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Note

Stability Analysis of Finite Difference Schemes for Quantum Mechanical Equations of Motion

1. Introduction

Finite difference (FD) schemes are extensively employed to obtain approximate numerical solutions for initial boundary value problems representing a wide variety of physical phenomena. In the course of developing an FD scheme, for solving a time-dependent Kohn–Sham-type equation (given in Section 4) for ion–atom collisions [1], derived through density functional theory and quantum fluid dynamics [2, 3], we have observed that stability conditions are not laid down satisfactorily for partial differential equations containing i ($i^2 = -1$). In this note we examine this situation for two broad categories of problems and provide appropriate stability criteria for equations containing i. Note that all these equations contain both space and time variables.

Consider the FD schemes for the following equations:

$$\text{(i)} \qquad \frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial u}{\partial x} + cu; \qquad 0 \leqslant x \leqslant X,\ t \geqslant 0$$

$$u(0, t) = 0, \qquad u(X, t) = 0; \qquad t \geqslant 0$$

$$u(x, 0) = f(x); \qquad 0 \leqslant x \leqslant X. \tag{1}$$

$$\text{(ii)} \qquad i\frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial u}{\partial x} + cu; \qquad 0 \leqslant x \leqslant X,\ t \geqslant 0$$

$$u(0, t) = 0, \qquad u(X, t) = 0; \qquad t \geqslant 0$$

$$u(x, 0) = f(x); \qquad 0 \leqslant x \leqslant X. \tag{2}$$

Equation (1) describes, for example, diffusion processes in nature while Eq. (2) occurs in quantum mechanical equations of motion. In both (i) and (ii), the quantities a, b and c are functions of x, t or even u, thereby embracing both linear and nonlinear equations. However, for simplicity, most of our discussion will treat a, b, c as constants.

Although there are extensive discussions in the literature [4–6] of FD schemes for (i) and FD schemes for (ii) have been employed by a number of workers

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[7–10], there is, unfortunately, very little discussion on the efficacy of these schemes, epecially concerning their stability with regard to *both* space- and time-step sizes. In this note we will study the stability properties of FD schemes for (ii) and compare them with those of FD schemes for (i).

It is well known that any two-level FD scheme for such problems is of the form

$$\sum_{j \in N_1} \alpha_j u_j^{n+1} = \sum_{j \in N_2} \beta_j u_j^n, \tag{3}$$

where N_1, N_2 are sets of integers; n, j denote particular mesh points in time and space, respectively; N is the total number of space-steps, i.e.,

$$u_j^n = u(jh, n\,\Delta t); \qquad Nh = N\,\Delta x = X; \qquad j = 1, 2, ..., (N-1). \tag{4}$$

Von Neumann's method of testing stability, by using the *Fourier series method* (see Section 2), involves substitution of $\rho^n e^{ij\beta}$ for u_j^n into (3) and then ensuring $|\rho| \leqslant 1$ for stability [11]. The *matrix method* (see Section 3), on the other hand, involves obtaining $U^{n+1} = BU^n$ for the vector of unknowns at the spatial grid-points $\{u_j\}$. The method is stable if the matrix B is *convergent*, i.e., the magnitudes of all the eigenvalues of B are less than unity [12]. As noted in [4], the Fourier series method is not rigorous, in the sense that it does not take care of the boundary conditions, whereas the matrix method is a direct reflection of the actual computation process.

In what follows, the FD approximation for the spatial derivative in (1) and (2) is taken as

$$\mathscr{L}(u_j) = a(u_{j+1} - 2u_j + u_{j-1})/h^2 + b(u_{j+1} - u_{j-1})/2h + cu_j. \tag{5}$$

In Section 2, we will show that the Fourier series method of testing stability can lead to wrong conclusions for the FD scheme

$$iu_j^{n+1} = iu_j^n + \Delta t[\theta \mathscr{L}(u_j^{n+1}) + (1-\theta)\,\mathscr{L}(u_j^n)] \tag{6}$$

in solving (2). Here $\theta = 0$, $\frac{1}{2}$ and 1 signifies fully explicit, Crank–Nicolson and fully implicit schemes, respectively [4]. The stability analysis of these schemes reveals certain interesting features, especially regarding the choice of step-size in a spatial direction. These are presented in Section 3. Section 4 discusses the implications of these results with regard to FD schemes for solving quantum mechanical equations of motion.

2. Failure of the Fourier Series Method

In (6), substitution of $\rho^n e^{ij\beta}$ for u_j^n, followed by simplification, leads to the growth factor

$$\rho = \frac{i[1 + (1-\theta)\,\Delta t(b/h)\sin\beta] + (1-\theta)\,\Delta t[c - (4a/h^2)\sin^2(\beta/2)]}{i[1 - \theta\,\Delta t(b/h)\sin\beta] - \theta\,\Delta t[c - (4a/h^2)\sin^2(\beta/2)]}. \tag{7}$$

From (7), it appears that $|\rho| \leqslant 1$ if

$$(1-2\theta)\,\Delta t\left[\frac{b^2}{h^2}\sin^2\beta+\left(c-\frac{4a}{h^2}\sin^2\frac{\beta}{2}\right)^2\right]+\frac{2b}{h}\sin\beta<0 \tag{8}$$

for all β. This clearly indicates that (6) is *unstable* for $\theta<\frac{1}{2}$ (explicit schemes). Further, even the Crank–Nicolson scheme ($\theta=\frac{1}{2}$), which is known to be unconditionally stable when applied to solve heat diffusion equations [13], becomes *unstable for any step-size Δt.* We also note that stability limitations for $\theta>\frac{1}{2}$ (implicit schemes) *cannot be explicitly obtained.* The underlying reason for these curious observations is that the step-size in a spatial direction plays an important role in stability studies, which is not brought out by the Fourier series method. However, as seen below, the matrix method will clearly reveal the important limitations on *both* the step-sizes, Δt and Δx (i.e., h).

3. The Matrix Method

In matrix notation, one can write (6) as

$$U^{n+1}=BU^n, \tag{9}$$

where

$$B=[I-\Delta t\theta A]^{-1}[I+\Delta t(1-\theta)A]. \tag{10}$$

Here I is the $(N-1)\times(N-1)$ identity matrix and the $(N-1)\times(N-1)$ tridiagonal matrix A is given by

$$A=-i\begin{pmatrix} p & q & & & & [\bigcirc] \\ r & p & q & & & \\ 0 & r & p & q & & \\ & & & & & \\ & & & r & p & q \\ & [\bigcirc] & & 0 & r & p \end{pmatrix}. \tag{11}$$

In (11),

$$p=-\frac{2a}{h^2}+c;\qquad q=\frac{a}{h^2}+\frac{b}{2h};\qquad r=\frac{a}{h^2}-\frac{b}{2h} \tag{12}$$

Now, the eigenvalues $\{\lambda_s\}$ of A are [4]

$$\lambda_s=-i\left[p+2(qr)^{1/2}\cos\left(\frac{sh\pi}{X}\right)\right];\qquad s=1,2,\ldots,(N-1). \tag{13}$$

In order that the FD scheme be stable,

$$\left|\frac{1+\Delta t(1-\theta)\lambda_s}{1-\Delta t\theta\lambda_s}\right| \leqslant 1; \qquad s=1,2,\ldots,(N-1). \tag{14}$$

If the spatial step-size is chosen as

$$h<2\left|\frac{a}{b}\right|, \tag{15}$$

then λ_s is a pure imaginary number $i\mu_s(\mu_s$ real) and stability prevails if

$$1+(\Delta t)^2\mu_s^2(1-\theta)^2 \leqslant 1+(\Delta t)^2\mu_s^2\theta^2, \tag{16}$$

i.e., if $\theta \geqslant \frac{1}{2}$. For $\theta < \frac{1}{2}$, scheme (6) *is unstable for any step-size* Δt. We thus observe that the Crank–Nicolson scheme is *stable*, contrary to the conclusion reached by the Fourier series method.

Consider now the situation

$$h \geqslant 2\left|\frac{a}{b}\right|. \tag{17}$$

Then

$$\lambda_s = -i\left[p+i\gamma\cos\left(\frac{sh\pi}{X}\right)\right], \tag{18}$$

where

$$\gamma=\frac{2\,|a|}{h^2}\left[\left(\frac{bh}{2a}+1\right)\left(\frac{bh}{2a}-1\right)\right]^{1/2}. \tag{19}$$

The FD scheme is stable if

$$\left|\frac{1+\Delta t(1-\theta)[-ip+\gamma\cos(sh\pi/X)]}{1-\Delta t\,\theta[-ip+\gamma\cos(sh\pi/X)]}\right| \leqslant 1. \tag{20}$$

Condition (20) will be true if

$$\left[1+\Delta t(1-\theta)\,\gamma\cos\left(\frac{sh\pi}{X}\right)\right]^2+(\Delta t)^2(1-\theta)^2p^2 \leqslant \left[1-\Delta t\,\theta\gamma\cos\left(\frac{sh\pi}{X}\right)\right]^2+(\Delta t)^2\theta^2p^2, \tag{21}$$

i.e., if

$$f=(2\theta-1)\,\Delta t\left[\gamma^2\cos^2\left(\frac{sh\pi}{X}\right)+p^2\right]-2\gamma\cos\left(\frac{sh\pi}{X}\right) \geqslant 0. \tag{22}$$

Condition (22) will be valid only if

$$(1-2\theta)<0, \tag{23}$$

i.e.,

$$\theta > \tfrac{1}{2}.$$

For $\theta > \frac{1}{2}$, a minimum in f exists for

$$g=\cos\left(\frac{sh\pi}{X}\right)\in\left[0, \cos\left(\frac{h\pi}{X}\right)\right]. \tag{24}$$

Then

$$\frac{df}{dg}=2(2\theta-1)\,\Delta t\,\gamma^2 g-2\gamma=0. \tag{25}$$

In other words,

$$g_{\min}=\frac{1}{(2\theta-1)\gamma\,\Delta t}. \tag{26}$$

(Note that at $g_{\min}$, $d^2f/dg^2=2(2\theta-1)\,\Delta t\,\gamma^2=(+)ve.$)

Let f decrease with g increasing in $(0, \cos(h\pi/X)]$, with the minimum lying outside this interval. Then, in case

$$\Delta t<\frac{1}{(2\theta-1)\gamma\cos(h\pi/X)}, \tag{27}$$

condition (22) will be satisfied if

$$\Delta t \geqslant \frac{2\gamma\cos(h\pi/X)}{(2\theta-1)[\gamma^2\cos^2(h\pi/X)+p^2]}. \tag{28}$$

Alternatively, in case

$$\Delta t>\frac{1}{(2\theta-1)\,\gamma\cos(h\pi/X)}, \tag{29}$$

the stability condition (22) is satisfied if

$$(2\theta-1)\,\Delta t\left[\gamma^2\frac{1}{(2\theta-1)^2\gamma^2\,\Delta t^2}+p^2\right] -2\gamma\frac{1}{(2\theta-1)\gamma\,\Delta t}\geqslant 0, \tag{30}$$

i.e., if

$$\Delta t \geqslant \frac{1}{|(2\theta - 1)p|}. \tag{31}$$

Thus, we are led to the following two conditions, with stability prevailing in *either* of the two cases:

$$\text{(i)} \quad \Delta t \geqslant \max\left[\frac{1}{(2\theta-1)\gamma\cos(h\pi/X)}, \frac{1}{|(2\theta-1)p|}\right] \tag{32}$$

$$\text{(ii)} \quad \frac{2\gamma\cos(h\pi/X)}{(2\theta-1)[\gamma^2\cos^2(h\pi/X)+p^2]} \leqslant \Delta t \leqslant \frac{1}{(2\theta-1)\gamma\cos(h\pi/X)}. \tag{33}$$

Note that condition (32) is not physically meaningful. Hence, the implicit scheme is stable if the step-size Δt is chosen according to (33).

4. Discussion

We now make a few comparative remarks on the stability of FD schemes for problems (i) and (ii) in Section 1, with particular reference to (ii).

A. As θ increases, the hierarchy of schemes for (i) and (ii) is maintained. Explicit schemes for (ii) are *unconditionally unstable*, contrary to the conditional *stability* of explicit schemes for (i). Implicit schemes for (ii) are *conditionally stable* whereas the corresponding schemes for (i) are *unconditionally stable.*

B. Consider the use of the separation of variables technique for the following simplified versions of problems (i) and (ii):

$$\text{(iii)} \qquad u_t = \alpha u_{xx}; \qquad u \to 0 \text{ as } x \to 0, \infty \tag{34}$$

$$\text{(iv)} \qquad iu_t = \alpha u_{xx}; \qquad u \to 0 \text{ as } x \to 0, \infty, \tag{35}$$

where each subscript denotes one partial differentiation with respect to the variable. In order that the solutions be physically meaningful, the solution of the diffusion equation (34) contains time in the exponential part whereas the solution for (35) is trigonometric in both space and time variables. This implies that analytical solutions of equations of type (ii) are inherently stable, unlike those of type (i). Note also that, in case of simple diffusion equations, the difference equations for the error have solutions which are trigonometric in the space variable and exponential in the time variable. This exponential behaviour with respect to time is really decided by the *nature of the analytic solution* rather than the contention of O'Brien *et al.* [11], who say that "the one and only one solution which reduces to $e^{i\beta x}$ when $t=0$ is $e^{\alpha t}e^{i\beta x}$."

A special equation of type (ii) is the nonlinear Schrödinger (NLS) equation

$$iu_t = -u_{xx} \pm 2\,|u|^2\,u. \tag{36}$$

According to the discussion in Section 3, numerical solutions of this equation are stable.[1] In fact, the semi-discrete approximation

$$\frac{du_j}{dt} = -i[(u_{j+1} - 2u_j + u_{j-1})/h^2 + 2\,|u_j|^2 u_j] \tag{37}$$

is such that the eigenvalues of the Jacobian matrix of this system are purely imaginary. Accordingly, the solutions are trigonometric in nature and therefore bounded.

C. Price *et al.* [17] have considered problems of type (i), with $c = 0$. In this case, numerical solutions with $h > 2\,|b/a|$ give rise to spurious oscillations, although the fully implicit scheme is unconditionally stable and nonoscillatory for any step-size Δt. However, for problems of type (ii), with $h > 2\,|b/a|$, stability criteria for the implicit scheme impose certain restrictions on Δt (see Section 3).

Finally, as an example of a generalized NLS equation, two of us have recently derived [1] a time-dependent Kohn–Sham-type equation in three-dimensional space based on both density functional theory and quantum fluid dynamics [2, 3]. For a system with spherical symmetry, the equation can be transformed to

$$-\frac{1}{8x^2}\frac{\partial^2 y}{\partial x^2} + \frac{1}{8x^3}\frac{\partial y}{\partial x} + v_{\text{eff}}[y, t]\,y = i\frac{\partial y}{\partial t}. \tag{38}$$

By treating the variable coefficients as constants during stability analysis, one can readily show that any implicit scheme is stable because the eigenvalues of the matrix A (see Section 3) are always purely imaginary. For then, $h < |2a/b| = 2x$. Obviously, h is always less than $2x$, since the first mesh point contains the Dirichlet data and from the second mesh point onwards $h < 2x$.

5. Conclusion

We have shown that, for a partial differential equation involving both space and time variables, stability criteria change drastically if the equation contains i ($i^2 = -1$), as is the case with quantum mechanical equations of motion. The restriction on the step-size in time is not sufficient to ensure stability of the numerical solution. Indeed, the mesh structure in the space variable plays a very important

[1] It was first pointed out by Benjamin and Feir [14, 15] that, for the NLS equation, the solution of the hermitian eigenvalue problem with the (+) sign has real eigenvalues and hence "stable" solutions; solitons result from the "unstable" equation with the (−) sign [16]. This "instability" has a different meaning compared to the instability being considered in this paper, viz. the unbounded growth of error.

role and can lead to wrong results if not chosen properly, even if the step-size in time is quite small. It was also observed that, for such equations, the usual Fourier series method for stability analysis is inadequate, whereas the matrix method is satisfactory. It may be worthwhile to look for a general Fourier series method which can be applied to the stability of finite difference schemes for *any* partial differential equation.

The principal result in this paper, viz. the stability of FD schemes for quantum mechanical equations of motion depends on both spatial and temporal zoning, may also be understood on physical grounds. One may compare (i) a free particle Green's function (GF) to the solution of a simple diffusion equation (DE) and (ii) the quantum mechanical motion of a free particle to Fresnel diffraction in optics. In case (i), the time-dependence of the DE solution is exponential and thus a source point has a limited range of influence at later times. However, the GF is oscillatory in time so that source points influence the wavefunction even at relatively large distances. Clearly, the spatial grid should be fine enough to adequately account for these oscillations. In case (ii), the usual requirement that the mesh size in time should be larger than a constant times the square of the spatial grid size is related to the oscillations of the Fresnel integral at relatively short distances. This, in turn, is related to the frequency of oscillations of the GF.[2]

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