increases. We use Maple to obtain the equations for the case of seven space steps.

In Sec. 4 we first impose the restriction on the potential that it be centralized. We give an example of localized initial data being transferred to localized terminal data, using Maple. A well-known aspect of quantum theory is the spreading of wavepackets; thus one expects difficulty in transferring localized initial data to localized terminal data. Such difficulty surfaces in our treatment, and to more of an extent when we impose the second requirement that the potential have the nature of steps. We give an example of an initial-terminal pair which can be steered via a step potential.

2 Difference Equations

2.1 Crank-Nicolson

We consider the C-N method as in [1], where it is used for parabolic equations. Writing the Schrodinger equation with time-dependent potential in the form

$$\frac{\partial \Psi}{\partial t} - i \left[\frac{\partial^2}{\partial x^2} - V(x, t) \right] \Psi(x, t) = 0, \quad 0 < x < L, \quad t > 0, \quad (1)$$

with

$$\Psi(0, t) = \Psi(L, t) = 0, \quad \Psi(x, 0) = \Psi^0(x),$$

we apply the C-N method as follows. We denote the mesh width in x by h (the space step) and the mesh width in t by k (the time step). The x values are jh with $j = 0, 1, \dots, J$, the t -values nk , $n=0, 1, \dots$. We average the Forward-Difference method at the n th step in t ,

$$\frac{\Psi_j^{n+1} - \Psi_j^n}{k} - i \frac{\Psi_{j+1}^n - 2\Psi_j^n + \Psi_{j-1}^n}{h^2} + iV_j^n \Psi_j^n = 0 \quad (2)$$

and the Backward-Difference approximation at the $(n+1)$ st step in t ,

$$\frac{\Psi_j^{n+1} - \Psi_j^n}{k} - i \frac{\Psi_{j+1}^{n+1} - 2\Psi_j^{n+1} + \Psi_{j-1}^{n+1}}{h^2} + iV_j^{n+1} \Psi_j^{n+1} = 0, \quad j = 1..J-1. \quad (3)$$

This gives the difference equations

$$\begin{aligned} & \frac{-i}{2h^2} \Psi_{j+1}^{n+1} + \left(\frac{1}{k} + \frac{i}{h^2} + \frac{iV_j^{n+1}}{2} \right) \Psi_j^{n+1} - \frac{i}{2h^2} \Psi_{j-1}^{n+1} \\ &= \frac{i}{2h^2} \Psi_{j+1}^n + \left(\frac{1}{k} - \frac{i}{h^2} - \frac{iV_j^n}{2} \right) \Psi_j^n + \frac{i}{2h^2} \Psi_{j-1}^n, \quad j = 1 \dots J - 1. \end{aligned} \quad (4)$$

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

2.2 A Classic Approach

Next we discuss the work of [3], which treats the quantum-mechanical scattering problem of a localized wave packet impinging on potential barriers and wells. The computer-generated motion pictures obtained show reflection and transmission and are quite illustrative. Similar motion pictures in the case of a well are later given in [7], using the “leap-frog” method in [16]. We note that work in [9, 10] starts with the approach of [3] and adds a potential due to the external electric field to the potential profile of a square quantum well. However the final potential is only discretized with respect to space in the difference equations.

In [3], the Schrodinger equation with time-independent potential

$$i \frac{\partial \Psi}{\partial t} = - \left[\frac{\partial^2}{\partial x^2} - V(x) \right] \Psi(x, t) = H \Psi(x, t) \quad (5)$$

is considered, where H is the Hamiltonian. Here the mesh width in x will again be denoted by h (the space step) and the mesh width in t by k (the time step). The standard finite difference expression for the Hamiltonian is

$$H \Psi_j = (1/h^2)[\Psi_{j+1} - 2\Psi_j + \Psi_{j-1}] - V_j \Psi_j. \quad (6)$$

The Cayley form

$$\frac{1 - \frac{1}{2}ikH}{1 + \frac{1}{2}ikH}$$

is a unitary approximation to e^{-ikH} . Replacing e^{-ikH} with the Cayley form in $\Psi_j^{n+1} = e^{-ikH} \Psi_j^n$, one obtains

$$\Psi_j^{n+1} = \left[\frac{1 - \frac{1}{2}ikH}{1 + \frac{1}{2}ikH} \right] \Psi_j^{n+1} \quad (7)$$

Letting $\lambda = 2h^2/k$, one has the difference equation

$$\Psi_{j+1}^{n+1} + (i\lambda - h^2V_j - 2)\Psi_j^{n+1} + \Psi_{j-1}^{n+1} = -\Psi_{j+1}^n + (i\lambda + h^2V_j + 2)\Psi_j^n - \Psi_{j-1}^n, \quad (8)$$

and takes $\Psi_0^n = \Psi_J^n = 0$ for all n. The system of difference equations for $j = 1..J - 1$ is then solved recursively.

If we now multiply (4), obtained via C-N, through by $2h^2i$ we obtain

$$\Psi_{j+1}^{n+1} + (i\lambda - 2 - h^2V_j^{n+1})\Psi_j^{n+1} + \Psi_{j-1}^{n+1} = -\Psi_{j+1}^n + (i\lambda + 2 + h^2V_j^n)\Psi_j^n - \Psi_{j-1}^n \quad (9)$$

Comparing (8) and (9), we see that if we remove time dependence of the potential in (9), i.e. let $V_j^n = V_j^{n+1} = V_j$, equations equivalent to (8) result.

3 Matrix Equations

In the following we take $k = 2$ and $h = 1$ for simplicity in writing. Starting by expressing (9) in matrix form as in [1], for $j = 1 \dots J - 1$, we have

$$\begin{aligned} & \left(\begin{bmatrix} i-2 & 1 & 0 & \dots & 0 \\ 1 & i-2 & 1 & \dots & 0 \\ 0 & 1 & i-2 & \dots & 0 \\ \vdots & & \ddots & & 1 \\ 0 & & & 1 & i-2 \end{bmatrix} - \begin{bmatrix} V_1^{n+1} & 0 & & & \\ 0 & \ddots & 0 & & \\ & & \ddots & 0 & \\ & & & \ddots & 0 \\ & & & 0 & V_{J-1}^{n+1} \end{bmatrix} \right) \begin{bmatrix} \Psi_1^{n+1} \\ \vdots \\ \vdots \\ \Psi_{J-1}^{n+1} \end{bmatrix} \\ &= \left(\begin{bmatrix} i+2 & -1 & 0 & \dots & 0 \\ -1 & i+2 & -1 & \dots & 0 \\ 0 & -1 & i+2 & \dots & 0 \\ \vdots & & \ddots & & 1 \\ 0 & & & -1 & i+2 \end{bmatrix} + \begin{bmatrix} V_1^n & 0 & & & \\ 0 & \ddots & 0 & & \\ & & \ddots & 0 & \\ & & & \ddots & 0 \\ & & & 0 & V_{J-1}^n \end{bmatrix} \right) \begin{bmatrix} \Psi_1^n \\ \vdots \\ \vdots \\ \Psi_{J-1}^n \end{bmatrix} \quad (10) \end{aligned}$$

We next separate real and imaginary parts. Let $\Psi_j^l = R_j^l + iM_j^l$, $l = 0, 1, \dots$ and

$$\widehat{R}^l = \begin{bmatrix} R_1^l \\ \vdots \\ R_{J-1}^l \end{bmatrix}, \quad \widehat{M}^l = \begin{bmatrix} M_1^l \\ \vdots \\ M_{J-1}^l \end{bmatrix}.$$

Let

$$A = \begin{bmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \dots & 0 \\ 0 & 1 & -2 & 1 & \\ \vdots & \ddots & & & \\ & & & 1 & -2 \end{bmatrix} \quad \text{and} \quad \widehat{V}^l = \begin{bmatrix} V_1^l & 0 & & & \\ 0 & \ddots & 0 & & \\ & & \ddots & 0 & \\ & & & \ddots & 0 \\ & & & 0 & V_{J-1}^l \end{bmatrix}$$

We have

$$(iI + A - \widehat{V}^{n+1})(\widehat{R}^{n+1} + i\widehat{M}^{n+1}) = (iI - A + \widehat{V}^n)(\widehat{R}^n + i\widehat{M}^n). \quad (11)$$

The real part of (11) gives

$$A\widehat{R}^{n+1} - \widehat{M}^{n+1} - \widehat{V}^{n+1}\widehat{R}^{n+1} = -A\widehat{R}^n - \widehat{M}^n + \widehat{V}^n\widehat{R}^n. \quad (12)$$

The imaginary part of (11) gives

$$\widehat{R}^{n+1} + A\widehat{M}^{n+1} - \widehat{V}^{n+1}\widehat{M}^{n+1} = \widehat{R}^n - A\widehat{M}^n + \widehat{V}^n\widehat{M}^n. \tag{13}$$

Now we rewrite the above systems in block matrix form:

$$\begin{aligned} & \left(\begin{bmatrix} A & -I \\ I & A \end{bmatrix} - \begin{bmatrix} \widehat{V}^{n+1} & 0 \\ 0 & \widehat{V}^{n+1} \end{bmatrix} \right) \begin{bmatrix} R_1^{n+1} \\ \vdots \\ R_{J-1}^{n+1} \\ M_1^{n+1} \\ \vdots \\ M_{J-1}^{n+1} \end{bmatrix} \\ &= \left(\begin{bmatrix} -A & -I \\ I & -A \end{bmatrix} + \begin{bmatrix} \widehat{V}^n & 0 \\ 0 & \widehat{V}^n \end{bmatrix} \right) \begin{bmatrix} R_1^n \\ \vdots \\ R_{J-1}^n \\ M_1^n \\ \vdots \\ M_{J-1}^n \end{bmatrix} \tag{14} \end{aligned}$$

Let $S = \begin{bmatrix} A & -I \\ I & A \end{bmatrix}$. Then we have

$$\begin{aligned} & S \begin{bmatrix} R_1^{n+1} \\ \vdots \\ R_{J-1}^{n+1} \\ M_1^{n+1} \\ \vdots \\ M_{J-1}^{n+1} \end{bmatrix} + S^T \begin{bmatrix} R_1^n \\ \vdots \\ R_{J-1}^n \\ M_1^n \\ \vdots \\ M_{J-1}^n \end{bmatrix} \\ &= \begin{bmatrix} \widehat{V}^{n+1} & 0 \\ 0 & \widehat{V}^{n+1} \end{bmatrix} \begin{bmatrix} R_1^{n+1} \\ \vdots \\ R_{J-1}^{n+1} \\ M_1^{n+1} \\ \vdots \\ M_{J-1}^{n+1} \end{bmatrix} + \begin{bmatrix} \widehat{V}^n & 0 \\ 0 & \widehat{V}^n \end{bmatrix} \begin{bmatrix} R_1^n \\ \vdots \\ R_{J-1}^n \\ M_1^n \\ \vdots \\ M_{J-1}^n \end{bmatrix} \\ &= \begin{bmatrix} R_1^{n+1} & 0 & & & & & \\ 0 & \ddots & & & & & \\ & & R_{J-1}^{n+1} & & & & \\ & & & M_1^{n+1} & & & \\ & & & & \ddots & & \\ & & & & & 0 & \\ & & & & & & M_{J-1}^{n+1} \end{bmatrix} \begin{bmatrix} V_1^{n+1} \\ \vdots \\ V_{J-1}^{n+1} \\ V_1^{n+1} \\ \vdots \\ V_{J-1}^{n+1} \end{bmatrix} \end{aligned}$$

$$\begin{aligned}
& + \begin{bmatrix} R_1^n & 0 & & & \\ 0 & \ddots & 0 & & \\ & & R_{J-1}^n & & \\ & & & M_1^n & \\ & & & \ddots & 0 \\ & & & 0 & M_{J-1}^n \end{bmatrix} \begin{bmatrix} V_1^n \\ \vdots \\ V_{J-1}^n \\ V_1^n \\ \vdots \\ V_{J-1}^n \end{bmatrix} \\
& = \begin{bmatrix} R_1^{n+1} & & 0 & R_1^n & & 0 \\ 0 & \ddots & & & \ddots & \\ M_1^{n+1} & & R_{J-1}^{n+1} & & & R_{J-1}^n \\ 0 & \ddots & & M_1^n & & 0 \\ & & M_{J-1}^{n+1} & & \ddots & M_{J-1}^n \end{bmatrix} \begin{bmatrix} V_1^{n+1} \\ \vdots \\ V_{J-1}^{n+1} \\ V_1^n \\ \vdots \\ V_{J-1}^n \end{bmatrix} \equiv EV.
\end{aligned} \tag{15}$$

Letting B denote the left-most term in (15), we have the system of linear algebraic equations $EV=B$.

Proposition: The matrix E is invertible exactly when

$$\det \begin{bmatrix} R_j^{n+1} & R_j^n \\ M_j^{n+1} & M_j^n \end{bmatrix} \neq 0, \tag{16}$$

for $j = 1 \dots J - 1$.

Proof. The matrix E is invertible if and only if the only solution of

$$EC \equiv \begin{bmatrix} R_1^{n+1} & & 0 & R_1^n & & 0 \\ 0 & \ddots & & & \ddots & \\ M_1^{n+1} & & R_{J-1}^{n+1} & & & R_{J-1}^n \\ 0 & \ddots & & M_1^n & & 0 \\ & & M_{J-1}^{n+1} & & \ddots & M_{J-1}^n \end{bmatrix} \begin{bmatrix} C_1 \\ \vdots \\ C_{J-1} \\ C_J \\ \vdots \\ C_{2(J-1)} \end{bmatrix} = 0 \tag{17}$$

is the trivial solution. This is true if and only if the homogeneous linear systems with coefficient matrices

$$\begin{bmatrix} R_j^{n+1} & R_j^n \\ M_j^{n+1} & M_j^n \end{bmatrix},$$

$j = 1 \dots J - 1$, have only trivial solutions. This is equivalent to (16) for $j = 1 \dots J - 1$.

Thus, if an initial-terminal pair satisfies (16), we may solve (15) for the potential which transfers initial to terminal. The solution in this case is unique and thus we only consider at this stage starting at an initial time, say $n = 0$

and passing to the terminal time in one time step. If previous time steps are allowed, a more complicated situation results.

Now working in the case in which (16) holds, we give the equations for the components of the potential in terms of the components of the initial and terminal data in the case of $J=7$, from Maple. We consider $n = 0$ to $n = 1$ and denote R_j^1 and M_j^1 by R_j and M_j respectively, R_j^0 and M_j^0 by r_j and m_j , respectively and V_j^1 and V_j^0 by V_j and v_j , respectively. Then

$$[V_1, \dots, V_6, v_1, \dots, v_6]^T \tag{18}$$

$$= \left[\begin{array}{l} -(-M_2r_1 + m_1r_2 + R_2m_1 - M_1m_1 + m_1^2 - \\ R_1r_1 + 2M_1r_1 - 2R_1m_1 + r_1^2 - m_2r_1)/(M_1r_1 - R_1m_1) \\ \\ -(R_1m_2 - M_1r_2 + 2M_2r_2 - M_2m_2 + m_2^2 + r_2^2 - 2R_2m_2 + R_3m_2 \\ + m_2r_1 + r_3m_2 - R_2r_2 - M_3r_2 - m_1r_2 - r_2m_3)/(M_2r_2 - R_2m_2) \\ \\ -(R_4m_3 + m_3r_4 - R_3r_3 + r_3^2 - 2R_3m_3 + m_3^2 - M_2r_3 - M_4r_3 \\ - r_3m_2 - m_4r_3 + R_2m_3 + 2M_3r_3 - M_3m_3 + r_2m_3)/(-R_3m_3 + M_3r_3) \\ \\ -(-M_3r_4 - 2R_4m_4 - M_5r_4 + r_4^2 + 2M_4r_4 - M_4m_4 + m_4^2 + R_3m_4 \\ + R_5m_4 + m_4r_3 + r_5m_4 - R_4r_4 - m_3r_4 - r_4m_5)/(M_4r_4 - R_4m_4) \\ \\ -(R_6m_5 + 2M_5r_5 - M_5m_5 - M_4r_5 - M_6r_5 - r_5m_4 - r_5m_6 + R_4m_5 \\ + r_6m_5 + r_4m_5 - R_5r_5 + r_5^2 - 2R_5m_5 + m_5^2)/(-R_5m_5 + M_5r_5) \\ \\ -(-M_6m_6 - r_6m_5 - R_6r_6 - M_5r_6 + r_6^2 \\ + R_5m_6 - 2R_6m_6 + 2M_6r_6 + r_5m_6 + m_6^2)/(-R_6m_6 + M_6r_6) \\ \\ (M_1r_2 + M_1R_2 - M_1^2 - 2M_1r_1 - R_1^2 \\ + M_1m_1 - R_1M_2 - R_1m_2 + R_1r_1 + 2R_1m_1)/(M_1r_1 - R_1m_1) \\ \\ (R_2r_2 + R_1M_2 + M_2R_3 - M_2^2 + M_2r_1 - 2M_2r_2 + M_2r_3 + M_2m_2 \\ - R_2M_3 - R_2^2 - M_1R_2 + 2R_2m_2 - R_2m_1 - R_2m_3)/(M_2r_2 - R_2m_2) \\ \\ (M_3r_2 - R_3^2 - M_2R_3 - R_3M_4 + R_3r_3 - R_3m_2 + 2R_3m_3 - R_3m_4 \\ + M_3R_4 + R_2M_3 + M_3r_4 - M_3^2 - 2M_3r_3 + M_3m_3)/(-R_3m_3 + M_3r_3) \\ \\ (R_4r_4 + R_3M_4 + M_4R_5 - M_4^2 + M_4r_3 - 2M_4r_4 + M_4r_5 + M_4m_4 \\ - R_4M_5 - R_4^2 - M_3R_4 + 2R_4m_4 - R_4m_3 - R_4m_5)/(M_4r_4 - R_4m_4) \\ \\ (M_5r_4 - R_5^2 - M_4R_5 - M_6R_5 + R_5r_5 - R_5m_4 + 2R_5m_5 - R_5m_6 \\ + R_6M_5 + R_4M_5 + M_5r_6 - M_5^2 - 2M_5r_5 + M_5m_5)/(-R_5m_5 + M_5r_5) \\ \\ -(R_6m_5 + R_6^2 + R_6M_5 - R_6r_6 - M_6R_5 \\ - 2R_6m_6 + M_6^2 - M_6m_6 - M_6r_5 + 2M_6r_6)/(-R_6m_6 + M_6r_6) \end{array} \right]$$

4 Restrictions on the Potential

In the following we consider the case $J = 7$. First we centralize the potential by imposing $V_1 = V_6 = v_1 = v_6 = 0$ in (18). Then we look for initial and terminal data satisfying (16) for which the initial data is localized to the left and the terminal data is localized to the right. By localized to the left we refer to the fact that the terms $r_j^2 + m_j^2$ have a maximum at $j = 2$ and decrease as j increases. Thus a graph of $F(j) = r_j^2 + m_j^2$, an approximation of $|\Psi(x_j, 0)|^2$ for $j = 1 \dots 6$, peaks to the left and tails off to the right. Similarly, localized to the right refers to a tail coming from the left rising to a peak on the right; for the example below the tail is flat from $j = 2$ to $j = 3$. Some attempts result in computational grid lock with Maple and it is not clear if this is due to insufficient specification or over-specification of components. We obtain the following example:

$$V = \begin{bmatrix} V_1 \\ \vdots \\ V_6 \\ v_1 \\ \vdots \\ v_6 \end{bmatrix} = \begin{bmatrix} 0 \\ -14.11436950 \\ 2.27272727273 \\ 3.518181818 \\ 5.5 \\ 0 \\ 0 \\ 1.111436950 \\ 1 \\ -5.272727273 \\ -24 \\ 0 \end{bmatrix},$$

$$\begin{bmatrix} r_1 \\ \vdots \\ r_6 \\ m_1 \\ \vdots \\ m_6 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 1 \\ 0.8 \\ 0.5 \\ 0.3 \\ 0.5 \\ 1.9 \\ .3545454545 \\ 0.6 \\ 0.5 \\ 0.3 \end{bmatrix}, \quad \begin{bmatrix} R_1 \\ \vdots \\ R_6 \\ M_1 \\ \vdots \\ M_6 \end{bmatrix} = \begin{bmatrix} 0.2 \\ 0.2 \\ 0.2 \\ 1 \\ 1.6 \\ 0.4 \\ 0.3 \\ 0.5 \\ 0.5 \\ 1 \\ 2 \\ 1 \end{bmatrix}$$

Second, we both centralize and require that the potential be single steps. Now, however, it is more difficult to also require localized initial and terminal

data. We obtain the example:

$$V = \begin{bmatrix} V_1 \\ \vdots \\ V_6 \\ v_1 \\ \vdots \\ v_6 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -0.9145379212 \\ -0.9145379212 \\ 0 \\ 0 \\ 0 \\ 0 \\ 2.266495745 \\ 2.266495745 \\ 0 \\ 0 \end{bmatrix},$$

$$\begin{bmatrix} r_1 \\ \vdots \\ r_6 \\ m_1 \\ \vdots \\ m_6 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 1 \\ 0.8 \\ 0.8 \\ 0.5 \\ 1 \\ -1.413689775 \\ 1.265154420 \\ 1.8 \\ 0.8 \\ 0.5 \end{bmatrix},$$

$$\begin{bmatrix} R_1 \\ \vdots \\ R_6 \\ M_1 \\ \vdots \\ M_6 \end{bmatrix} = \begin{bmatrix} 1.078281860 \\ 0.1957046498 \\ 4.140506990 \\ 5 \\ 2.1 \\ 0.7 \\ -0.9608590700 \\ 1.413689775 \\ 0.5 \\ 1 \\ 2 \\ 1 \end{bmatrix}.$$

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