Most conventional explicit finite difference schemes, e.g. Euler's scheme, for solving the parabolic equation of Schrödinger type $u_t = iu_{xx}$ are unconditionally unstable. This difficulty can be overcome by introducing a dissipative term to the conventional explicit schemes. Based on this approach, we derive a class of new explicit finite difference schemes which are conditionally stable, spans two time levels and are $O(k, h^2)$ accurate. We also determine the schemes from this class that have the least restrictive stability requirements. It is interesting to note that the analog of the Lax-Wendroff scheme is unstable.

Stable Explicit Schemes for Equations of the Schrödinger Type

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1. Introduction

Equations of the Schrödinger type arise in many disciplines, such as quantum mechanics, plasma physics and acoustics. Recently, there have been many studies of applying finite difference methods to solve equations of this type for practical problems that arise in these areas, see for example[1, 8, 3, 6, 4, 5]. Most of these studies employ some form of implicit schemes. The stability and convergence properties of these schemes have been thoroughly analyzed and can be found in [10, 5].

It is well-known[5, 7] that most of the conventional explicit schemes, for example Euler's scheme, are unconditionally unstable for this type of equations. It is therefore natural to ask the question of whether there exist stable explicit schemes for the Schrödinger equation. Not only is this question of theoretical interest, it is also important for practical applications. Compared to implicit schemes, explicit schemes are generally easier to implement and take less storage. These advantages are especially pronounced for multi-dimensional problems. Moreover, it is often easier to vectorize an explicit scheme on the many pipeline-oriented computers available today, e.g. Crays, Cyber 205 and the FPS 164.

The purpose of this paper is to present a class of stable explicit schemes for the Schrödinger equation. It is well-known that in the study of wave phenomena, the addition of dissipative terms often makes the theoretical development more convenient. Moreover, such terms often improve the stability properties of the corresponding difference schemes. The famous Lax-Wendroff scheme for hyperbolic systems is one such example. Unfortunately, as will be shown in Section 3, the analogous scheme for the Schrödinger equation is unstable. However, we have succeeded in deriving stable explicit schemes for the Schrödinger equation by introducing appropriately chosen dissipative terms. In Section 2 and Section 3, we present our results for the simplest equation of the Schrödinger type:

$$u_t = iu_{xx}, \tag{1.1}$$

and discuss the effect of adding different kinds of dissipative terms. Here $i = \sqrt{-1}$. Using the methods in [9], these results can be extended to the more general equation :

$$u_t = ia(x,t)u_{xx} + b(x,t)u_x + c(x,t)u + f(x,t),$$

as well as to nonlinear equations.

The equation (1.1) admits travelling wave solutions with nondiminishing amplitudes and in this sense behaves more like a hyperbolic system than a parabolic one. Since the solutions to (1.1) have nongrowing amplitudes, correspondingly the definition of stability used in this paper is the notion of *practical stability* as discussed by [9, 2], which requires the discrete solution to have a nongrowing norm. Namely, unless stated otherwise explicitly, stability in this paper means $||G|| \leq 1$ where G is the characteristic polynomial of the numerical scheme. Note that this definition of stability is different from other definitions which allow growth in the computed solution and ones that are insensitive to additions of lower order terms in the equation.

In this paper, we use u_j^n to denote $u(x_j, t^n)$, k and h to denote the temporal and spatial mesh sizes respectively, and r to denote $\frac{k}{h^2}$. A uniform spatial mesh is assumed for the stability analysis.

2. Dissipative Term ϵu_{xx} and the Corresponding Explicit Schemes

The simplest explicit scheme for (1.1) is the Euler scheme

$$\frac{u_j^{n+1} - u_j^n}{k} = i\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}\right), \tag{2.1}$$

and the corresponding truncation error is $O(k, h^2)$. It is well-known that this scheme is unconditionally unstable[7].

For deriving stable explicit schemes, we introduce a dissipative term R in (1.1) to obtain

$$u_t = iu_{xx} + R. \tag{2.2}$$

In this section, we shall take $R = \epsilon u_{xx}$, where ϵ is a small scalar. In the next section, we shall consider $R = \epsilon u_{xxxx}$. In order to preserve the $O(k, h^2)$ truncation error of (2.1), we take $\epsilon = (\alpha+i\beta)k$ or $\epsilon = (\alpha + i\beta)h^2$, where α and β are real scalars, independent of k and h. We discuss the two cases separately.

Case 1. $R = (\alpha + i\beta)ku_{xx}$

The corresponding explicit scheme for this is

$$\frac{u_j^{n+1} - u_j^n}{k} = (i + (\alpha + i\beta)k)\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}\right). \tag{2.3}$$

Theorem 2.1. *The scheme (2.3) is stable if and only if $\alpha > 0$ and*

$$r \leq \frac{\alpha k}{2(\alpha^2 k^2 + (1+\beta k)^2)}. \tag{2.4}$$

Proof. The characteristic polynomial for (2.3) is

$$G = 1 - (i + (\alpha + i\beta)k)\gamma,$$

where $\gamma = 4r\sin^2\frac{\omega h}{2}$. Therefore, we have

$$|G|^2 = (1 - \alpha k\gamma)^2 + (1 + \beta k)^2\gamma^2.$$

Stability requires $|G|^2 \leq 1$ for $0 \leq \gamma \leq 4r$. It can be easily verified that the maximum of $|G|^2$ occurs at the boundary of the interval $0 \leq \gamma \leq 4r$. At $\gamma = 0$, $G = 1$. At $\gamma = 4r$, stability requires that

$$|G|^2 = (1 - 4r\alpha k)^2 + (1 + \beta k)^2 16r^2 \leq 1,$$

from which we easily obtain (2.4).

∎

We note that when k and h are small enough, (2.4) cannot be satisfied. Therefore, while being *conditionally* stable, scheme (2.3) is not very practical.

Case 2. $R = (\alpha + i\beta)h^2 u_{xx}$

The corresponding explicit scheme is

$$\frac{u_j^{n+1} - u_j^n}{k} = (i + (\alpha + i\beta)h^2)\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}\right). \tag{2.5}$$

Theorem 2.2. *The scheme (2.5) is stable if and only if $\alpha > 0$ and*

$$r \leq \frac{\alpha h^2}{2(\alpha^2 h^2 + (1+\beta h)^2)}. \tag{2.6}$$

Proof. The characteristic polynomial for (2.5) is

$$G = 1 - (i + (\alpha + i\beta)h^2)\gamma.$$

Analogous to the proof of Theorem 2.1, the condition $|G|^2 \leq 1$ gives (2.6).

∎

Note that the stability condition for this scheme is of the form $k \leq O(h^4)$ which is too severe for small h, again making this scheme impractical.

3. Dissipative Term ϵu_{xxxx} and the Corresponding Explicit Schemes

From the last section, we see that the schemes (2.1), (2.3) and (2.5) are either unstable or have too severe a restriction on k. Therefore, we turn our attention to the introduction of the dissipative term ϵu_{xxxx}. Again there are two separate cases.

Case 1. $R = (\alpha + i\beta)ku_{xxxx}$.

The corresponding explicit scheme for this is

$$\frac{u_j^{n+1} - u_j^n}{k} = i\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}\right) + (\alpha + i\beta)k\left(\frac{u_{j+2}^n - 4u_{j+1}^n + 6u_j^n - 4u_{j-1}^n + u_{j-2}^n}{h^4}\right). \tag{3.1}$$

Theorem 3.1. *The scheme (3.1) is stable if and only if*

$$\alpha \leq -\frac{1}{2}, \text{ except for the half line } \left\{\alpha = -\frac{1}{2}, \beta \leq 0\right\},$$

and

$$r \leq \frac{(\beta + \sqrt{-\alpha(2\alpha^2 + 2\beta^2 + \alpha)})}{4(\alpha^2 + \beta^2)}. \tag{3.2}$$

The least restrictive stability constraint is

$$r \leq \frac{1}{2} \tag{3.3}$$

and is obtained when $\alpha = -\frac{1}{2}, \beta = \frac{1}{2}$.

Proof. The characteristic polynomial for the scheme (3.1) is

$$G = 1 - i\gamma + (\alpha + i\beta)\gamma^2,$$

where $\gamma = 4r\sin^2\frac{\omega h}{2}$. Thus we have

$$\begin{aligned}|G|^2 &= (1 + \alpha\gamma^2)^2 + (\beta\gamma^2 - \gamma)^2 \\ &= 1 + (1 + 2\alpha)\gamma - 2\beta\gamma^3 + (\alpha^2 + \beta^2)\gamma^4.\end{aligned}$$

The condition $|G|^2 \leq 1$ reduces to

$$f(\gamma) \equiv (1 + 2\alpha) - 2\beta\gamma + (\alpha^2 + \beta^2)\gamma^2 \leq 0. \tag{3.4}$$

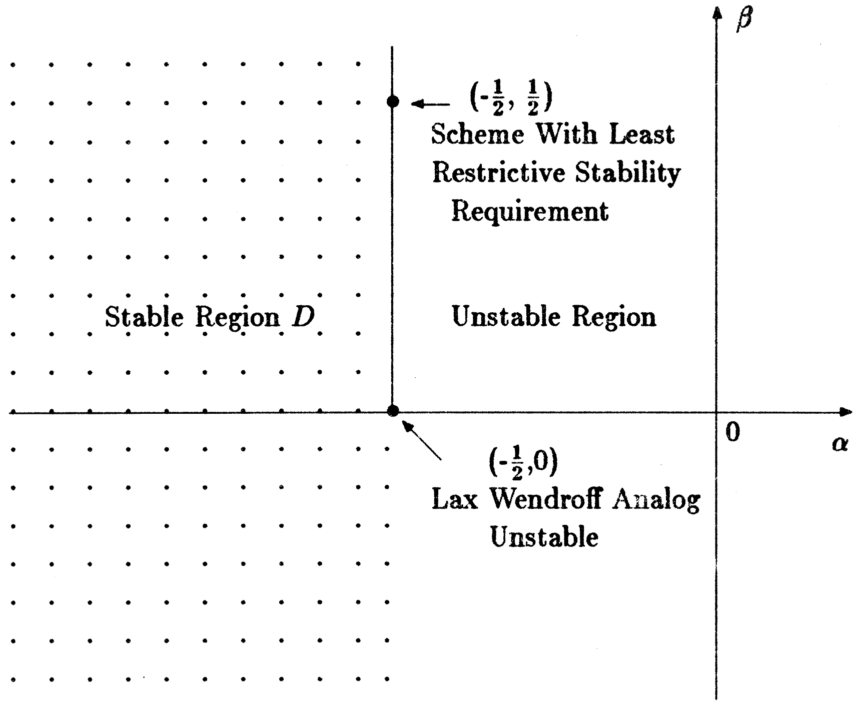

Figure 1: Stability Region for $u_t = iu_{xx} + (\alpha + i\beta)ku_{xxxx}$.

Now $f(\gamma)$ has two roots given by

$$\gamma_{\pm} = \frac{\beta \pm \sqrt{\beta^2 - (1+2\alpha)(\alpha^2+\beta^2)}}{(\alpha^2+\beta^2).}$$

Condition (3.4) requires that $\gamma_{\pm}$ be real and that $\gamma_- \le \gamma \le \gamma_+$. Now $\gamma_{\pm}$ are real if and only if

$$\beta^2 - (1+2\alpha)(\alpha^2+\beta^2) \ge 0. \tag{3.5}$$

Since $0 \le \gamma$, the condition $\gamma_- \le \gamma$ gives

$$\beta - \sqrt{\beta^2 - (1+2\alpha)(\alpha^2+\beta^2)} \le 0. \tag{3.6}$$

On the other hand, γ_+ must be positive, so

$$\beta + \sqrt{\beta^2 - (1+2\alpha)(\alpha^2+\beta^2)} > 0. \tag{3.7}$$

From (3.6), we obtain $\alpha \le -\frac{1}{2}$ for $\beta > 0$, and from (3.7), we obtain $\alpha < -\frac{1}{2}$ for $\beta \le 0$. Hence the stability region D is as depicted in Figure 1. Note that condition (3.6) and (3.7) subsume (3.5).

Since $\gamma \le 4r$, the condition $\gamma \le \gamma_+$ is exactly (3.2).

To find the scheme with the least restrictive stability condition, we seek the maximum of the right hand side of (3.2) in D. Let

$$g(\alpha,\beta) = \frac{(\beta + \sqrt{-\alpha(2\alpha^2+2\beta^2+\alpha)})}{4(\alpha^2+\beta^2)}.$$

From the equation $\frac{\partial g}{\partial \beta} = 0$, it can be deduced that g reaches its largest value when $\beta = \sqrt{-\frac{\alpha}{2}}$. Since $g(\alpha, \sqrt{-\frac{\alpha}{2}}) = \frac{1}{4}\sqrt{-\frac{2}{\alpha}}$, we have that g is maximized in D at $\alpha = -\frac{1}{2}, \beta = \frac{1}{2}$. The stability condition (3.3) follows from this.

∎

It is interesting to note that the special case $\alpha = -\frac{1}{2}, \beta = 0$, or equivalently $R = -\frac{1}{2}ku_{xxxx}$, is a scheme that is analogous to the Lax-Wendroff scheme for the system $u_t = u_x$. It can be derived from the Taylor series expansion

$$\begin{aligned} u_j^{n+1} &= u_j^n + k(u_t)_j^n + \frac{k^2}{2}(u_{tt})_j^n + O(k^3) \\ &= u_j^n + k(u_{xx})_j^n + \frac{k^2}{2}(u_{xxxx})_j^n + O(k^3), \end{aligned}$$

and is therefore $O(k^2, h^2)$ accurate. Unfortunately, from Theorem 3.1, it is *unstable*.

Case 2. $R = (\alpha + i\beta)h^2 u_{xxxx}$.

The corresponding explicit scheme is

$$\frac{u_j^{n+1} - u_j^n}{k} = i\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}\right) + (\alpha + i\beta)h^2\left(\frac{u_{j+2}^n - 4u_{j+1}^n + 6u_j^n - 4u_{j-1}^n + u_{j-2}^n}{h^4}\right). \quad (3.8)$$

Theorem 3.2. *The scheme (3.8) is stable if and only if $\alpha < 0$ and*

$$r \leq \min(-2\alpha, \frac{-2\alpha}{16\alpha^2 + (4\beta - 1)^2}). \quad (3.9)$$

The least restrictive stability constraint is

$$r \leq \frac{1}{2}, \quad (3.10)$$

and is obtained when $\alpha = -\frac{1}{4}, \beta = \frac{1}{4}$.

Proof. The characteristic polynomial for (3.8) is

$$G = 1 - ir\eta + (\alpha + i\beta)r\eta^2,$$

where $\eta = 4\sin^2\frac{\omega h}{2}$. Thus we have

$$\begin{aligned} |G|^2 &= (1 + \alpha r\eta^2)^2 + (\beta r\eta^2 - r\eta)^2 \\ &= 1 + (r^2 + 2r\alpha)\eta^2 - 2r^2\beta\eta^3 + r^2(\alpha^2 + \beta^2)\eta^4. \end{aligned}$$

The condition $|G|^2 \leq 1$ reduces to

$$(r + 2\alpha) - 2r\beta\eta + r(\alpha^2 + \beta^2)\eta^2 \leq 0,$$

from which it follows directly that the condition on r is

$$r \leq g(\eta) \equiv \frac{-2\alpha}{\alpha^2\eta^2 + (\beta\eta - 1)^2}.$$

First we must have $\alpha < 0$. By differentiating $g(\eta)$, it can be verified that $g(\eta)$ cannot achieve its minimum within the interval $0 \leq \eta \leq 4$. Thus the condition on r reduces to

$$r \leq \min(g(0), g(4)),$$

Dissipative term R	Error	Stability	Remarks
0	$O(k,h^2)$	unstable	Euler
$(\alpha+i\beta)ku_{xx}$	$O(k,h^2)$	$2(\alpha^2k^2+(1+\beta k)^2)\le \alpha h^2$	unstable for small k and h
$(\alpha+i\beta)h^2u_{xx}$	$O(k,h^2)$	$k\le\frac{\alpha h^4}{2(\alpha^2h^4+(1+\beta h^2)^2)}$	$\alpha>0$
$(\alpha+i\beta)ku_{xxxx}$	$O(k,h^2)$	$k\le h^2\frac{(\beta+\sqrt{-\alpha(2\alpha^2+2\beta^2+\alpha)})}{4(\alpha^2+\beta^2)}$	$\alpha\le-\frac{1}{2},\beta>0;\alpha<-\frac{1}{2},\beta\le 0$
$-\frac{1}{2}ku_{xxxx}$	$O(k^2,h^2)$	unstable	Lax-Wendroff Analog
$(-\frac{1}{2}+i\frac{1}{2})ku_{xxxx}$	$O(k,h^2)$	$k\le\frac{h^2}{2}$	Least Restrictive Stability
$(\alpha+i\beta)h^2u_{xxxx}$	$O(k,h^2)$	$k\le h^2\min(-2\alpha,\frac{-2\alpha}{16\alpha^2+(4\beta-1)^2})$	$\alpha<0$
$-\frac{i}{12}h^2u_{xxxx}$	$O(k,h^4)$	unstable	4th order in h
$(-\frac{1}{4}+i\frac{1}{4})h^2u_{xxxx}$	$O(k,h^2)$	$k\le\frac{h^2}{2}$	Least Restrictive Stability

Table 1: Stability of Explicit Schemes for $u_t=iu_{xx}+R$.

which is exactly condition (3.9).

To make the right hand side of (3.9) as large as possible, one should take $\beta=\frac{1}{4}$. Condition (3.9) then reduces to

$$r\le\min(-2\alpha,-\frac{1}{8\alpha}).$$

From $-2\alpha=-\frac{1}{8\alpha}$, we obtain $\alpha=-\frac{1}{4}$ and hence (3.10).

∎

When $\alpha<0$, the truncation error of (3.8) is $O(k,h^2)$. It is interesting to note that if $\alpha=0$ and $\beta=-\frac{1}{12}$, the truncation error becomes $O(k,h^4)$ because the right hand side of (3.8) becomes a fourth order approximation to iu_{xx}. Unfortunately, by Theorem 3.2, this higher order scheme is *unstable*.

4. Comparison and Extensions

We summarize our results in Table 1 from which we can draw the following conclusions.

1. Schemes derived from the addition of dissipative terms of the form

$$(\alpha+i\beta)ku_{xx}\qquad \textit{and}\qquad (\alpha+i\beta)h^2u_{xx}$$

are impractical, whereas schemes derived from the addition of dissipative terms of the form

$$(\alpha+i\beta)ku_{xxxx}\qquad \textit{and}\qquad (\alpha+i\beta)h^2u_{xxxx}$$

are practical.

2. The schemes with the least restrictive stability requirements are

$$\frac{u_j^{n+1}-u_j^n}{k}=i\left(\frac{u_{j+1}^n-2u_j^n+u_{j-1}^n}{h^2}\right)+(-\frac{1}{2}+i\frac{1}{2})k\left(\frac{u_{j+2}^n-4u_{j+1}^n+6u_j^n-4u_{j-1}^n+u_{j-2}^n}{h^4}\right), \quad (4.1)$$

and

$$\frac{u_j^{n+1}-u_j^n}{k}=i\left(\frac{u_{j+1}^n-2u_j^n+u_{j-1}^n}{h^2}\right)+(-\frac{1}{4}+i\frac{1}{4})h^2\left(\frac{u_{j+2}^n-4u_{j+1}^n+6u_j^n-4u_{j-1}^n+u_{j-2}^n}{h^4}\right). \quad (4.2)$$

The stability criterion for both is

$$k\le\frac{h^2}{2}. \quad (4.3)$$

It is interesting to note that when $k=\frac{h^2}{2}$, then the two schemes are the same. However, if $k<\frac{h^2}{2}$, then the dissipative term R for scheme (4.1) is smaller than that for scheme (4.2).

3. Stable schemes derived from $(\alpha+i\beta)ku_{xxxx}$ and $(\alpha+i\beta)h^2u_{xxxx}$ have truncation error $O(k,h^2)$. Higher order schemes are necessarily unstable.

Using the techniques in ([9], Sec. 5.3 and 8.4), the above conclusions can be extended to the more general equation

$$u_t=ia(x,t)u_{xx}+b(x,t)u_x+c(x,t)u+f(x,t), \quad (4.4)$$

and more generally to the nonlinear equation

$$u_t=ia(x,t)u+g(x,t,u,u_x).$$

Here the functions $b(x,t), c(x,t)$ $f(x,t)$ and $g(x,t)$ may be complex valued functions and $a(x,t)$ is a real valued function. We list here the scheme for (4.4) corresponding to (4.2)

$$\begin{aligned}\frac{u_j^{n+1}-u_j^n}{k}&=ia_j^n\left(\frac{u_{j+1}^n-2u_j^n+u_{j-1}^n}{h^2}\right)\\&+\frac{1}{4}(-|a_j^n|+ia_j^n)h^2\left(\frac{u_{j+2}^n-4u_{j+1}^n+6u_j^n-4u_{j-1}^n+u_{j-2}^n}{h^4}\right)\\&+b_j^n\left(\frac{u_{j+1}^n-u_{j-1}^n}{2h}\right)+c_j^nu_j^n+f_j^n.\end{aligned} \quad (4.5)$$

Under a slightly weaker stability definition, namely that $||G||\le 1+O(k)$ [9], a sufficient condition for the stability of (4.5) is

$$k\le\frac{h^2}{2\max_x|a(x,t)|}. \quad (4.6)$$

Finally, since the dissipative terms in (4.1), (4.2) and (4.5) have five point stencils, we briefly comment on the choice of boundary conditions for these terms. The term

$$T=u_{j+2}^n-4u_{j+1}^n+6u_j^n-4u_{j-1}^n+u_{j-2}^n$$

can be written as

$$T = v_{j+1}^n - 2v_j^n + v_{j-1}^n,$$

where

$$v_j^n \equiv u_{j+1}^n - 2u_j^n + u_{j-1}^n.$$

For initial boundary value problems with $j = 0, 1, \cdots, J$, it can be shown that the stability condition (4.6) is not affected if we use as boundary condition for T

$$v_0^n = v_J^n = 0.$$

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