FINITE DIFFERENCE DISCRETIZATION OF THE CUBIC SCHRÖDINGER EQUATION

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Abstract. We analyze the discretization of an initial-boundary value problem for the cubic Schrödinger equation in one space dimension by a Crank–Nicolson–type finite difference scheme. We then linearize the corresponding equations at each time level by Newton's method and discuss an iterative modification of the linearized scheme which requires solving linear systems with the same tridiagonal matrix. We prove second-order error estimates.

1. Introduction

For $T > 0$ and λ a nonzero real number, we consider the following initial-boundary value problem for the cubic Schrödinger equation: We seek a complex-valued function u defined on $[0,1] \times [0,T]$ satisfying

$$
\begin{aligned}
&u_t = \mathrm{i}u_{xx} + \mathrm{i}\lambda|u|^2 u && \text{in} \quad [0,1]\times[0,T],\\
&u(0,\cdot) = u(1,\cdot) = 0 && \text{on} \quad [0,T],\\
&u(\cdot,0) = u_0 && \text{in} \quad [0,1],
\end{aligned}
\tag{1.1}
$$

where u_0 is a complex-valued initial value. We assume that (1.1) admits a unique solution which is smooth enough for our purposes.

For the mathematical theory and the physical significance of the cubic Schrödinger equation we refer to Strauss [6] and Strauss [7]. It is well-known that

$$
\forall t \in [0,T] \quad \|u(\cdot,t)\| = \|u_0\|,
\tag{1.2}
$$

and

$$
\forall t \in [0,T] \quad \|u_x(\cdot,t)\|^2 - \frac{\lambda}{2}|u(\cdot,t)|_4^4 = \|u_0\|^2 - \frac{\lambda}{2}|u_0|_4^4,
\tag{1.3}
$$

where $|\cdot|_p, p \neq 2$, denotes the L^p-norm over $[0,1]$, and $\|\cdot\|$ the L^2-norm. To obtain (1.2) and (1.3) multiply the Schrödinger equation by $\bar{u}$ —the complex conjugate of u — and by $\mathrm{i}\bar{u}_t$, respectively, then integrate by parts over $[0,1]$, use the boundary conditions and finally take real parts.

In our one dimensional situation it is also easily seen that the solution u of (1.1) does not blow up. In fact, denoting by $H_0^1(0,1)$ the Sobolev space of complex-valued

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functions belonging, together with their distributional derivatives, to $L^2(0,1)$ and vanishing at the endpoints 0 and 1, and using the well-known and easily established Sobolev inequality

$$|v|_4^4 \le \|v\|^3\,\|v'\| \quad \forall v \in H_0^1(0,1), \tag{1.4}$$

and (1.2), we obtain

$$\forall t \in [0,T] \quad |u(\cdot,t)|_4^4 \le c\|u_x(\cdot,t)\|, \tag{1.5}$$

with $c := 2\|u_0\|^3$. From (1.3), (1.5) follows the existence of a constant C such that

$$\max\big\{\|u_x(\cdot,t)\|, |u(\cdot,t)|_4 : t \in [0,T]\big\} < C.$$

Using the well-known inequality $|v|_\infty \le \|v'\|$ for $v \in H_0^1(0,1)$, we conclude that

$$\sup\big\{|u(x,t)| : 0 < x < 1, 0 < t < T\big\} < C$$

with a constant C independent of T.

Several numerical methods have been proposed in the literature for discretizing the cubic Schrödinger equation, see, e.g., Akrivis, Dougalis & Karakashian [1], Delfour, Fortin & Payre [2], Griffiths, Mitchell & Morris [3], Karakashian, Akrivis & Dougalis [4], Sanz-Serna [5], Tourigny & Morris [9], Verwer & Sanz-Serna [10], Weideman & Herbst [11] and the references therein. In this paper we discretize (1.1) by a Crank–Nicolson-type finite difference method, and analyze a linearization of the scheme by Newton's method. This Crank-Nicolson-type scheme has been proposed for the equation at hand by Delfour, Fortin & Payre [2]; the spatial discretization of the nonlinear term is motivated by a method of Strauss & Vasquez [8]. Dirichlet boundary conditions serve here as a model case; periodic or Neumann conditions can be analyzed with no additional complications.

Let $N, J \in \mathbb{N}, h := 1/(J+1), k := T/N, x_j := jh, j = 0,\dots,J+1$, and $t^n := nk, t^{n+1/2} := (n+1/2)k, u_j^n := u(x_j,t^n), u^n := (u_0^n,\dots,u_{J+1}^n)$, $n = 0,\dots,N$. Let $\mathbb{C}_0^{J+2} := \big\{v = (v_0,\dots,v_{J+1}) \in \mathbb{C}^{J+2} : v_0 = v_{J+1} = 0\big\}$ and for $v \in \mathbb{C}_0^{J+2}$ set $\varDelta_h v_0 := \varDelta_h v_{J+1} := 0$, $\varDelta_h v_j := (v_{j-1} - 2v_j + v_{j+1})/h^2, j = 1,\dots,J$. For $v^0,\dots,v^N \in \mathbb{C}_0^{J+2}$ we set $v^{n+1/2} := (v^{n+1}+v^n)/2$ and $\partial v^n := (v^{n+1}-v^n)/k$. Setting $U^0 := u^0$, we define approximations $U^n \in \mathbb{C}_0^{J+2}$ of u^n recursively by

$$\partial U_j^n = \mathrm{i}\varDelta_h U_j^{n+1/2} + \mathrm{i}\lambda\varphi(U_j^{n+1}, U_j^n), \quad j = 1,\dots,J, \tag{1.6}$$

$n = 0,\dots,N-1$, where $\varphi(z,w) := \big(|z|^2+|w|^2\big)(z+w)/4, z,w \in \mathbb{C}$, see Delfour, Fortin & Payre [2]. It is easily seen that this method is conservative in a discrete L^2-norm; specifically

$$\|U^n\|_h = \|U^0\|_h, \quad n = 1,\dots,N,$$

where $\|v\|_h := \big(h\sum_{j=1}^J |v_j|^2\big)^{\frac12}$ for $v \in \mathbb{C}_0^{J+2}$. A discrete analog of (1.3) holds as well, see (2.3) below. The scheme (1.6) has been extensively used in computations.

In section 2 we show existence and for k small enough (independent of h) uniqueness of the approximate solutions and derive the error estimate

$$\max_{1\le n\le N} \|u^n - U^n\|_h \le c(k^2+h^2), \tag{1.7}$$

where here and in the sequel c and C denote generic constants independent of k and h, not necessarily the same at any two places unless indices are used. In section 3 we use Newton's method to linearize the scheme (1.6). We extrapolate from previous time levels to construct suitable starting values and perform one Newton iteration at each time level. Second-order estimates for the linearized scheme are also given. A disadvantage of this method is that the matrix of the linear system to be solved at each time level t^n changes with n. To overcome this, in section 4, we solve approximately these systems by an "inner" iterative procedure that requires solving linear systems with a tridiagonal matrix, the same at each time level. Although the overall scheme is not theoretically conservative any more, it performs well numerically. In our computations in the case of three inner iterations at each time level the discrete L^2-norm $\|\cdot\|_h$ was conserved to a satisfactory accuracy. We show second-order error estimates for this efficient scheme as well.

This paper is similar in spirit to Akrivis, Dougalis & Karakashian [1] where analogous results for the midpoint scheme in the finite element case are derived. In the error analysis of the linearized schemes in Akrivis, Dougalis & Karakashian [1] the approximations of the linearized schemes are compared to the approximations of the nonlinear scheme. Here we compare the approximations of the linearized schemes directly to the exact solution and simplify the error analysis considerably.

2. Crank–Nicolson-type discretization

Existence. To show existence of the approximations $U^1,\dots,U^N$ for the scheme (1.6) we shall use the following Brouwer-type theorem, cf. Akrivis, Dougalis & Karakashian [1].

Lemma 2.1. *Let $\big(H,(\cdot,\cdot)\big)$ be a finite dimensional inner product space, $\|\cdot\|$ the associated norm, and $g: H\to H$ be continuous. Assume moreover that*

$$\exists \alpha>0\ \forall z\in H\ \ \|z\|=\alpha \quad \operatorname{Re}\big(g(z),z\big)\ge 0.$$

Then, there exists a $z^*\in H$ such that $g(z^*)=0$ and $\|z^*\|\le\alpha$. □

For $v,w\in\mathbb{C}_0^{J+2}$, we define

$$|v|_{1,h} := \Big[h\sum_{j=0}^{J}\Big|\frac{v_{j+1}-v_j}{h}\Big|^2\Big]^{1/2}, \quad \|v\|_{h,p} := \Big[h\sum_{j=1}^{J}|v_j|^p\Big]^{1/p}, \quad p\ge 1,$$

$(v,w)_h := h\sum_{j=1}^J v_j\bar w_j$, and $\|v\|_h := (v,w)_h^{\frac12} = \|v\|_{h,2}$. For fixed n, we rewrite (1.6) in the form

$$U_j^{n+1/2} = U_j^n + \frac{\mathrm{i}k}{2}\Delta_h U_j^{n+1/2} + \frac{\mathrm{i}k\lambda}{4}\big(|2U_j^{n+1/2}-U_j^n|^2+|U_j^n|^2\big)U_j^{n+1/2}, \quad j=1,\dots,J.$$

The mapping $\Pi : \mathbb{C}_0^{J+2} \to \mathbb{C}_0^{J+2}$

$$\big(\Pi(v)\big)_j := v_j - U_j^n - \frac{\mathrm{i}k}{2}\Delta_h v_j - \frac{\mathrm{i}k\lambda}{4}\big(|2v_j - U_j^n|^2 + |U_j^n|^2\big)v_j, \quad j = 1, \dots, J,$$

is obviously continuous. Since for $v \in \mathbb{C}_0^{J+2}$

$$-\,(\Delta_h v, v)_h = |v|_{1,h}^2, \tag{2.1}$$

we have $\mathrm{Re}(\Pi(v), v)_h = \|v\|_h^2 - \mathrm{Re}(U^n, v)_h$, i.e.,

$$\mathrm{Re}(\Pi(v), v)_h \geq \|v\|_h\big(\|v\|_h - \|U^n\|_h\big).$$

Hence, for $\|v\|_h = \|U^n\|_h + 1, \mathrm{Re}(\Pi(v), v)_h > 0$, and the existence of U^{n+1} follows from Lemma 2.1.

Conservation. Taking in (1.6) the inner product with $U^{n+1/2}$, using (2.1) and taking real parts, we obtain $\|U^{n+1}\|_h = \|U^n\|_h$, i.e.,

$$\|U^n\|_h = \|U^0\|_h, \quad n = 1, \dots, N. \tag{2.2}$$

Thus, a discrete analog of (1.2) holds, i.e., the scheme (1.6) is conservative. Taking in (1.6) the inner product with $U^{n+1} - U^n$, using (2.1) and taking imaginary parts, we see that

$$|U^n|_{1,h}^2 - \frac{\lambda}{2}\,\|U^n\|_{h,4}^4 = |U^0|_{1,h}^2 - \frac{\lambda}{2}\,\|U^0\|_{h,4}^4, \quad n = 1, \dots, N. \tag{2.3}$$

which is a discrete analog of (1.3), see Delfour, Fortin & Payre [2].

Uniqueness. For k small enough (independent of h), we shall show global uniqueness of the approximations $U^1, \dots, U^N$ satisfying (1.6). We shall only use the regularity assumption $u_0 \in H_0^1(0,1)$. First, the following Sobolev-type inequality holds

$$\forall v \in \mathbb{C}_0^{J+2} \quad \|v\|_{h,4}^4 \leq 2\|v\|_h^3\,|v|_{1,h}, \tag{2.4}$$

cf. (1.4). This follows immediately from the inequalities

$$\|v\|_{h,4}^4 \leq \max_j |v_j|^2\,\|v\|_h^2 \quad \text{and} \quad \max_j |v_j|^2 \leq 2\|v\|_h\,|v|_{1,h}, \quad v \in \mathbb{C}_0^{J+2},$$

the first one being trivial and the second one following from

$$|v_j|^2 = \sum_{i=0}^{j-1} v_i(\bar{v}_{i+1} - \bar{v}_i) + \sum_{i=0}^{j-1} \bar{v}_{i+1}(v_{i+1} - v_i),$$

by applying the Schwarz inequality. Let now $v, w \in \mathbb{C}_0^{J+2}$ be such that $\Pi(v) = \Pi(w) = 0$. Setting $\chi := v - w$, we obviously have

$$\chi_j = \frac{\mathrm{i}k}{2}\Delta_h\chi_j + \frac{\mathrm{i}k\lambda}{4}\big[\psi(v_j, w_j) + |U_j^n|^2\chi_j\big], \quad j = 1, \dots, J, \tag{2.5}$$

where

$\psi(v_j, w_j) := |2v_j - U_j^n|^2 v_j - |2w_j - U_j^n|^2 w_j$, and $\psi(v, w) := \big(\psi(v_0, w_0), \dots, \psi(v_{J+1}, w_{J+1})\big)$.

Taking in (2.5) the inner product with χ, using (2.1), taking real and imaginary parts, respectively, and using Hölder's inequality in the right-hand sides of the resulting identities, we obtain

$$\|\chi\|_h^2 \le \frac{k}{4}|\lambda|\|\psi(v,w)\|_{h,\frac{4}{3}}\|\chi\|_{h,4} \tag{2.6a}$$

$$|\chi|_{1,h}^2 \le \frac{|\lambda|}{2}\|\psi(v,w)\|_{h,\frac{4}{3}}\|\chi\|_{h,4} + \frac{|\lambda|}{2}\|U^n\|_{h,4}^2\|\chi\|_{h,4}^2. \tag{2.6b}$$

Using $\big||2z_1 - z|^2 z_1 - |2z_2 - z|^2 z_2\big| \le 4\big(|z_1| + |z_2| + \frac{1}{2}|z|\big)^2 |z_1 - z_2|$ for $z_1, z_2, z \in \mathbb{C}$, and applying Hölder's inequality, we have

$$\|\psi(v,w)\|_{h,\frac{4}{3}} \le c\|v,w,U^n\|_{h,4}^2\|\chi\|_{h,4},$$

where $\|v,w,U^n\|_{h,4} := \max\big(\|v\|_{h,4}, \|w\|_{h,4}, \|U^n\|_{h,4}\big)$, and c is a numerical constant. This estimate, inserted in (2.6) yields

$$\|\chi\|_h^2 \le c_1|\lambda|k\|v,w,U^n\|_{h,4}^2\|\chi\|_{h,4}^2, \tag{2.7a}$$

$$|\chi|_{1,h}^2 \le c_2|\lambda|\,\|v,w,U^n\|_{h,4}^2\|\chi\|_{h,4}^2, \tag{2.7b}$$

where c_1, c_2 are numerical constants. Further, for initial value $u_0 \in H_0^1(0,1)$ obviously holds

$$|U^0|_{1,h} \le \|u_0'\|. \tag{2.8}$$

From (2.4), (2.2) follows $\|U^m\|_{h,4}^4 \le c|U^m|_{1,h}, m = 0,\dots,N$. Then, (2.3), (2.8) yield $|U^m|_{1,h}^2 - \lambda c|U^m|_{1,h} \le C$; we conclude

$$|U^m|_{1,h} + \|U^m\|_{h,4} \le c, \quad m = 0,\dots,N,$$

i.e., $\|v,w,U^n\|_{h,4} \le c$. Then, using (2.4), (2.7), we obtain

$$\|\chi\|_{h,4}^4 \le c\lambda^2 k^{\frac{3}{2}}\|\chi\|_{h,4}^4,$$

i.e., uniqueness for k sufficiently small.

Convergence. Setting $M := \max\big\{|u(x,t)| : (x,t) \in [0,1]\times[0,T]\big\} + 1$, we define the auxiliary function $\tilde\varphi : \mathbb{C}\times\mathbb{C} \to \mathbb{C}$ by

$$\tilde\varphi(z,w) := \begin{cases} \varphi(z,w) & \text{if } |z|, |w| \le M, \\ \dfrac{1}{4}(M^2 + |w|^2)(z+w) & \text{if } |z| > M, |w| \le M, \\ \dfrac{1}{4}(M^2 + |z|^2)(z+w) & \text{if } |z| \le M, |w| > M, \\ \dfrac{1}{2}M^2(z+w) & \text{if } |z|, |w| > M. \end{cases}$$

$\tilde\varphi$ is obviously globally Lipschitz continuous. Let $V^0 := u^0$ and $V^n \in C_0^{J+2}, n = 1,\dots,N$, satisfy

$$\partial V_j^n = \mathrm{i}\Delta_h V_j^{n+1/2} + \mathrm{i}\lambda\tilde\varphi(V_j^{n+1}, V_j^n), \quad j = 1,\dots,J. \tag{2.9}$$

Existence of $V^n, n = 1,\dots,N$, can be shown using Lemma 2.1, and uniqueness for k sufficiently small (independent of h) follows from the global Lipschitz continuity of $\tilde\varphi$.

Proposition 2.1. *Let the solution u of* (1.1) *be smooth enough, and $V^1,\dots,V^N$ satisfy* (2.9)*. Then, for k small enough,*

$$\max_{1\le n\le N} \|u^n - V^n\|_h \le c(k^2+h^2), \tag{2.10}$$

with a constant independent of h and k.

Proof. Let $r^n \in \mathbb{C}_0^{J+2}$ be the consistency error of the method (1.6) (or (2.9)), i.e., with $u^{n+1/2} = (u^{n+1}+u^n)/2$

$$r_j^n := \partial u_j^n - \mathrm{i}\Delta_h u_j^{n+1/2} + \mathrm{i}\lambda\tilde\varphi(u_j^{n+1},u_j^n), \quad j=1,\dots,J. \tag{2.11}$$

It is easily seen that

$$\max_{j,n} |r_j^n| \le C(k^2+h^2). \tag{2.12}$$

Let $e^n := u^n - V^n, n = 0,\dots,N$. Then we have

$$\partial e_j^n = \mathrm{i}\Delta_h e_j^{n+1/2} + \mathrm{i}\lambda\big[\tilde\varphi(u_j^{n+1},u_j^n)\tilde\varphi(V_j^{n+1},V_j^n)\big] + r_j^n, \quad j=1,\dots,J. \tag{2.13}$$

Taking the inner product with $e^{n+1/2}$, using (2.1), taking real parts and applying the Schwarz inequality we obtain using the Lipschitz continuity of $\tilde\varphi$

$$\|e^{n+1}\|_h^2 - \|e^n\|_h^2 \le Ck\big[\|e^{n+1}\|_h + \|e^n\|_h + \|r^n\|_h\big]\|e^{n+1/2}\|_h,$$

i.e.,

$$(1-ck)\|e^{n+1}\|_h \le (1+ck)\|e^n\|_h + Ck(k^2+h^2).$$

The result follows in view of Gronwall's discrete inequality. □

The main result in this section is given in the following theorem.

Theorem 2.1. *Let the solution u of* (1.1) *be smooth enough, $U^1,\dots,U^N$ satisfy* (1.7)*, and $k = o(h^{1/4})$. Then, for k small enough*

$$\max_{1\le n\le N} \|u^n - U^n\|_h \le c(k^2+h^2). \tag{2.14}$$

Proof. Using the obvious inequality

$$\max_{1\le j\le J} |\omega_j| \le h^{-\frac12}\|\omega\|_h \tag{2.15}$$

for $\omega \in \mathbb{C}_0^{J+2}$, (2.10) yields

$$\max_{1\le n\le N}\max_{1\le j\le J} |u_j^n - V_j^n| \le Ch^{-\frac12}(k^2+h^2),$$

i.e., for k,h sufficiently small $|V_j^n| \le M, n=1,\dots,N, j=1,\dots,J$. Therefore the V^n satisfy (1.6), i.e., for k small enough $V^n = U^n$, and the result follows from (2.10). □

3. Linearization by Newton's method

Computing the approximations $U^1,\dots,U^N$ satisfying (1.6) requires solving at each time level a $J\times J$ nonlinear system. In this section we shall analyze the approximate solution of these systems by Newton's method.

In the rest of the paper, for $v^0,\dots,v^N\in\mathbb{C}_0^{J+2}$ we let $\hat v^0:=v^0, \hat v^1:=v^1$ unless explicitly otherwise stated, and $\hat v^{n+1}:=2v^n-v^{n-1}, n=1,\dots,N-1$. Let $\tau(x,y,z,w):=x^2+y^2-xz-yw+(z^2+w^2)/2=\frac14\big(|2(x+\mathrm{i}y)-(z+\mathrm{i}w)|^2+|z+\mathrm{i}w|^2\big)(x+\mathrm{i}y)$, and $g(x,y,z,w):=(x+iy)\tau(x,y,z,w), x,y,z,w\in\mathbb{R}$. Setting $U^0:=u^0$ we approximate u^n by $U^n\in\mathbb{C}_0^{J+2}, U^n=V^n+\mathrm{i}W^n, V_j^n,W_j^n\in\mathbb{R}$, such that for $n=0,\dots,N-1$

$$\begin{aligned}(3.1)\quad &\partial U_j^n-\mathrm{i}\Delta_h U_j^{n+1/2}-\mathrm{i}\lambda\big[\partial_1 g(E_j^n,Z_j^n,V_j^n,W_j^n)(V_j^{n+1}-\hat V_j^{n+1})\\ &+\partial_2 g(E_j^n,Z_j^n,V_j^n,W_j^n)(W_j^{n+1}-\hat W_j^{n+1})\big]=2\mathrm{i}\lambda g(E_j^n,Z_j^n,V_j^n,W_j^n),\ j=1,\dots,J,\end{aligned}$$

where $E^n:=\frac12(V^n+\hat V^{n+1}), Z^n:=\frac12(W^n+\hat W^{n+1})$, and $\hat U^1$ is given by

$$\partial\hat U_j^1-\mathrm{i}\Delta_h\hat U_j^{1/2}=\mathrm{i}\lambda\varphi(u_j^0,u_j^0),\quad j=1,\dots,J. \tag{3.2}$$

Taking in (1.6) real and imaginary parts, using $\hat U^{n+1}$ as a starting approximation and performing one Newton step leads easily to (3.1).

Theorem 3.1. *Let the solution u of* (1.1) *be sufficiently smooth, k and h be sufficiently small and $k=o(h^{1/4})$. Then $U^n, n=1,\dots,N$, are uniquely defined by* (3.1), (3.2), *and*

$$\max_{0\le n\le N}\|u^n-U^n\|_h\le c(k^2+h^2). \tag{3.3}$$

Proof. Let $e^n:=u^n-U^n, n=0,\dots,N$. It is easily seen that $\hat U^1$ is well defined. Let us now estimate $\|\hat e^1\|_h, e^1:=u^1-\hat U^1$: from (3.2) and (2.11) we obtain

$$\hat e_j^1-\frac{\mathrm{i}k}{2}\Delta_h\hat e_j^1=\mathrm{i}\lambda k\big[\varphi(u_j^1,u_j^0)-\varphi(u_j^0,u_j^0)\big]+kr_j^0,\quad j=1,\dots,J.$$

Taking the inner product with $\hat e^1$, using (2.1), taking real parts, applying the Schwarz inequality, and using the local Lipschitz continuity of φ and (2.12) we easily obtain

$$\|\hat e^1\|_h\le\Gamma(k^2+h^2), \tag{3.4}$$

with a constant Γ. We shall now prove inductively that $U^n, n=1,\dots,N$, are uniquely defined,

$$\|u^\nu-U^\nu\|_h\le C_\nu(k^2+h^2)\quad 0\le\nu\le N, \tag{3.5}$$

with

$$C_\nu=Dk+(1+Dk)C_{\nu-1}+DkC_{\nu-2}\quad 2\le\nu\le N, \tag{3.6}$$

where $C_0=0, C_1=1$ say, and the constant D is defined as follows: We write the solution u of (1.1) in the form $u=v+\mathrm{i}w$ where v and w are real-valued, and set

$v_j^n := v(x_j, t^n), w_j^n := w(x_j, t^n)$. Let $s^n \in \mathbb{C}_0^{J+2}$ be the consistency error of the scheme (3.1), i.e., with $u^{n+1/2} = (u^n + u^{n+1})/2$, for $n = 0, \dots, N-1$

$$\begin{aligned} s_j^n := \partial u_j^n - \mathrm{i}\Delta_h u_j^{n+1/2} - \mathrm{i}\lambda\big[\partial_1 g(\varepsilon_j^n, \zeta_j^n, v_j^n, w_j^n)(v_j^{n+1} - \hat{v}_j^{n+1}) \\ + \partial_2 g(\varepsilon_j^n, \zeta_j^n, v_j^n, w_j^n)(w_j^{n+1} - \hat{w}_j^{n+1})\big] - 2\mathrm{i}\lambda g(\varepsilon_j^n, \zeta_j^n, v_j^n, w_j^n),\ j = 1, \dots, J, \end{aligned} \tag{3.7}$$

where $\varepsilon^n := \frac{1}{2}(v^n + \hat{v}^{n+1}), \zeta^n := \frac{1}{2}(w^n + \hat{w}^{n+1})$. It is easily seen that

$$\max_{j,n} |s_j^n| \le c(u)(k^2 + h^2). \tag{3.8}$$

Let $K := \{\alpha \in \mathbb{R}^4 : |\alpha_j| \le M, j = 1, \dots, 4\}$, where M is as in section 2, $D_1 := |\lambda| \max\{|\partial_j g(\alpha)| : j = 1, \dots, 4, \alpha \in K\}$, $\tilde{D}_2 := |\lambda| \max\{|\partial_{j,m} g(\alpha)| : j, m = 1, \dots, 4, \alpha \in K\}$, and D_2 be such that $\tilde{D}_2 \max_{n,j} |u_j^{n+1} - \hat{u}_j^{n+1}| \le D_2 k^2$.

With $d := 2D_1, d_1 := 24D_1 + 20D_2, d_2 := 6D_1 + 4D_2$ and $d_3 := c(u)$ we let D be such that for k sufficiently small ($k \le 1/(2d)$, say)

$$\frac{\delta_{1j} + d_j k}{1 - dk} \le \delta_{1j} + Dk, \quad j = 1, 2, 3,$$

where δ is the Kronecker symbol. It can be easily seen that $\max_{0 \le n \le N} C_n \le C^*$ with a constant C^* independent of h and k. In the sequel, let k and h be small enough such that

$$\max(\Gamma, C^*) h^{-1/2}(k^2 + h^2) < 1/4 \quad (k = o(h^{1/4})). \tag{3.9}$$

Now, (3.5) is trivially true for $\nu = 0$. We assume that $U^\nu, \nu = 0, \dots, n, n < N$, are uniquely defined and satisfy (3.5); using (3.9) it is easily seen that U^{n+1} is well defined for k sufficiently small (independent of h and n), and it remains to show (3.5) for $\nu = n + 1$. Obviously

$$\begin{aligned} \partial e_j^n - \mathrm{i}\Delta_h e_j^{n+1/2} &= \mathrm{i}\lambda\big[\partial_1 g(\varepsilon_j^n, \zeta_j^n, v_j^n, w_j^n)(v_j^{n+1} - \hat{v}_j^{n+1}) \\ &\quad + \partial_2 g(\varepsilon_j^n, \zeta_j^n, v_j^n, w_j^n)(w_j^{n+1} - \hat{w}_j^{n+1})\big] + 2\mathrm{i}\lambda g(\varepsilon_j^n, \zeta_j^n, v_j^n, w_j^n) \\ &\quad - \mathrm{i}\lambda\big[\partial_1 g(E_j^n, Z_j^n, V_j^n, W_j^n)(V_j^{n+1} - \hat{V}_j^{n+1}) + \partial_2 g(E_j^n, Z_j^n, V_j^n, W_j^n)(W_j^{n+1} - \hat{W}_j^{n+1})\big] \\ &\quad - 2\mathrm{i}\lambda g(E_j^n, Z_j^n, V_j^n, W_j^n) + s_j^n, \quad j = 1, \dots, J. \end{aligned}$$

Taylor expanding $g, \partial_1 g$ and $\partial_2 g$ around $(E_j^n, Z_j^n, V_j^n, W_j^n)$ until first-order terms, and then taking the inner product with $e^{n+1/2}$, using (2.1), taking real parts and applying the Schwarz inequality, we obtain

$$\begin{aligned} \frac{1}{k}\big(\|e^{n+1}\|_h - \|e^n\|_h\big) \le 2D_1\|e^{n+1} - \hat{e}^{n+1}\|_h + 4D_2 k^2\big(\|e^n + \hat{e}^{n+1}\|_h + 2\|e^n\|_h\big) \\ + 4D_1\big(\|e^n + \hat{e}^{n+1}\|_h + 2\|e^n\|_h\big) + c(u)(k^2 + h^2) \end{aligned} \tag{3.10}$$

and conclude easily that (3.5) holds for $\nu = n + 1$. □

4. On the practical implementation of Newton's method

In order to compute U^{n+1} by (3.1) we have to solve a linear system whose matrix varies from step to step. In this section we shall analyze an iterative scheme in order to approximate U^{n+1} which requires solving linear systems with the same coefficient matrix.

For $m_0,\dots,m_N\in\mathbb{N}$ we define approximations $U^{n(m)}\in\mathbb{C}_0^{J+2}, U^{n(m)}=V^{n(m)}+\mathrm{i}W^{n(m)}, V_j^{n(m)}, W_j^{n(m)}\in\mathbb{R}, m=0,\dots,m_n$, to u^n as follows

$$U^{0(m)}=U^0,\quad m=0,\dots,m_0, \tag{4.1}$$

$$\begin{aligned} U^{1(0)}&:=\hat U^1\quad(\text{see }\ (3.2))\\ U^{n+1(0)}&:=2U^{n(m_n)}-U^{n-1(m_{n-1})},\quad n=1,\dots,N-1 \end{aligned}\tag{4.2}$$

and for $n=0,\dots,N-1$

$$\begin{aligned} &\frac1k\big(U_j^{n+1(m+1)}-U_j^{n(m_n)}\big)-\frac{\mathrm{i}}{2}\varDelta_h\big(U^{n+1(m+1)}+U^{n(m_n)}\big)_j\\ &\quad=\mathrm{i}\lambda\big[\partial_1 g(H_j^n,\varTheta_j^n,V_j^{n(m_n)},W_j^{n(m_n)})(V_j^{n+1(m)}-V_j^{n+1(0)})\\ &\quad+\partial_2 g(H_j^n,\varTheta_j^n,V_j^{n(m_n)},W_j^{n(m_n)})(W_j^{n+1(m)}-W_j^{n+1(0)})\big]\\ &\quad+2\mathrm{i}\lambda g(H_j^n,\varTheta_j^n,V_j^{n(m_n)},W_j^{n(m_n)}),\quad j=1,\dots,J,\\ &\qquad\qquad\qquad\qquad n=0,\dots,m_{n+1}-1, \end{aligned}\tag{4.3}$$

where $H^n:=\frac12\big(V^{n+1(0)}+V^{n(m_n)}\big), \varTheta^n:=\frac12\big(W^{n+1(0)}+W^{n(m_n)}\big)$, and g is as in section 3.

Theorem 4.1. *Let the solution u of* (1.1) *be sufficiently smooth, k and h be sufficiently small, and $k=o(h^{1/4})$. Then, for given integers $m_n>0, U^{n(m_n)}\in\mathbb{C}_0^{J+2}$ are uniquely defined by* (4.1)–(4.3), *and*

$$\max_{0\le n\le N}\|u^n-U^{n(m_n)}\|_h\le c(k^2+h^2). \tag{4.4}$$

Proof. It is easily seen that $U^{n(m)}, n=0,\dots,N, m=0,\dots,m_n$, are well defined by (4.1)–(4.3). We shall show inductively that

$$\|u^\nu-U^{\nu(m_\nu)}\|_h\le c_\nu(k^2+h^2),\quad \nu=0,\dots,N, \tag{4.5}$$

with

$$c_\nu=(dk)^{m_\nu}\big(\tilde d+2c_{\nu-1}+c_{\nu-2}\big)+Dk+(1+Dk)c_{\nu-1}+Dkc_{\nu-2},\quad 2\le\nu\le N, \tag{4.6}$$

where $c_0=0, c_1=1$ say, the constants d and D are as in section 3, and $\tilde d$ is such that

$$\max_{0\le n\le N}\|u^n-\hat u^n\|_h\le c(k^2+h^2).$$

It can be easily seen that $\max_{0\le\nu\le N}c_\nu\le c^*$ with a constant c^* independent of h and k. In the sequel, let k and h be small such that

$$c^*h^{-1/2}(k^2+h^2)<\frac14. \tag{4.7}$$

Note that (4.5) holds trivially for $\nu = 0$. We assume now that (4.5) holds for $\nu = 0,\dots,n, n < N$, and we shall prove it for $\nu = n+1$. Letting $e^{n(m)} := u^n - U^{n(m)}, n = 0,\dots,N, m = 0,\dots,m_n$, we have, with s^n as in section 3

$$\begin{aligned}
&\frac{1}{k}\big(e_j^{n+1(m+1)} - e_j^{n(m_n)}\big) - \frac{\mathrm{i}}{2}\Delta_h\big(e^{n+1(m+1)} + e^{n(m_n)}\big)_j\\
&\quad = \mathrm{i}\lambda\big[\partial_1 g(\varepsilon_j^n,\zeta_j^n,v_j^n,w_j^n)(v_j^{n+1} - \hat v_j^{n+1}) + \partial_2 g(\varepsilon_j^n,\zeta_j^n,v_j^n,w_j^n)(w_j^{n+1} - \hat w_j^{n+1})\big]\\
&\quad - \mathrm{i}\lambda\big[\partial_1 g(H_j^n,\Theta_j^n,V_j^{n(m_n)},W_j^{n(m_n)})(V_j^{n+1(m)} - V_j^{n+1(0)})\\
&\quad\ + \partial_2 g(H_j^n,\Theta_j^n,V_j^{n(m_n)},W_j^{n(m_n)})(W_j^{n+1(m)} - W_j^{n+1(0)})\big]\\
&\quad\ + 2\mathrm{i}\lambda\big[g(\varepsilon_j^n,\zeta_j^n,v_j^n,w_j^n) - g(H_j^n,\Theta_j^n,V_j^{n(m_n)},W_j^{n(m_n)})\big] + s_j^n, \quad j = 1,\dots,J.
\end{aligned}$$

Let $\tilde e^{n+1} := \hat u^{n+1} - U^{n+1(0)}$. Taylor expanding $g, \partial_1 g$ and $\partial_2 g$ around $(H_j^n,\Theta_j^n,V_j^{n(m_n)}, W_j^{n(m_n)})$ until first-order terms, and then taking the inner product with $e^{n+1(m+1)} + e^{n(m_n)}$, using (2.1), taking real parts and applying the Schwarz inequality, we obtain

$$\begin{aligned}
&\frac{1}{k}\big(\|e^{n+1(m+1)}\|_h - \|e^{n(m_n)}\|_h\big) \le 2D_1\|e^{n+1(m)} - \tilde e^{n+1}\|_h\\
&\qquad + 4D_2k^2\big(\|e^{n(m_n)} + \tilde e^{n+1}\|_h + 2\|e^{n(m_n)}\|_h\big)\\
&\qquad + 4D_1\big(\|e^{n(m_n)} + \tilde e^{n+1}\|_h + 2\|e^{n(m_n)}\|_h\big) + c(u)(k^2+h^2)
\end{aligned}\tag{4.8}$$

and conclude easily that (4.5) holds for $\nu = n+1$. □

Remark 4.1. Taking $m_n = 1, n = 0,\dots,N$, our scheme can be written in the form

$$U_j^{n+1(1)} - U_j^{n(1)} = \frac{\mathrm{i}k}{2}\Delta_h\big(U^{n+1(1)} + U^{n(1)}\big)_j + \mathrm{i}\lambda k\varphi(2U_j^{n(1)} - U_j^{n-1(1)}, U_j^{n(1)}), \quad n \ge 1, \tag{4.9}$$

which is the standard way for linearizing the second-order scheme (1.6) by extrapolating from previous values in the nonlinear term.

Numerical computations show that taking $m_n > 1$ improves essentially the error constant and the conservation properties of the method.

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