Abstract. We consider the stability of difference schemes for the solution of the initial boundary value problem for the equation

$$u_t = (A(x,t)u_x)_x + B(x,t)u_x + C(x,t)u + f(x,t),$$

where u, A, B, C and f are complex valued functions. Using energy methods, we establish the stability of a general two level scheme which includes Euler's method, Crank–Nicolson's method and the backward Euler method. If the coefficient $A(x,t)$ is purely imaginary, the explicit Euler's method is unconditionally unstable. For this case, we propose a new scheme with appropriately chosen artificial dissipation, which we prove to be conditionally stable.

Stability Analysis of Difference Schemes for Variable Coefficient Schrödinger Type Equations

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1. Introduction

Finite difference methods for the solution of equations of Schrödinger type have been studied by many authors, and extensively applied to solve practical problems in many disciplines [1, 5, 6, 7, 8, 9, 10, 11]. Since conventional explicit schemes are unstable [2, 4], implicit schemes are usually used, especially the Crank–Nicolson scheme. In [7], D.F. Griffiths et al discussed a predictor–corrector scheme. In [8, 12] the existence and convergence of solution for this difference equation have been studied. Since the solution of Schrödinger equation possesses conservation laws, the schemes which satisfy discrete conservation laws have also been investigated extensively [6, 7].

We consider the equation

$$u_t = (A(x,t)u_x)_x + B(x,t)u_x + C(x,t)u + f(x,t), \tag{1.1}$$

in the domain $Q_T(0 \leq x \leq l, \quad 0 \leq t \leq T)$, where $u(x,t)$, $A(x,t)$, $B(x,t)$, $C(x,t)$ and $f(x,t)$ are complex functions, and $\mathrm{Re}\, A(x,t) \geq 0$ and $|A(x,t)| \neq 0$. This kind of equation arises in plasma physics and acoustics [1, 11]. Clearly, (1.1) involves both equations of Schrödinger type and parabolic equations. In this paper, we consider the initial–boundary value problem for (1.1), with the conditions :

$$u_{|t=0} = \widetilde{u}(x) \tag{1.2}$$

$$u_{|x=0} = u_{|x=l} = 0, \tag{1.3}$$

where $\widetilde{u}(x)$ is a complex function.

In Section 2, we analyse the stability of a general two level difference scheme for (1.1), (1.2) and (1.3), which is a direct generalization of a well–known scheme for parabolic equations, and includes the explicit Euler scheme and the implicit Crank–Nicolson scheme as special members. Some new results are obtained from which we can see the relationship between the Schrödinger equation and the parabolic equation.

If $\mathrm{Re}\, A(x,t) \equiv 0$, the above mentioned explicit Euler scheme is unstable. Several interesting stable explicit schemes have been presented in [3] for the case of the simplified equation $u_t = iu_{xx}$, and applied to some underwater acoustics problem in [2]. In these schemes, Euler's method is stabilized by appropriately chosen artificial dissipation. In Section 4, we extend these results to equation (1.1).

We let h denote the spatial mesh size and divide the finite interval $[0,l]$ into the mesh intervals by the points $x_j = jh \quad (j = 0, 1, \ldots, J)$, where $Jh = l$. We let k_n denote the size of the time step at the n–th step. For convenience, we shall denote $u(x_j, t_n)$ by u_j^n. We also use the following difference operators :

$$u_{\bar{t}_j}^{n+1} = u_{t_j}^n = \frac{u_j^{n+1} - u_j^n}{k_n},$$

$$D_+ u_j = \frac{u_{j+1} - u_j}{h}, \qquad D_- u_j = \frac{u_j - u_{j-1}}{h},$$

$$D u_j = \frac{u_{j+1/2} - u_{j-1/2}}{h}, \qquad \widetilde{D} u_j = \frac{u_{j+1} - u_{j-1}}{2h} = \frac{1}{2}(D_+ + D_-)u_j.$$

Hence, we have

$$\frac{1}{h^2}(u_{j+1} - 2u_j + u_{j-1}) = D_+ D_- u_j = D^2 u_j.$$

$$\frac{1}{h^2}\left[A_{j+1/2}(u_{j+1} - u_j) - A_{j-1/2}(u_j - u_{j-1})\right] = D(ADu_j).$$

Finally, for any function ϕ, we use $\phi^{n+\alpha}$ to denote $\alpha\phi^{n+1} + (1-\alpha)\phi^n$, for $0 \le \alpha \le 1$.

Next, we give our definition of stability. First we define the inner product for u and v :

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

where $\bar{v}$ denotes the complex conjugate of v and the norm for u :

$$\|u\| = \sqrt{(u,u)} \quad .$$

Definition 1.1. We call a scheme stable if the solution u_j^n satisfies :

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

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

2. A General Two Level Scheme.

We are going to consider the following scheme for (1.1), (1.2) and (1.3) :

$$\begin{aligned} \frac{u_j^{n+1} - u_j^n}{k_n} &- \frac{1}{h^2}[A_{j+1/2}^{n+\alpha}(u_{j+1}^{n+\alpha} - u_j^{n+\alpha}) - A_{j-1/2}^{n+\alpha}(u_j^{n+\alpha} - u_{j-1}^{n+\alpha})] \\ &- B_j^{n+\alpha}\left(\frac{u_{j+1}^{n+\alpha} - u_{j-1}^{n+\alpha}}{2h}\right) - C_j^{n+\alpha} u_j^{n+\alpha} = f_j^{n+\alpha} \qquad j = 1, 2, \ldots, J-1 \end{aligned} \tag{2.1}$$

$$u_j^0 = \tilde{u}_j, \qquad j = 1, 2, \ldots, J-1. \tag{2.2}$$

$$u_0^n = u_J^n = 0, \qquad n = 0, 1, \ldots \tag{2.3}$$

We can also write (2.1) in this form :

$$u_{t_j}^{n+1} - DA^{n+\alpha}Du_j^{n+\alpha} - B_j^{n+\alpha}\widetilde{D}u_j^{n+\alpha} - C_j^{n+\alpha}u_j^{n+\alpha} = f_j^{n+\alpha}. \tag{2.4}$$

Clearly, (2.1) or (2.4) is explicit, implicit and the Crank–Nicolson scheme when $\alpha = 0$, $\alpha \neq 0$ and $\alpha = \frac{1}{2}$, respectively.

We will see that this scheme is unstable if $\mathrm{Re}\, A(x,t) = 0$ and $\alpha = 0$. In this case, we will give another conditionally stable explicit scheme in Section 3.

To facilitate the analysis, we first transform (2.1) by a change of variable to eliminate the first order term.

Lemma 2.1. *Suppose $A \in C^3$, $B \in C^2$, $C \in C^1$ and $Re A \geq 0$, $|A| \geq a_0 > 0$, then we can choose a function ϕ, such that $0 < M_0 \leq |\phi_j| \leq M_1$, $j = 0, 1, \cdots, J$ where M_0 and M_1 are constants and under the transformation*

$$u_j^{n+\alpha} = \phi_j^{n+\alpha} v_j^{n+\alpha} \tag{2.5}$$

(2.1) becomes :

$$\begin{aligned} L(v^{n+\alpha}) \equiv \frac{v_j^{n+1} - v_j^n}{k_n} &- \frac{1}{h^2}\left[A_{j+1/2}^{n+\alpha}(v_{j+1}^{n+\alpha} - v_j^{n+\alpha}) - A_{j-1/2}^{n+\alpha}(v_j^{n+\alpha} - v_{j-1}^{n+\alpha})\right] \\ &- G_{j-1}^{n+\alpha}v_{j-1}^{n+\alpha} - H_j^{n+\alpha}v_j^{n+\alpha} - K_{j+1}^{n+\alpha}v_{j+1}^{n+\alpha} - Q_j^{n+\alpha}v_j^{n+1-\alpha} = F_j^{n+\alpha} \end{aligned} \tag{2.6}$$

where G_j, H_j, K_j, Q_j, F_j are bounded in Q_T.

Proof. See Appendix A.

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We now state our main stability result for (2.6).

Theorem 2.1. *Suppose the conditions in Lemma 2.1 are satisfied. If $\frac{1}{2} \leq \alpha \leq 1$, then scheme (2.1) is stable.*

Proof. In order to establish the stability of (2.6), we are going to estimate $\|v^{n+1}\|$. We multiply (2.6) by $\bar{v}_j^{n+\alpha}$ to obtain :

$$(L(v^{n+\alpha}), v^{n+\alpha}) = (F^{n+\alpha}, v^{n+\alpha}) \quad . \tag{2.7}$$

Then we estimate every term in (2.7). For the first term, we have :

$$\begin{aligned}
\mathrm{Re}\,(v_{\bar{t}}^{n+1}, v^{n+\alpha}) &= \alpha \mathrm{Re}\,(v_{\bar{t}}^{n+1}, v^{n+1}) + (1-\alpha)\mathrm{Re}\,(v_{\bar{t}}^{n+1}, v^{n}) \\
&= \frac{\alpha}{k_n}\sum |v_j^{n+1}|^2 - \left(\frac{1-\alpha}{k_n}\right)\sum |\bar{v}_j^n|^2 \\
&\quad - \frac{\alpha}{k_n}\mathrm{Re}\sum v_j^n \bar{v}_j^{n+1} + \frac{(1-\alpha)}{k_n}\mathrm{Re}\sum v_j^{n+1}\bar{v}_j^n \\
&= \frac{1}{2k_n}(\sum |v_j^{n+1}|^2 - \sum |v_j^n|^2) - \frac{(1-2\alpha)}{2k_n}\sum |v_j^{n+1} - v_j^n|^2 \\
&= \frac{1}{2k_n}(\|v^{n+1}\|^2 - \|v^n\|^2) - \frac{(1-2\alpha)}{2}k_n \|v_{\bar{t}}^{n+1}\|^2.
\end{aligned} \tag{2.8}$$

For the second term, we have

$$\begin{aligned}
\mathrm{Re}\,(DA^{n+\alpha}Dv\,, v^{n+\alpha}) &= -\mathrm{Re}\,(A^{n+\alpha}D_- v^{n+\alpha}, D_- v^{n+\alpha}) \\
&= -\|\sqrt{\mathrm{Re}\,A^{n+\alpha}}D_- v^{n+\alpha}\|^2.
\end{aligned} \tag{2.9}$$

For the rest of the terms on the left hand side of (2.7), we have

$$\begin{aligned}
|G_{j-1}^{n+\alpha} v_{j-1}^{n+\alpha} \bar{v}_j^{n+\alpha}| &\le \frac{|G_{j-1}^{n+\alpha}|}{2}(|v_{j-1}^{n+\alpha}|^2 + |v_j^{n+\alpha}|^2) \\
|H_j^{n+\alpha} v_j^{n+\alpha} \bar{v}_j^{n+\alpha}| &\le \frac{|H_j^{n+\alpha}|}{2}(|v_j^{n+\alpha}|^2 + |\bar{v}_j^{n+\alpha}|^2) \\
|K_{j+1}^{n+\alpha} v_{j+1}^{n+\alpha} \bar{v}_j^{n+\alpha}| &\le \frac{|K_{j+1}^{n+\alpha}|}{2}(|v_{j+1}^{n+\alpha}|^2 + |\bar{v}_j^{n+\alpha}|^2) \\
|Q_j^{n+\alpha} v_j^{n+1-\alpha} \bar{v}_j^{n+\alpha}| &\le |Q_j^{n+\alpha}|\left[(1-\alpha)|v_j^{n+1}| + \alpha|v_j^n|\right]\left[\alpha|v_j^{n+1}| + (1-\alpha)|v_j^n|\right] \\
&\le \frac{|Q_j^{n+\alpha}|}{2}\left(|v_j^{n+1}|^2 + |v_j^n|^2\right).
\end{aligned}$$

So we have

$$\begin{aligned}
&\left|\mathrm{Re}\left[\sum G_{j-1}^{n+\alpha} v_{j-1}^{n+\alpha} \bar{v}_j^{n+\alpha} + \sum H_j^{n+\alpha} v_j^{n+\alpha} \bar{v}_j^{n+\alpha} + \sum K_{j+1}^{n+\alpha} v_{j+1}^{n+\alpha} \bar{v}_j^{n+\alpha} + \sum Q_j^{n+\alpha} v_j^{n+1-\alpha} \bar{v}_j^{n+\alpha}\right]\right| \\
&\qquad \le M_2\left[\|v^{n+\alpha}\|^2 + \|v^{n+\alpha}\|^2 + \|v^{n+\alpha}\|^2 + \frac{1}{2}\|v^{n+1}\|^2 + \frac{1}{2}\|v^n\|^2\right] \\
&\qquad = 3M_2\|v^{n+\alpha}\|^2 + \frac{M_2}{2}\|v^{n+1}\|^2 + \frac{M_2}{2}\|v^n\|^2,
\end{aligned} \tag{2.10}$$

where M_2 is a constant which is an upper bound of $|G|$, $|H|$, $|K|$ and $|Q|$.

For the right hand side of (2.7), we get

$$|Re\,(F^{n+\alpha}, v^{n+\alpha})| \le \frac{1}{2}\|v^{n+\alpha}\|^2 + \frac{1}{2}\|F^{n+\alpha}\|^2 \quad . \tag{2.11}$$

Now we substitute expressions (2.8), (2.9), (2.10) and (2.11) into (2.7) and obtain

$$\begin{aligned}
\frac{1}{2k_n}(\|v^{n+1}\|^2 - \|v^n\|^2) - \left(\frac{1-2\alpha}{2}\right) k_n \|v_{\bar{t}}^{n+1}\|^2 + \|\sqrt{Re\, A^{n+\alpha}} D_- v^{n+\alpha}\|^2 & \\
\leq 3M_2\|v^{n+\alpha}\|^2 + \frac{M_2}{2}\|v^{n+1}\|^2 + \frac{M_2}{2}\|v^n\|^2 + \frac{1}{2}\|v^{n+\alpha}\|^2 + \frac{1}{2}\|F^{n+\alpha}\|^2 & \\
\leq M_3(\|v^{n+1}\|^2 + \|v^n\|^2) + \frac{1}{2}\|F^{n+\alpha}\|^2, &
\end{aligned} \tag{2.12}$$

where

$$M_3 = 6M_2 + \frac{M_2}{2} + 1 \quad .$$

When $\frac{1}{2} \leq \alpha \leq 1$, from expression (2.12) we have

$$\frac{1}{2k_n}(\|v^{n+1}\|^2 - \|v^n\|^2) \leq M_3(\|v^{n+1}\|^2 + \|v^n\|^2) + \frac{1}{2}\|F^{n+\alpha}\|^2.$$

It is easy to see that when $k_n \leq \frac{1}{4M_3}$ we have

$$\begin{aligned}
\|v^{n+1}\|^2 &\leq \frac{1+2k_nM_3}{1-2k_nM_3}\|v^n\|^2 + 2k_n\|F^n\|^2 \\
&\leq (1+8k_nM_3)\|v^n\|^2 + 2k_n\|F^n\|^2.
\end{aligned}$$

According to Lemma 4.1 in Appendix B, we obtain

$$\|v^{n+1}\|^2 \leq 2e^{8M_3t^{n+1}}\left[\|v_0\|^2 + \sum_{l=0}^{n}\|F^l\|^2 k_l\right]. \tag{2.13}$$

From (2.5) and $0 < M_0 \leq |\phi_j| \leq M_1$ we obtain

$$\|u^{n+1}\|^2 \leq 2\frac{M_1^2}{M_0^2}e^{8M_3t^{n+1}}\left[\|u_0\|^2 + \sum_{l=0}^{n}\|f^l\|^2 k_l\right]. \tag{2.14}$$

∎

Now we turn to discuss the case $0 \leq \alpha < \frac{1}{2}$.

Theorem 2.2. *If* $0 \leq \alpha < \frac{1}{2}$ *and*

$$k_n \leq \frac{1}{2(1-2\alpha)\left[\frac{1}{h^2}\max_x \frac{|A^{n+\alpha}|^2}{Re\,A^{n+\alpha}} + \frac{1}{\eta}\right]} \tag{2.15}$$

where η *is an arbitrary positive constant then the scheme (2.1) is stable.*

Proof. First let

$$P_{1j} = \frac{1}{h^2}|A^{n+\alpha}_{j+1/2}|\,|v^{n+\alpha}_{j+1} - v^{n+\alpha}_{j}|$$
$$P_{2j} = \frac{1}{h^2}|A^{n+\alpha}_{j-1/2}|\,|v^{n+\alpha}_{j} - v^{n+\alpha}_{j-1}|$$
$$P_{3j} = |G^{n+\alpha}_{j-1}|\,|v^{n+\alpha}_{j-1}|$$
$$P_{4j} = |H^{n+\alpha}_{j}|\,|v^{n+\alpha}_{j}|$$
$$P_{5j} = |K^{n+\alpha}_{j+1}|\,|v^{n+1-\alpha}_{j+1}|$$
$$P_{6j} = |Q^{n+\alpha}_{j}|\,|v^{n+\alpha}_{j}|$$
$$P_{7j} = |F^{n+\alpha}_{j}|.$$

From (2.6) we obtain immediately

$$|v^{n+1}_{\bar{t}_j}|^2 \le \left(\sum_{l=1}^{7} P_{lj}\right)^2 . \tag{2.16}$$

Next we construct a quadratic form in P_{lj} $(l = 1, \cdots, 7)$ by :

$$P_j = \frac{h^2\,Re\,A^{n+\alpha}_{j+1/2}}{|A^{n+\alpha}_{j+1/2}|^2}P^2_{1j} + \frac{h^2\,Re\,A^{n+\alpha}_{j-1/2}}{|A^{n+\alpha}_{j-1/2}|^2}P^2_{2j} + 5\eta\sum_{l=3}^{7}P^2_{lj} - (1-2\alpha)k_n\left(\sum_{l=1}^{7}P_{lj}\right)^2 \tag{2.17}$$

where η is an arbitrary positive constant. According to Lemma 4.2 (in Appendix C), P_j is nonnegative if

$$k_n \le \frac{1}{(1-2\alpha)\left[\frac{|A^{n+\alpha}_{j+1/2}|^2}{h^2\,Re\,A^{n+\alpha}_{j+1/2}} + \frac{|A^{n+\alpha}_{j-1/2}|^2}{h^2\,Re\,A^{n+\alpha}_{j-1/2}} + \frac{1}{\eta}\right]} , \tag{2.18}$$

which is true because of (2.15). Making this assumption, we have from (2.16) :

$$(1-2\alpha)k_n|v^{n+1}_{\bar{t}j}|^2 \le \left(\frac{h^2\,Re\,A^{n+\alpha}_{j+1/2}}{|A^{n+\alpha}_{j+1/2}|^2}\right)P^2_{1j} + \left(\frac{h^2\,Re\,A^{n+\alpha}_{j-1/2}}{|A^{n+\alpha}_{j-1/2}|^2}\right)P^2_{2j} + 5\eta\sum_{l=3}^{7}P^2_{lj}.$$

Summing up these expressions from $j = 1$ to $j = J-1$, we obtain

$$(1-2\alpha)k_n\|v^{n+1}_{\bar{t}}\|^2 \le 2\|\sqrt{Re\,A^{n+\alpha}}D_-v^{n+\alpha}\|^2 + 5\eta M_2^2(3\|v^{n+\alpha}\|^2 + \|v^{n+1-\alpha}\|^2) + 5\eta\|F^{n+\alpha}\|^2.$$

$$\le 2\|\sqrt{Re\,A^{n+\alpha}}D_-v^{n+\alpha}\|^2 + 40\eta M_2^2(\|v^{n+1}\|^2 + \|v^n\|^2) + 5\eta\|F^{n+\alpha}\|^2 \tag{2.19}$$

Substituting (2.19) into (2.12), we have

$$\frac{1}{k_n}(\|v^{n+1}\|^2 - \|v^n\|^2) \le M_4(\|v^{n+1}\|^2 + \|v^n\|^2) + M_5\|F^{n+\alpha}\|^2,$$

where $M_4 = 2M_3 + 40\eta M_2^2$ and $M_5 = 1 + 5\eta$. It is easy to see that when $k_n \le \frac{1}{2M_4}$, then

$$\begin{aligned}\|v^{n+1}\| &\le \frac{1+k_nM_4}{1-k_nM_4}\|v^n\|^2 + \frac{M_5k_n}{1-k_nM_4}\|F^{n+\alpha}\|^2 \\ &\le (1+4k_nM_4)\|v^n\|^2 + 2M_5k_n\|F^{n+\alpha}\|^2 \quad .\end{aligned}$$

According to Lemma 4.1, we obtain

$$\|v^{n+1}\|^2 \le e^{4M_4t^{n+1}}(\|u^0\|^2 + 2M_5\sum_{l=0}^{n}\|F^{l+\alpha}\|^2k_l) \tag{2.20}$$

and from (2.5) and $0 < M_0 \le |\phi| \le M$, we obtain

$$\|u^{n+1}\|^2 \le \frac{M_1^2}{M_0^2}e^{4M_4t^{n+1}}(\|u^0\|^2 + 2M_5\sum_{l=0}^{n}\|F^{l+\alpha}\|^2k_l) \tag{2.21}$$

which implies that the scheme (2.1) is stable.

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3. A stable explicit scheme for the case $Re\,A \equiv 0$.

In this section, we assume $Re\,A \equiv 0$ and let $a(x,t)$ denote the imaginary part of A. We see from the previous section that the scheme (2.1) with $\alpha = 0$ is unstable. This is unfortunate because in many applications an explicit scheme is desirable because they tend to be easier to implement, especially in a vector or parallel computing environment. In [2], we construct a stable explicit scheme for the simple equation $u_t = iu_{xx}$ by adding appropriately chosen artificial dissipative terms to (2.1). Here we consider an extension of this scheme for the more general equation (1.1). We construct the following scheme :

$$\begin{aligned}\frac{u_j^{n+1}-u_j^n}{k_n} &- ia_j^n\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} - \frac{(ia_j^n - |a_j^n|)}{4}(v_{j+1}^n - 2v_j^n + v_{j-1}^n) \\ &- B_j^n\frac{u_{j+1}^n - u_{j-1}^n}{2h} - C_j^nu_j^n = f_j, \quad j = 1,\ldots,J-1,\end{aligned} \tag{3.1}$$

where

$$v_j^n = \frac{1}{h^2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n), \quad j = 1,\ldots,J-1, \tag{3.2}$$

with

$$v_0 = v_J = 0. \tag{3.3}$$

We will prove that this scheme is conditionally stable. For convenience, we assume

1.

$$a_j > 0, \quad j = 0,1,\ldots,J. \tag{3.4}$$

2.
$$\max\left(|a|, \left|\frac{\partial a}{\partial x}\right|, \left|\frac{\partial^2 a}{\partial x^2}\right|, |B|, \left|\frac{\partial B}{\partial x}\right|, |C|\right) \le M. \tag{3.5}$$

We shall need the following lemmas :

Lemma 3.1. *(Discrete Sobolev inequality)*

Given $\epsilon > 0$, there exists a constant c dependent on ϵ and n such that

$$\|D^l u\|_{L_\infty} \le \epsilon \|D^n u\|_{L_2} + c\|u\|_{L_2} \quad l < n, \tag{3.6}$$

$$\|D^l u\|_{L_2} \le \epsilon \|D^n u\|_{L_2} + c\|u\|_{L_2} \quad l \le n. \tag{3.7}$$

Lemma 3.2. *(Estimate $\|u_{\bar{t}}^n\|$).*

For any $\epsilon > 0$ there exists a constant K dependent on ϵ, such that the solution u_j^n of (3.1) satisfies :

$$\|u_{\bar{t}}^{n+1}\|^2 \le \sum_{j=1}^{J-1} (a_j^n)^2 |D^2 u_j^n|^2 + \epsilon \|D^2 u^n\|^2 + K(\epsilon)\left[\|u^n\|^2 + \|f^n\|^2\right]. \tag{3.8}$$

Proof. From (3.1), we have

$$\|u_{\bar{t}}^{n+1}\|^2 = \sum_{j=1}^{J-1} \left\{ \left[i a_j^n D^2 u_j^n + \frac{1}{4}(i-1) a_j^n D^2 v_j^n + G_j^n \right] \cdot \left[-i a_j^n D^2 \bar{u}_j^n + \frac{1}{4}(-i-1) a_j^n D^2 \bar{v}_j^n + \bar{G}_j^n \right] \right\}$$

where

$$G_j = B_j D u_j + c_j u_j + f_j. \tag{3.9}$$

Expanding the above expression, we have

$$\|u_{\bar{t}}^{n+1}\|^2 = \sum_{j=1}^{J-1} \{(a_j^n)^2 |D^2 u_j^n|^2 + \frac{1}{2} Re\left[(1-i)(a_j^n)^2 h^2 D^2 u_j^n \cdot D^2 \bar{v}_j^n\right] + \frac{1}{8}(a_j^n)^2 h^4 |D^2 v_j^n|^2\}$$
$$+ 2Re \sum_{j=1}^{J-1} [i a_j^n D^2 u_j^n + \frac{1}{4}(i-1) a_j^n h^2 D^2 v_j^n] \bar{G}_j^n \quad .$$

Using (3.3), we obtain

$$h^2 \sum_{j=1}^{J-1} (a_j^n)^2 D^2 u_j^n D^2 \bar{v}_j^n$$
$$= \sum_{j=1}^{J-1} v_j^n [(a_{j+1}^n)^2 (\bar{v}_{j+1}^n - \bar{v}_j^n) - (a_j^n)^2 (\bar{v}_j^n - \bar{v}_{j-1}^n) - ((a_{j+1}^n)^2 - (a_j^n)^2)(\bar{v}_{j+1}^n - \bar{v}_j^n)]$$
$$= \sum_{j=2}^{J-1} v_{j-1}^n a_j^n (\bar{v}_j^n - \bar{v}_{j-1}^n) - \sum_{j=1}^{J-1} v_j^n (a_j^n)^2 (\bar{v}_j^n - \bar{v}_{j-1}^n) - \sum_{j=1}^{J-1} v_j^n ((a_{j+1}^n)^2 - (a_j^n)^2)(\bar{v}_{j+1}^n - \bar{v}_j^n)$$
$$= -\sum_{j=1}^{J} (a_j^n)^2 |v_j^n - v_{j-1}^n|^2 - \sum_{j=1}^{J-1} ((a_{j+1}^n)^2 - (a_j^n)^2) v_j^n (\bar{v}_{j+1}^n - \bar{v}_j^n).$$

Hence

$$\frac{1}{2}\sum_{j=1}^{J-1} Re\left[(1-i)(a_j^n)^2h^2D^2u_j^n\cdot D^2\bar{v}_j^n\right]+\frac{1}{8}\sum_{j=1}^{J-1}(a_j^n)^2h^4|D^2v_j^n|^2$$

$$\le -\frac{1}{2}\sum_{j=1}^{J}(a_j^n)^2|v_j^n-v_{j-1}^n|^2+\left|\sum_{j=1}^{J-1}((a_{j+1}^n)^2-(a_j^n)^2)v_j^n(\bar{v}_{j+1}^n-\bar{v}_j^n)\right|$$

$$+\frac{1}{4}\sum_{j=1}^{J-1}(a_j^n)^2[|v_{j+1}^n-v_j^n|^2+|v_j^n-v_{j-1}^n|^2]$$

$$\le \left|\sum_{j=1}^{J-1}((a_{j+1}^n)^2-(a_j^n)^2)v_j^n(\bar{v}_{j+1}^n-\bar{v}_j^n)\right|-\frac{1}{4}\sum_{j=1}^{J}((a_j^n)^2-a_{j-1}^{n^2})|v_j^n-v_{j-1}^n|^2$$

$$\le 2\sum_{j=1}^{J-1}|(a_{j+1}^n)^2-(a_j^n)^2|\,|v_j^n|\,|v_{j+1}^n-v_j^n|.$$

So

$$\|u_{\bar{t}}^{n+1}\|^2\le\sum_{j=1}^{J-1}(a_j^n)^2|D^2u_j^n|^2+2\sum_{j=1}^{J-1}|(a_{j+1}^n)^2-(a_j^n)^2|\,|v_j^n|\,|v_{j+1}^n-v_j^n|$$

$$+2Re\sum_{j=1}^{J-1}\left[ia_j^nD^2u_j^n+\frac{1}{4}(i-1)a_j^nh^2D^2v_j^n\right]\bar{G}_j^n.$$

For G_j, using Lemma 3.1, we have

$$\|\bar{G}^n\|^2\le 3M^2(\|Du^n\|^2+\|u^n\|^2)+3\|f^n\|^2$$

$$\le 6M^2\epsilon_1\|D^2u^n\|^2+(6M^2K(\epsilon_1)+3M^2)\|u^n\|^2+3\|f^n\|^2,$$

where $\epsilon_1>0$. It follows that if we define

$$Q\equiv 2Re\sum_{j=1}^{J-1}\left[ia_j^nD^2u_j^n+\frac{1}{4}(i-1)a_j^nh^2D^2v_j^n\right]\bar{G}_j^n,$$

we have

$$Q\le 6M\|D^2u^n\|\,\|\bar{G}^n\|$$

$$\le 3M\left[\epsilon_2\|D^2u^n\|^2+\frac{1}{\epsilon_2}\|G^n\|^2\right]$$

$$=\left[3M\epsilon_2+\frac{18M^3\epsilon_1}{\epsilon_2}\right]\|D^2u^n\|^2+\frac{1}{\epsilon_2}\left[18M^3K(\epsilon_1)+9M^3\right]\|u^n\|^2+\frac{9M}{\epsilon_2}\|f^n\|^2,$$

where ϵ_2 is any positive constant. If we define ϵ_1 by

$$\epsilon_1=\frac{\epsilon^2}{864M^4}\quad,$$

and ϵ_2 by

$$\epsilon_2 = \frac{\epsilon}{12M} \quad ,$$

then we have

$$Q \le \frac{\epsilon}{2}\|D^2u^n\|^2 + K_1(\epsilon)\left[\|u^n\|^2 + \|f^n\|^2\right].$$

where $K_1(\epsilon)$ is a constant dependent on ϵ. On the other hand using Lemma 3.1,

$$\begin{aligned}
2\sum_{j=1}^{J-1} |(a_{j+1}^n)^2 - (a_j^n)^2|\,|v_j^n|\,|v_{j+1}^n - v_j^n| &\le 8M^2h\|v^n\|^2 \\
&\le 8M^2h\left[\epsilon_3\|D^2u^n\|^2 + K_2(\epsilon_3)\|u^n\|^2\right] \\
&= 8M^2h\epsilon_3\|D^2u^n\|^2 + 8M^2hK_2(\epsilon_3)\|u^n\|^2 \quad ,
\end{aligned}$$

where ϵ_3 is an arbitrary positive constant. If we take

$$\epsilon_3 = \frac{\epsilon}{16M^2h} \quad ,$$

then we have

$$2\sum_{j=1}^{J-1} |(a_{j+1}^n)^2 - (a_j^n)^2|\,|v_j^n|\,|v_{j+1}^n - v_j^n| \le \frac{\epsilon}{2}\|D^2u^n\|^2 + K_3(\epsilon)\|u^n\|^2 \quad .$$

where $K_3(\epsilon)$ is a constant dependent on ϵ. Combining the above results, we finally have

$$\|u_{\bar{t}}^{n+1}\|^2 \le \sum_{j=1}^{J-1}(a_j^n)^2|D^2u_j^n|^2 + \epsilon\|D^2u^n\|^2 + K_4(\epsilon)\|u^n\|^2 + K_1(\epsilon)\|f^n\|^2,$$

where

$$K_4(\epsilon) = K_1(\epsilon) + K_3(\epsilon) \quad ,$$

which completes the proof.

∎

Theorem 3.1. *If (3.4) holds and*

$$\min|a(x)| > \beta > 0 \tag{3.10}$$

then the scheme of (3.1) is stable if

$$k_n < \frac{1}{2}\frac{h^2}{\max|a|} \quad . \tag{3.11}$$

Proof. Multiply (3.1) by $\bar{u}_j^n$ and we obtain

$$(Lu^n, u^n) = (f^n, u^n). \tag{3.12}$$

Next we estimate each term in (3.12). For the first term we have

$$Re\,(u_{\bar{t}}^{n+1}, u^n) = \frac{1}{2k_n}(\|u^{n+1}\|^2 - \|u^n\|^2) - \frac{k_n}{2}\|u_{\bar{t}}^{n+1}\|^2,$$

which is similar to (2.8). Applying Lemma 3.2, we obtain, for any $\epsilon > 0$,

$$Re\,(u_{\bar{t}}^{n+1}, u^n) \geq \frac{1}{2k_n}(\|u^{n+1}\|^2 - \|u^n\|^2) - \frac{k_n}{2}\left[\sum_{j=1}^{J-1}(a_j^n)^2|D^2u_j^n|^2 + \epsilon\|D^2u^n\|^2 + k_4\|u^n\|^2 + k_1\|f^n\|^2\right]. \tag{3.13}$$

The second term is given by

$$I_2 = \sum_{i=1}^{J-1}\left(-ia_j^n\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}\cdot \bar{u}_j^n\right).$$

We first employ the following expansion :

$$\begin{aligned} a_j^n\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} &= \frac{1}{h^2}\left[a_{j+1/2}^n(u_{j+1}^n - u_j^n) - a_{j-1/2}^n(u_j^n - u_{j-1}^n)\right] \\ &\quad + \frac{1}{h^2}\left[(a_j^n - a_{j+1/2}^n)(u_{j+1}^n - u_j^n) - (a_j^n - a_{j-1/2}^n)(u_j^n - u_{j-1}^n)\right]. \end{aligned}$$

Then, using the boundary conditions, we have :

$$\begin{aligned} &\sum_{j=1}^{J-1}\frac{1}{h^2}\left[a_{j+1/2}^n(u_{j+1}^n - u_j^n) - a_{j-1/2}^n(u_j^n - u_{j-1}^n)\right]\bar{u}_j^n \\ &\quad = \sum_{j=1}^{J-1}\frac{1}{h^2}a_{j+1/2}^n(u_{j+1}^n - u_j^n)\bar{u}_j^n - \sum_{j=0}^{J-2}a_{j+1/2}^n(u_{j+1}^n - u_j^n)\bar{u}_{j+1}^n \\ &\quad = -\frac{1}{h^2}\sum_{j=0}^{J-1}a_{j+1/2}^n|u_{j+1}^n - u_j^n|^2 \quad , \end{aligned}$$

and

$$\begin{aligned} &\left|\sum_{j=1}^{J-1}\frac{1}{h^2}\left[(a_j^n - a_{j+1/2}^n)(u_{j+1}^n - u_j^n) - (a_j^n - a_{j-1/2}^n)(u_j^n - u_{j-1}^n)\right]\bar{u}_j^n\right| \\ &\quad \leq \frac{1}{2}\sum_{j=1}^{J-1}\left|\frac{(u_{j+1}^n - u_j^n)}{h}\right|^2 + \frac{1}{2}\sum_{j=1}^{J-1}\left|\frac{(a_j^n - a_{j+1/2}^n)}{h}\right|^2|u_j^n|^2 + \frac{1}{2}\sum_{j=1}^{J-1}\left|\frac{(u_j^n - u_{j-1}^n)}{h}\right|^2 \\ &\quad\quad + \frac{1}{2}\sum_{j=1}^{J-1}\left|\frac{(a_j^n - a_{j-1/2}^n)}{h}\right|^2|u_j^n|^2 \\ &\quad \leq 2[\epsilon\|D^2u^n\|^2 + c_2\|u^n\|^2] + M^2\|u^n\|^2 \\ &\quad \leq 2\epsilon\|D^2u^n\|^2 + (2c_2 + M^2)\|u^n\|^2. \end{aligned}$$

Hence we have

$$|Re\, I_2| \le 2\epsilon \|D^2 u^n\|^2 + (2c_2 + M^2)\|u^n\|^2.$$

The third term is given by

$$I_3 = \sum_{i=1}^{J-1} \left(-\frac{(ia_j^n - |a_j^n|)}{4} (v_{j+1}^n - 2v_j^n + v_{j-1}^n) \cdot \bar{u}_j^n \right).$$

Using the expression :

$$\begin{aligned} \frac{(1-i)}{4} a_j^n \frac{(v_{j+1}^n - 2v_j^n + v_{j-1}^n)}{h^2} &= \frac{(1-i)}{4} \frac{1}{h^2} \left[a_{j+1}^n v_{j+1}^n - 2a_j^n v_j^n + a_{j-1}^n v_{j-1}^n \right] \\ &+ \frac{(1-i)}{4} \frac{1}{h^2} \left[(a_j^n - a_{j+1}^n) v_{j+1}^n + (a_j^n - a_{j-1}^n) v_{j-1}^n \right] \quad , \end{aligned}$$

we have

$$\begin{aligned} h^2 \frac{(1-i)}{4} \sum_{j=1}^{J-1} \frac{1}{h^2} &\left[a_{j+1}^n v_{j+1}^n - 2a_j^n v_j^n + a_{j-1}^n v_{j-1}^n \right] \bar{u}_j^n \\ &= h^2 \frac{(1-i)}{4} \left[\frac{1}{h^2} \sum_{j=1}^{J-1} a_j^n v_j^n (\bar{u}_{j+1}^n - \bar{u}_j^n + \bar{u}_{j-1}^n) \right] \\ &= h^2 \frac{(1-i)}{4} \sum_{j=1}^{J-1} a_j^n |v_j^n|^2 \quad , \end{aligned}$$

and

$$\begin{aligned} \Big| \frac{(1-i)}{4} h^2 \sum_{j=1}^{J-1} \frac{1}{h^2} &\left[(a_j^n - a_{j+1}^n) v_{j+1}^n + (a_j^n - a_{j-1}^n) v_{j-1}^n \right] \bar{u}_j^n \Big| \\ &\le \frac{h}{2} \sum_{j=1}^{J-1} \Big| \frac{a_j^n - a_{j+1}^n}{h} \Big| \, |v_{j+1}^n| \, |u_j^n| + \frac{h}{2} \sum_{j=1}^{J-1} \Big| \frac{a_j^n - a_{j-1}^n}{h} \Big| \, |v_{j-1}^n| \, |u_j^n| \\ &\le Mh[\epsilon \|v^n\|^2 + \frac{1}{\epsilon} \|u^n\|^2] \\ &= h\epsilon M \|v^n\|^2 + \frac{Mh}{\epsilon} \|u^n\|^2 \quad . \end{aligned}$$

The rest of the terms are easily bounded :

$$\begin{aligned} \Big| \sum_{j=1}^{J-1} B_j^n \frac{u_{j+1}^n - u_{j-1}^n}{2h} \cdot \bar{u}_j^n \Big| &\le M \|Du^n\| \, \|u^n\| \\ &\le \frac{M}{2} \left[\epsilon \|D^2 u^n\|^2 + K_2(\epsilon) \|u^n\|^2 \right] \quad , \end{aligned}$$

$$|(cu, u)| \le M \|u\|^2$$

and

$$|(f, u)| \le \frac{1}{2} \|f\|^2 + \frac{1}{2} \|u\|^2 \quad .$$

Summing all the above terms, we get

$$\frac{1}{2k_n}(\|u^{n+1}\|^2 - \|u^n\|^2)$$
$$\leq \sum_{j=1}^{J-1}\left(\frac{k_n}{2}(a_j^n)^2 - \frac{h^2}{4}a_j^n\right)|D^2u_j^n|^2 + \left[\frac{k_n}{2}\epsilon + 2\epsilon + h\epsilon M + \frac{M\epsilon}{2}\right]\|D^2u^n\|^2$$
$$+\left[\frac{k_n}{2}K_4 + 2c_2 + M^2 + \frac{Mh}{\epsilon} + \frac{Mk_2}{2} + M + \frac{1}{2}\right]\|u^n\|^2 + \left[\frac{k_n}{2}K_1 + \frac{1}{2}\right]\|f^n\|^2.$$

Of course, when (3.11) holds, we have

$$\frac{k_n}{2}(a_j^n)^2 - \frac{h^2}{4}a_j^n \leq -\frac{\beta^2\triangle}{2}.$$

where

$$\triangle = \frac{h^2}{2\max|a|} - k_n > 0.$$

As long as ϵ is small enough, we can make

$$\frac{k_n}{2}\epsilon + 2\epsilon + k\epsilon M + \frac{M\epsilon}{2} \leq \frac{\beta^2\triangle}{2}.$$

For such an ϵ, we have

$$\frac{1}{2k_n}(\|u^{n+1}\|^2 - \|u^n\|^2) \leq \widetilde{M_1}\|u^n\|^2 + \widetilde{M_2}\|f^n\|^2.$$

Here the constants $\widetilde{M_1}$, $\widetilde{M_2}$ depend on $\triangle$ and M. Using Lemma 2.1, we have the proof.

∎

4. Concluding Remarks

Using energy methods, we have established the stability properties of the two schemes considered in this paper. Since equation (1.1) includes both parabolic and Schrödinger type equations as special cases, our stability results provide a unified treatment for both types of equations. Finally, the results here agree with the stability results obtained for the constant coefficient Cauchy problem via Fourier analysis [3, 4].

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Appendix

Appendix A (Proof of Lemma 2.1)

We substitute (2.5) into (2.1) and get, for the first term :

$$\begin{aligned}
u_{\bar{t}_j}^{n+1} &= (\phi v)_{\bar{t}_j}^{n+1} \\
&= \frac{1}{k}\left[\phi_j^{n+\alpha}(v_j^{n+1}-v_j^n) + (\phi_j^{n+1}-\phi_j^{n+\alpha})v_j^{n+1} + (\phi_j^{n+\alpha}-\phi_j^n)v_j^n\right] \\
&= \frac{1}{k}\left[\phi_j^{n+\alpha}(v_j^{n+1}-v_j^n) + (\phi_j^{n+1}-\phi_j^n)((1+\alpha)v_j^{n+1}+\alpha v_j^n)\right] \\
&= \phi_j^{n+\alpha} v_{\bar{t}_j}^{n+1} + v_j^{n+1-\alpha}\phi_{\bar{t}_j}^{n+1}.
\end{aligned}$$

In the following, for simplicity, we shall drop the index "$n+\alpha$". For the second term using the expressions

$$\begin{aligned}
\phi_{j+1} &= \phi_j + \widetilde{D}\phi_j h + \frac{1}{2}D_+D_-\phi_j h^2 \\
\phi_{j-1} &= \phi_j - \widetilde{D}\phi_j h + \frac{1}{2}D_+D_-\phi_j h^2,
\end{aligned}$$

we obtain :

$$\begin{aligned}
D(ADu_j) &= D(AD(\phi v)_j) \\
&= \frac{\phi_j}{h^2}\left[A_{j+1/2}(v_{j+1}-v_j) - A_{j-1/2}(v_j-v_{j-1})\right] \\
&\quad + \frac{1}{2h^2}\left[A_{j+1/2}(\phi_{j+1}-\phi_{j-1})v_{j+1} - A_{j-1/2}(\phi_{j+1}-\phi_{j-1})v_{j-1}\right] \\
&\quad + \frac{(\phi_{j+1}-2\phi_j+\phi_{j-1})}{2h^2}(A_{j+1/2}v_{j+1}+A_{j-1/2}v_{j-1}) \\
&= \frac{\phi_j}{h^2}\left[A_{j+1/2}(v_{j+1}-v_j) - A_{j-1/2}(v_j-v_{j-1})\right] + \frac{(\phi_{j+1}-\phi_{j-1})}{2h^2}A_j(v_{j+1}-v_{j-1}) \\
&\quad + \frac{(\phi_{j+1}-\phi_{j-1})}{2h^2}\left[(A_{j+1/2}-A_j)v_{j+1} + (A_j - A_{j-1/2})v_{j-1}\right] \\
&\quad + \frac{(\phi_{j+1}-2\phi_j+\phi_{j-1})}{2h^2}(A_{j+1/2}v_{j+1}+A_{j-1/2}v_{j-1}) \\
&= \phi_j DADv_j + 2A_j\widetilde{D}\phi_j\widetilde{D}v_j + \left[\frac{A_{j+1/2}-A_j}{h}v_{j+1} + \frac{A_j - A_{j-1/2}}{h}v_{j-1}\right]\widetilde{D}\phi_j \\
&\quad + \frac{(A_{j+1/2}v_{j+1}+A_{j-1/2}v_{j-1})}{2}D^2\phi_j.
\end{aligned}$$

For third term using the expressions

$$\phi_{j+1} = \phi_j + D_+\phi_j h, \qquad \phi_{j-1} = \phi_j - D_-\phi_j h$$

we obtain

$$\begin{aligned}
B_j\widetilde{D}u_j &= \frac{B_j}{2h}(\phi_{j+1}v_{j+1} - \phi_{j-1}v_{j-1}) \\
&= B_j\phi_j\widetilde{D}v_j + \frac{B_j}{2}(D_+\phi_j v_{j+1} + D_-\phi_j v_{j-1}) \quad .
\end{aligned}$$

In the second and third term, the first order difference term for v is $(2A_j\widetilde{D}\phi_j + B_j\phi_j)\widetilde{D}v_j$. We can choose ϕ_j to make this term vanish by setting

$$2A_j\widetilde{D}\phi_j + B_j\phi_j = 0. \tag{1}$$

Since $|A| \geq a_0 > 0$ and A, B are bounded, it is easy to see that we can choose ϕ_j such that $0 < M_0 \leq |\phi_j| \leq M_1$, where M_0, M_1 are constants. Moreover, from (1) and $|\phi_j| \leq M_1$, we have

$$|\widetilde{D}\phi_j| \leq \text{constant} \qquad \text{in} \quad Q_T.$$

If we take the finite difference of (1), then because of the assumptions on A ,B, we can obtain

$$|D_+D_-\phi_j| \leq \text{constant} \qquad \text{in} \quad Q_T.$$

After some manipulation, we obtain (2.6), where

$$\begin{aligned}
G_{j-1}^{n+\alpha} &= \frac{1}{\phi_j^{n+\alpha}}\left[\widetilde{D}\phi_j^{n+\alpha}\frac{(A_j^{n+\alpha} - A_{j-1/2}^{n+\alpha})}{h} + \frac{1}{2}D_+D_-\phi_j^{n+\alpha}A_{j-1/2}^{n+\alpha} + \frac{b_j^{n+\alpha}}{2}\widetilde{D}\phi_j^{n+\alpha}\right]\\
H_j^{n+\alpha} &= C_j^{n+\alpha}\\
K_{j+1}^{n+\alpha} &= \frac{1}{\phi_j^{n+\alpha}}\left[\widetilde{D}\phi_j^{n+\alpha}\frac{(A_{j+1/2}^{n+\alpha} - A_j^{n+\alpha})}{h} + \frac{1}{2}D_+D_-\phi_j^{n+\alpha}A_{j+1/2}^{n+\alpha} + \frac{b_j^{n+\alpha}}{2}\widetilde{D}\phi_j^{n+\alpha}\right]\\
Q_j^{n+\alpha} &= -\frac{\phi_{\bar{t}_j}^{n+1}}{\phi_j^{n+\alpha}}\\
F_j^{n+\alpha} &= \frac{f_j^{n+\alpha}}{\phi_j^{n+\alpha}}.
\end{aligned}$$

Because of the properties of A, B, C, F and ϕ, the functions G, H, K, Q and F are all bounded.

Appendix B

Lemma 4.1. *(Duhamel's Principle).*

Assume $u^n \geq 0$, $v^n \geq 0$ *for* $n = 1, 2, \ldots$.

If $u^{n+1} \leq (1 + Mk_n)u^n + k_n v^n, \quad n = 0, 1, \ldots,$

then

$$u^{n+1} \leq e^{Mt^{n+1}}\left(u^0 + \sum_{l=0}^{n} v^l k_l\right) \quad . \tag{2}$$

Here M *is a positive constant and* $t^{n+1} = \sum_{l=0}^{n} k_l$.

Proof.

We have

$$\begin{aligned}
u^{n+1} \leq & (1+Mk_n)u^n + k_n v^n \\
\leq & (1+Mk_n)[(1+Mk_{n-1})u^{n-1} + k_{n-1}v^{n-1}] + k_n v^n \\
\leq & \prod_{l=0}^{n}(1+Mk_l)u^0 + \sum_{l=0}^{n-1}\prod_{s=l+1}^{n}(1+Mk_s)k_l v^l + k_n v^n \\
\leq & \prod_{l=0}^{n}(1+Mk_l)u^0 + \sum_{l=0}^{n-1}\prod_{s=0}^{n}(1+Mk_s)k_l v^l + k_n v^n \\
\leq & \exp\left[\sum_{l=0}^{n}\ln(1+Mk_l)\right]\cdot\left[u^0 + \sum_{l=0}^{n} v^l k_l\right] \quad .
\end{aligned}$$

Since $\ln(1+Mk_l) \leq Mk_l$, we obtain (2).

∎

Appendix C

Lemma 4.2. *Assume* $m_i \geq 0 \quad (i = 1, \cdots, n)$ *and* $k > 0$. *The necessary and sufficient condition for the polynomial in* p_i

$$\sum_{i=1}^{n} m_i p_i^2 - k(\sum_{i=1}^{n} p_i)^2 \tag{3}$$

to be nonnegative definite, is

$$k \leq \frac{1}{\sum_{i=1}^{n}\frac{1}{m_i}} \quad . \tag{4}$$

Proof. Define $p = (p_1, \cdots, p_n)^T$, $l = (1, 1, \cdots, 1)^T$ and $D = diagonal(m_1, m_2, \cdots, m_n)$. Then the polynomial in (3) can be rewritten as

$$p^T Dp - k(p^T l)^2 = p^T(D - kll^T)p$$

The condition for the matrix $D - kll^T$ to be nonnegative definite is $1 - kl^T D^{-1} l \geq 0$ which is (4).

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