Control of Electronic Materials

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Abstract

Quantum-scale structures are described by the Schrodinger equation and control is exercised by a time-dependent potential term. Here we consider two numerical schemes for the Schrodinger equation with a time-dependent potential and show that the proof of stability of one may be modified to show stability of the other.

1 Introduction

New solid-state structures are under development, and efforts to control them have begun. Examples include quantum dots and their control via laser radiation [2, 3] and control of quantum cellular automata via a modulated potential barrier [9]. Quantum-scale structures are commonly described by the Schrodinger equation, and physically meaningful control has been modelled by a time-dependent potential term in the equation.

Investigation of numerical methods for control problems for such systems is important for implementation. A classic method [4] (see [5, 6, 7]) for numerically approximating the time-dependent Schrodinger equation with a time-independent potential uses the Cayley form. It is equivalent to the Crank-Nicolson method. A scheme which extends this method to the case of a time-dependent potential has been used to study control in one dimension [8]. Chan and Shen [1] earlier studied a scheme which also allows time dependence of the potential in the Schrodinger equation, which differs from the scheme in [8] in that it includes "mixed-time" potential-state terms. Stability of that scheme is shown in [1]. Here we show that a modification of the proof in [1] gives stability of the other scheme, on a domain bounded in space and time and allowing for a variable time step.

2 Stability

Consider the Schrodinger equation

$$\Psi_t = i\Psi_{xx} - iV(x,t)\Psi, \tag{2.1}$$

on the domain $Q_T(0 \leq x \leq l, 0 \leq t \leq T)$, with the initial condition

$$\Psi|_{t=0} = \tilde{\Psi}(x),$$

where $\tilde{\Psi}(x)$ is a complex function, and boundary conditions

$$\Psi|_{x=0} = \Psi|_{x=l} = 0.$$

The potential $V(x,t)$ is assumed to be real.

First we discuss the work of Chan and Shen. In [1] equations of the form

$$u_t = (A(x,t)u_x)_x + B(x,t)u_x + C(x,t)u + f(x,t) \tag{2.2}$$

are considered, on Q_T, where $u(x,t), A(x,t), B(x,t), C(x,t)$ and $f(x,t)$ are complex functions, and Re $A(x,t) \geq 0$ and $|A(x,t)| \neq 0$. The initial condition is

$$u|_{t=0} = \tilde{u}(x),$$

where $\tilde{u}(x)$ is a complex function, and the boundary conditions are

$$u|_{x=0} = u|_{x=l} = 0.$$

Let h denote the spatial mesh, $x_j = jh(j = 0, 1, \cdots, J)$ the mesh points, k_n the size of the time step at the n^{th} step, with u_j^n denoting $u(x_j, t_n)$. For any function ϕ, let $\phi^{n+\alpha}$ denote $\alpha\phi^{n+1} + (1-\alpha)\phi^n$, for $0 \leq \alpha \leq 1$. To define stability, let the inner product for u and v be

$$(u, v) = \sum_{j=1}^{J-1} u_j \bar{v}_j h,$$

where $\bar{v}$ denotes the complex conjugate of v and $||u|| = \sqrt{(u,u)}$.

Definition 2.1 *A scheme is stable if the solution u_j^n satisfies*

$$||u^n|| \leq C_1||u^0|| + C_2 \sum_{l=0}^{J-1} ||f^l||k_l,$$

where C_1 and C_2 are constants which are independent of n and h.

The following scheme is considered:

$$\frac{u_j^{n+1} - u_j^n}{k_n} - \frac{1}{h^2}[A_{j+\frac{1}{2}}^{n+\alpha}(u_{j+1}^{n+\alpha} - u_j^{n+\alpha}) - A_{j-\frac{1}{2}}^{n+\alpha}(u_j^{n+\alpha} - u_{j-1}^{n+\alpha})]$$

$$-B_j^{n+\alpha}(\frac{u_{j+1}^{n+\alpha} - u_{j-1}^{n+\alpha}}{2h}) - C_j^{n+\alpha}u_j^{n+\alpha} = f_j^{n+\alpha}, \quad j = 1, 2, \cdots, J-1, \tag{2.3}$$

$$u_j^0 = \tilde{u_j}, \quad j = 1, 2, \cdots, J-1, \tag{2.4}$$

$$u_0^n = u_J^n = 0, \quad n = 0, 1, \cdots. \tag{2.5}$$

This is Crank-Nicolson when $\alpha = \frac{1}{2}$. Let (I) denote the conditions : $A \in C^3, B \in C^2, C \in C^1$, Re $A \geq 0, |A| \geq a_0 > 0$. Then the following is obtained.

Theorem 2.1 *(see Thm. 2.1, [1]). Suppose conditions (I) are satisfied. If $\frac{1}{2} \le \alpha \le 1$, then scheme (2.3), with (2.4) and (2.5), is stable.*

Now we consider the Schrodinger equation (2.1) in light of the above. First, we see (2.1) is of the form (2.2) if $A(x,t) = i, B = 0, C = -iV$, and $f = 0$. Using $\alpha = \frac{1}{2}$, scheme (2.3) becomes

$$\frac{\Psi_j^{n+1} - \Psi_j^n}{k_n} - \frac{i}{2h^2}(\Psi_{j+1}^{n+1} - 2\Psi_j^{n+1} + \Psi_{j-1}^{n+1} + \Psi_{j+1}^n - 2\Psi_j^n + \Psi_{j-1}^n) + i\frac{(V_j^{n+1} + V_j^n)}{2}\frac{(\Psi_j^{n+1} + \Psi_j^n)}{2} = 0, \tag{2.6}$$

with

$$\Psi_j^0 = \tilde{\Psi}_j, \quad j = 1, 2, \cdots, J-1 \tag{2.7}$$

$$\Psi_0^n = \Psi_J^n = 0, \quad n = 0, 1, \cdots. \tag{2.8}$$

We observe that the above scheme may be obtained by first semi-discretizing (2.1) with respect to space

$$i\frac{d\Psi_j}{dt}(t) = -\frac{1}{h^2}(\Psi_{j+1}(t) - 2\Psi_j(t) + \Psi_{j-1}(t)) + V_j(t)\Psi_j(t), \quad j = 1, \cdots, J-1,$$

and then replacing the time derivative of Ψ_j by $\frac{\Psi_j^{n+1} + \Psi_j^n}{k_n}$, Ψ_j by $\frac{\Psi_j^{n+1} + \Psi_j^n}{2}$ and V_j by $\frac{V_j^{n+1} + V_j^n}{2}$, $j = 1, \cdots, J-1$.

If $V \in C^1$, then (I) is satisfied, and Theorem 2.1 applies.

Next we consider the scheme obtained in [8] by averaging the Forward-Difference method at the nth step in t,

$$\frac{\Psi_j^{n+1} - \Psi_j^n}{k} - i\frac{\Psi_{j+1}^n - 2\Psi_j^n + \Psi_{j-1}^n}{h^2} + iV_j^n\Psi_j^n = 0, \tag{2.9}$$

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

$$\frac{\Psi_j^{n+1} - \Psi_j^n}{k} - i\frac{\Psi_{j+1}^{n+1} - 2\Psi_j^{n+1} + \Psi_{j-1}^{n+1}}{h^2} + iV_j^{n+1}\Psi_j^{n+1} = 0, \quad j = 1..J-1, \tag{2.10}$$

where k is a constant time step. This gives the difference equations

$$\frac{\Psi_j^{n+1} - \Psi_j^n}{k} - \frac{i}{2h^2}(\Psi_{j+1}^{n+1} - 2\Psi_j^{n+1} + \Psi_{j-1}^{n+1} + \Psi_{j+1}^n - 2\Psi_j^n + \Psi_{j-1}^n) + \frac{i}{2}(V_j^n\Psi_j^n + V_j^{n+1}\Psi_j^{n+1}) = 0. \tag{2.11}$$

Compare (2.6) and (2.11). We now show in Theorem 2.2 that a scheme the same as (2.11), except for the fact that now a variable time step is allowed as in (2.6), is stable. The proof of Theorem 2.2 modifies that of Theorem 2.1 in the step involving estimation of the potential term. In the case of the Schrodinger equation (2.1), with A the constant i, $B = 0$ and $f = 0$, it is also possible to rewrite certain other parts of the proof of Theorem 2.1 in a more basic form, which we do.

Theorem 2.2 *Let $V(x,t) \in C^1$. The scheme*

$$\frac{\Psi_j^{n+1}-\Psi_j^n}{k_n} - \frac{i}{2h^2}(\Psi_{j+1}^{n+1}-2\Psi_j^{n+1}+\Psi_{j-1}^{n+1}+\Psi_{j+1}^n-2\Psi_j^n+\Psi_{j-1}^n)+\frac{i}{2}(V_j^n\Psi_j^n+V_j^{n+1}\Psi_j^{n+1})=0, \tag{2.12}$$

with (2.7) and (2.8), is stable.

Proof. First, multiply (2.12) by $\overline{\Psi_j^{n+\frac{1}{2}}}h$ (notation as earlier) and sum over j, obtaining

$$\sum_{j=1}^{J-1}\left(\frac{\Psi_j^{n+1}-\Psi_j^n}{k_n}\right)\overline{\Psi_j^{n+\frac{1}{2}}}h+\sum_{j=1}^{J-1}\frac{i}{2h^2}(\Psi_{j+1}^{n+1}-2\Psi_j^{n+1}+\Psi_{j-1}^{n+1}+\Psi_{j+1}^n-2\Psi_j^n+\Psi_{j-1}^n)\overline{\Psi_j^{n+\frac{1}{2}}}h$$

$$+\sum_{j=1}^{J-1}\frac{i}{2}(V_j^n\Psi_j^n+V_j^{n+1}\Psi_j^{n+1})\overline{\Psi_j^{n+\frac{1}{2}}}h=0. \tag{2.13}$$

Take real parts. For the first term, we have

$$\begin{aligned} &Re\left(\sum_{j=1}^{J-1}\left(\frac{\Psi_j^{n+1}-\Psi_j^n}{k_n}\right)\overline{\Psi_j^{n+\frac{1}{2}}}h\right)\\ =\ & Re\left(\frac{1}{2k_n}\sum_{j=1}^{J-1}(\Psi_j^{n+1}-\Psi_j^n)(\overline{\Psi_j^{n+1}}+\overline{\Psi_j^n})h\right)\\ =\ & Re\left(\frac{1}{2k_n}\sum_{j=1}^{J-1}(|\Psi_j^{n+1}|^2-|\Psi_j^n|^2+2iIm(\overline{\Psi_j^n}\Psi_j^{n+1}))h\right)\\ =\ & \frac{1}{2k_n}(||\Psi^{n+1}||^2-||\Psi^n||^2). \end{aligned} \tag{2.14}$$

For the second term,

$$\begin{aligned} &Re\left(\sum_{j=1}^{J-1}\frac{i}{2h^2}(\Psi_{j+1}^{n+1}-2\Psi_j^{n+1}+\Psi_{j-1}^{n+1}+\Psi_{j+1}^n-2\Psi_j^n+\Psi_{j-1}^n)\overline{\Psi_j^{n+\frac{1}{2}}}h\right)\\ =\ & Re\left(\frac{i}{h^2}\sum_{j=1}^{J-1}(\Psi_{j+1}^{n+\frac{1}{2}}-2\Psi_j^{n+\frac{1}{2}}+\Psi_{j-1}^{n+\frac{1}{2}})\overline{\Psi_j^{n+\frac{1}{2}}}h\right). \end{aligned} \tag{2.15}$$

For convenience, we temporarily suppress the superscripts. The sum in the right-hand side of (2.15) becomes

$$\sum_{j=1}^{J-1}\Psi_{j+1}\overline{\Psi}_jh-2\sum_{j=1}^{J-1}|\Psi_j|^2h+\sum_{j=1}^{J-1}\Psi_{j-1}\overline{\Psi}_jh. \tag{2.16}$$

We have

$$\sum_{j=1}^{J-1}\Psi_{j+1}\overline{\Psi}_jh=\sum_{j=1}\Psi_j\overline{\Psi}_{j-1}h$$

by boundary conditions. Thus

$$\begin{aligned}\sum_{j=1}^{J-1}\Psi_{j+1}\overline{\Psi}_j h - 2\sum_{j=1}^{J-1}|\Psi_j|^2 h + \sum_{j=1}^{J-1}\Psi_{j-1}\overline{\Psi}_j h \\ = -2\sum_{j=1}^{J-1}|\Psi_j|^2 h + 2Re\sum_{j=1}^{J-1}\Psi_j\overline{\Psi}_{j-1}h. \qquad (2.17)\end{aligned}$$

Returning to (2.15), we have

$$\begin{aligned} & Re\left(\frac{i}{h^2}\sum_{j=1}^{J-1}(\Psi_{j+1}^{n+\frac{1}{2}} - 2\Psi_j^{n+\frac{1}{2}} + \Psi_{j-1}^{n+\frac{1}{2}})\overline{\Psi_j^{n+\frac{1}{2}}}h\right) \\ = \ & Re\left(\frac{i}{h^2}\left(-2\sum_{j=1}^{J-1}|\Psi_j^{n+\frac{1}{2}}|^2 h + 2Re\sum_{j=1}^{J-1}\Psi_j^{n+\frac{1}{2}}\overline{\Psi_{j-1}^{n+\frac{1}{2}}}h\right)\right) = 0. \qquad (2.18)\end{aligned}$$

Now, substituting (2.14), (2.18) into (2.13), we have

$$\begin{aligned}\frac{1}{2k_n}(||\Psi^{n+1}||^2 - ||\Psi^n||^2) &= -Re\sum_{j=1}^{J-1}\frac{i}{2}(V_j^n\Psi_j^n + V_j^{n+1}\Psi_j^{n+1})\overline{\Psi_j^{n+\frac{1}{2}}}h \\ &\leq \left|Re\sum_{j=1}^{J-1}\frac{i}{2}(V_j^n\Psi_j^n + V_j^{n+1}\Psi_j^{n+1})\overline{\Psi_j^{n+\frac{1}{2}}}h\right| \\ &\leq \sum_{j=1}^{J-1}\left|(V_j^n\Psi_j^n + V_j^{n+1}\Psi_j^{n+1})\left(\frac{\overline{\Psi_j^{n+1}} + \overline{\Psi_j^n}}{2}\right)\right|h \\ &\leq \frac{M}{2}\sum_{j=1}^{J-1}(|\Psi_j^n|^2 + |\Psi_j^{n+1}|^2 + 2|\Psi_j^{n+1}\overline{\Psi_j^n}|)h \\ &\leq M(||\Psi^n||^2 + ||\Psi^{n+1}||^2), \qquad (2.19)\end{aligned}$$

where $|V_j^n| \leq M$ for all n, j. Now, as in [1], if $k_n < \frac{1}{4M}$, we have

$$||\Psi^{n+1}||^2 \leq \frac{1 + 2k_nM}{1 - 2k_nM}||\Psi^n||^2 \leq (1 + 8k_nM)||\Psi^n||^2.$$

By Duhamel's Principle,

$$||\Psi^{n+1}||^2 \leq 2e^{8Mt^{n+1}}||\Psi^0||^2,$$

where $t^{n+1} = \sum_{l=0}^{n} k_l$.

Remark: While the scheme (2.12) is computationally simpler, the relative merits of the schemes for control are still to be determined.

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