ON FULLY DISCRETE GALERKIN METHODS OF SECOND–ORDER TEMPORAL ACCURACY FOR THE NONLINEAR SCHRÖDINGER EQUATION

GEORGIOS D. AKRIVIS, VASSILIOS A. DOUGALIS, AND OHANNES A. KARAKASHIAN

Abstract. We approximate the solutions of an initial- and boundary-value problem for nonlinear Schrödinger equations (with emphasis on the 'cubic' nonlinearity) by two fully discrete finite element schemes based on the standard Galerkin method in space and two implicit, Crank–Nicolson-type second-order accurate temporal discretizations. For both schemes we study the existence and uniqueness of their solutions and prove L^2 error bounds of optimal order of accuracy. For one of the schemes we also analyze one step of Newton's method for solving the nonlinear systems that arise at every time step. We then implement this scheme using an iterative modification of Newton's method that, at each time step t^n, requires solving a number of sparse complex linear systems with a matrix that does not change with n. The effect of this 'inner' iteration is studied theoretically and numerically.

1. Introduction

In this paper we shall study numerical methods of Galerkin-finite element type for approximating the solution of the following initial- and boundary-value problem for the Nonlinear Schrödinger equation (NLS). Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or 3, be a bounded domain with boundary $\partial\Omega$ and let $0 < T < \infty$ be given. We seek a complex-valued function $u = u(x,t)$, defined on $\bar{\Omega} \times [0,T]$ and satisfying

$$(1.1) \qquad \begin{cases} u_t = \mathrm{i}\Delta u + \mathrm{i}f(u) & \text{in} \quad \bar{\Omega} \times [0,T], \\ u = 0 & \text{on} \quad \partial\Omega \times [0,T], \\ u(x,0) = u^0(x) & \text{in} \quad \bar{\Omega}\ , \end{cases}$$

where $f : \mathbb{C} \to \mathbb{C}$ is locally Lipschitz and $u^0 : \bar{\Omega} \to \mathbb{C}$ is given. We shall assume that the data of this problem are smooth and compatible enough so that it possesses a unique solution, sufficiently smooth for our purposes.

Employing standard notation, we shall use the symbols $H^s = H^s(\Omega)$, $H_0^1 = H_0^1(\Omega)$ to denote the usual, complex (Hilbert) Sobolev spases. Let $(\cdot,\cdot)$ be the inner product on $L^2 = H^0$ defined by $(u,v) = \int_\Omega u(x)\bar{v}(x)dx$ for $u, v \in L^2$, and denote by $\|\cdot\|$ the associated L^2 norm. We shall assume throughout the paper that f satisfies $\mathrm{Im}(f(v),v) = 0$

1991 *Mathematics Subject Classification.* 65M60, CR G. 1.8.

The work of G.D.A. and V.A.D. was supported by the Institute of Applied and Computational Mathematics of the Research Center of Crete-FORTH and the Science Alliance program of the University of Tennessee.

The work of O.A.K. was supported by the AFOSR Grant 88-0019.

for any $v \in H_0^1$. Some of the results below will be obtained for such a general f. But we shall be particularly interested in (and accordingly shall specialize our results frequently to) the choice

$$f(z) = \lambda |z|^2 z, \quad \lambda \ \text{real}, \tag{1.2}$$

i.e. in the 'cubic' NLS, important in applications such as nonlinear optics, plasma physics and water waves. We refer the reader to the surveys [12] and [9] and [8, §8.1] for an overview of the physical significance and various properties of the equation, its existence-uniqueness theory and for further references. It is straightforward to see that the L^2 norm of the solution $u(\cdot,t) = u(t)$ of (1.1) is an invariant of the equation, i.e. that

$$\|u(t)\| = \|u^0\|, \quad 0 \le t \le T \tag{1.3}$$

holds. In addition, if f is given by (1.2), we obtain

$$\|\nabla u(t)\|^2 - \frac{\lambda}{2}|u(t)|_4^4 = \|\nabla u^0\|^2 - \frac{\lambda}{2}|u^0|_4^4, \quad 0 \le t \le T, \tag{1.4}$$

where, here and in the sequel, $|\cdot|_p$, $1 \le p \le \infty$, $p \ne 2$, will denote the norm of $L^p = L^p(\Omega)$ and $(\nabla u, \nabla v) = \sum_{i=1}^d (\partial_i u, \partial_i v)$.

During the past ten years quite a few papers have appeared in the numerical analysis and scientific computing literature on various aspects of numerical methods (of finite difference, finite element, spectral or more specialized type) for NLS equations. See, for example, [3], [4], [15], [10], [13], [5], [11], [19], [6], [17] and their lists of references.

In the present work we shall discretize (1.1) in space by the standard Galerkin method. To this effect, for $0 < h < 1$, let S_h be a finite-dimensional subspace of continuous functions in H_0^1, (typically, vector spaces of piecewise polynomial functions of a fixed degree defined on suitable partitions of $\bar{\Omega}$ and endowed with bases with elements of small support) in which approximations to the solution $u(t)$ of (1.1) will be sought for $0 \le t \le T$. We assume that S_h satisfies the following approximation property: there exists an integer $r \ge 2$ such that

$$\inf_{\varphi \in S_h} (\|v - \varphi\| + h\|v - \varphi\|_1) \le c h^s \|v\|_s, \quad 1 \le s \le r, \quad \forall v \in H^s \cap H_0^1, \tag{1.5}$$

where $\|\cdot\|_s$ denotes the usual norm of H^s. We also suppose that, in addition, S_h satisfies the inverse assumption

$$|\varphi|_\infty \le c_I\, h^{-d/2} \|\varphi\| \qquad \forall \varphi \in S_h\,, \tag{1.6}$$

and that, if u is the solution of (1.1), there holds

$$\lim_{h \to 0} \sup_{0 \le t \le T} \inf_{\varphi \in S_h} \{|u(t) - \varphi|_\infty + h^{-d/2}\|u(t) - \varphi\|\} = 0; \tag{1.7}$$

this follows, as is well-known, from (1.5) and (1.6) provided there exists an interpolation operator of smooth functions into S_h with reasonable L^∞ approximation properties. In (1.5), (1.6) and in the sequel, the symbols c, C, etc. denote positive generic constants, not necessarily the same at any two different places, which are independent of the discretization parameter h and the time step k, unless the contrary is explicitly indicated. Such constants may depend of course on the solution u and the data of (1.1).

To set the stage for the Galerkin method one may define first the semidiscrete approximation of $u(t)$ in S_h in the customary way, as the map $u_h : [0,T] \to S_h$ satisfying

$$\begin{cases} (u_{ht}, \varphi) + \mathrm{i}(\nabla u_h, \nabla\varphi) = \mathrm{i}(f(u_h), \varphi) \qquad \forall \varphi \in S_h, \quad 0 \le t \le T, \\ u_h(0) = u_h^0, \end{cases} \tag{1.8}$$

where u_h^0 is some approximation to u^0 in S_h. In section 2 we show that u_h exists uniquely and, if u is sufficiently smooth and the initial condition u_h^0 is chosen so that

$$\|u^0 - u_h^0\| \le ch^r \ , \tag{1.9}$$

it satisfies the optimal rate-of-convergence L^2 error estimate

$$\max_{0 \le t \le T} \|u(t) - u_h(t)\| \le ch^r.$$

In the rest of the paper we are concerned with second-order accurate in t fully discrete approximations to the system of ordinary differential equations represented by (1.8). Let $k > 0$ be the (constant) time step and $t^n = nk, n = 0, 1, ..., J$, where $t^J = T$. First, we discretize (1.8) by a Crank–Nicolson type method (more precisely by the 'midpoint' or one-stage Gauss-Legendre implicit Runge-Kutta (IRK) scheme) and approximate $u(t^j) = u^j$ by $U^j \in S_h \ , \ 0 \le j \le J$, defined by

$$\begin{cases} \frac{1}{k}(U^{n+1} - U^n, \varphi) + \frac{\mathrm{i}}{2}(\nabla(U^{n+1} + U^n), \nabla\varphi) \\ \qquad\qquad\qquad = \mathrm{i}(f(\frac{1}{2}(U^{n+1} + U^n)), \varphi) \qquad \forall \varphi \in S_h, \quad 0 \le n \le J-1, \\ U^0 = u_h^0. \end{cases} \tag{1.10}$$

This scheme has often been used for numerical computations in the literature, coupled of course with various iterative techniques for solving at each time step the nonlinear system of equations that it represents; see e.g. Sanz-Serna and Verwer [11], Tourigny and Morris [17]. Verwer and Sanz-Serna discuss its convergence in the context of a finite difference space discretization in [18]. It is easily seen that it is L^2-conservative, i.e. if a solution $\{U^n\}$ of (1.10) exists then

$$\|U^n\| = \|U^0\| \, , \qquad 0 \le n \le J, \tag{1.11}$$

which is the discrete analog of (1.3); the scheme however does not conserve the discrete analog of the second invariant (1.4). In section 3 we verify that, given U^n, a solution U^{n+1} of (1.10) exists in S_h. We next discuss the uniqueness of solutions of the discrete scheme (1.10) when f is given by (1.2), assuming that U^0 is bounded in L^2 uniformly in h – e.g. when $U^0 = Pu^0$, where P is the L^2 projection operator onto S_h – without making any hypotheses on the existence, uniqueness and smoothness of solutions of (1.1). If $d = 1$ we show that the solution U^{n+1} of (1.10) is unique, provided k is sufficiently small. For $d = 2$, recall, cf. e.g. [1], that the continuous problem (1.1) has unique solutions in H^2 for all $t \geq 0$, provided $u^0 \in H^2 \cap H_0^1$, and, either $\lambda \leq 0$ or $\lambda > 0$ and $c_0\lambda\|u^0\|^2 < 2$ (where c_0 is a positive constant occurring in a Gagliardo–Nirenberg inequality, cf. (3.10) below), whilst for $c_0\lambda\|u^0\|^2 > 2$ the solution may blow up in finite time. We show that solutions of (1.10) are unique provided that $c_0|\lambda|\|U^0\|^2 < 1/4$ if $\lambda \leq 0$ and $c_0\lambda\|U^0\|^2 < .22...$ if $\lambda > 0$, which is a qualitatively 'correct' restriction on the initial data U^0 and λ if $\lambda > 0$. If $\lambda < 0$ we conjecture that the restriction is not needed and uniqueness of solutions of (1.10) should hold for k sufficiently small, perhaps under some mild hypothesis on u^0 like $u^0 \in H^2 \cap H_0^1$, and for some reasonable approximation U^0 thereof. (It is not hard to see that uniqueness would follow, for k sufficiently small, if one can prove a priori that for $0 \leq n \leq J$ $|U^n|_4^4 = o(k^{-1})$ as $k \to 0$ if $d = 2$, and $|U^n|_4^4 = o(k^{-1/2})$ as $k \to 0$ if $d = 3$.) Of course, if one is willing to impose the *mesh condition* that $|\lambda|\,\|U^0\|^2 kh^{-d}$ be sufficiently small, then, as shown in section 3, U^n is unique for $d = 2$ or 3.

We then proceed to prove an L^2 error estimate for the scheme (1.10) for a general f assuming that the solution of (1.1) is sufficiently smooth. In Theorem 3.1 we show that if (1.9) holds and $k = o(h^{d/4})$ then there exists a *unique* solution of (1.10) satisfying

$$\max_{0\leq n\leq J} \|u^n - U^n\| \leq c(k^2 + h^r). \tag{1.12}$$

(Uniqueness follows from the fact that solutions U^n that are close to the exact solution u^n in the sense of (1.12) are bounded, e.g. in L^∞, uniformly in k and h.)

It is interesting to contrast these results for the scheme (1.10) with the analogous ones for the following method, also of Crank–Nicolson type, written and analyzed here in case that f is given by (1.2):

$$\begin{cases} \frac{1}{k}(U^{n+1} - U^n, \varphi) + \frac{\mathrm{i}}{2}(\nabla(U^{n+1} + U^n), \nabla\varphi) \\ \qquad = \frac{\mathrm{i}\lambda}{4}((|U^{n+1}|^2 + |U^n|^2)(U^{n+1} + U^n), \varphi) \quad \forall\varphi \in S_h, \quad 0 \leq n \leq J-1, \\ U^0 = u_h^0. \end{cases} \tag{1.13}$$

This scheme was introduced by Delfour, Fortin, and Payre, [3] (the differencing of the nonlinear term being motivated by a method of Strauss and Vazquez, [13]) and has been used widely in computations in finite-difference or finite-element contexts; cf. e.g. [3], [10], [14], [5]. As was pointed out in [3], solutions of (1.13) satisfy in addition to (1.11) the discrete analog of (1.4) as well, i.e. the relation

$$\|\nabla U^n\|^2 - \frac{\lambda}{2}|U^n|_4^4 = \|\nabla U^0\|^2 - \frac{\lambda}{2}|U^0|_4^4, \qquad 0 \leq n \leq J\,. \tag{1.14}$$

In section 3, after proving existence of solutions of (1.13), we turn to the question of their uniqueness, which can be resolved now in a satisfactory manner, in parallel with the results for the continuous problem, because of (1.14). In particular, it turns out that if $\|U^0\|_1 \leq c$, c independent of h, then, solutions of (1.13) are unique, for k sufficiently small, if $d = 1$ and, if $\lambda \leq 0$, for $d = 2$ and 3 as well. In the case $d = 2, \lambda > 0$, one must impose the condition that $c_0\lambda\|U^0\|^2 < 2$, exactly as for (1.1). In [10] Sanz-Serna has proved an $O(k^2 + h^r)$ L^2-error estimate for the scheme (1.13) in one space dimension with periodic boundary conditions at the endpoints, provided that u is sufficiently smooth, (1.9) holds and $k = o(h)$. To complete the picture, we show in Theorem 3.2 that if u is sufficiently smooth, (1.9) holds and $k = o(h^{d/4})$, then, the solution of (1.13) satisfies the error estimate (1.12) as well.

Implementing the schemes (1.10) or (1.13) needs solving a nonlinear system of equations at each time step. In section 4 we study *Newton's method* for scheme (1.10) with f given by (1.2). In Theorem 4.1 we show that if suitable starting values are constructed at each time step and *one* Newton iteration is performed, yielding the approximation $U_1^n \in S_h$ to U^n , then, under the hypotheses of Theorem 3.1, the resulting method is stable and

$$\max_{1\leq n\leq J} \|U_1^n - U^n\| \leq c(k^2 + h^r) \tag{1.15}$$

holds, i.e. the overall optimal-order L^2 error estimate is preserved. Tourigny and Morris, [17], have recently discussed the application of Newton's method in the context of (1.10) and shown computational results.

A disadvantage of Newton's method is that the matrix of the linear system that has to be solved at each time step t^n changes with n. In section 5 we construct and analyze a natural iterative scheme for solving at each time step this linear system approximately. This 'inner' loop is implemented by solving, for each n , j_n linear sparse *complex* systems of size $\dim S_h \times \dim S_h$ whose matrix does not change with n or the inner iterations and yields an approximation U^{n,j_n} of U_1^n. We show that if $j_n \geq 1$, the resulting overall scheme is stable and the $O(k^2 + h^r)$ global error estimate is preserved. It is evident that increasing the number j_n of inner iterations improves the error constant and the conservation properties of the method. The scheme of course is not L^2-conservative - nor is, for that matter, the exact Newton's method with a finite number of Newton steps -. But it is important to gain an idea of what j_n should be in practice to yield acceptable approximations U^{n,j_n} that conserve to a satisfactory accuracy the two invariants of the problem. With this goal in mind we close the paper by showing the results of some relevant computations on two simple test problems. Our conclusions are that performing $j_n = 3$ iterations at each time step yields very good approximations. The values of the invariants degenerate if $j_n = 1$ or 2 whilst there is no need to go up to $j_n = 4$.

In a sequel to this paper we shall analyze the convergence of *higher-order* full discretizations of (1.8) using q-stage, $q > 1$, IRK methods satisfying suitable consistency and stability conditions; these methods yield highly accurate approximations. The specific class of the Gauss-Legendre IRK methods are, in addition, L^2–conservative. The scheme (1.10) is the lowest-order ($q = 1$) member of the latter class.

The authors record their thanks to their students, Messrs. Theodore Katsaounis and Michael Plexousakis for programming the schemes and performing the numerical experiments reported in section 5.

2. Semidiscrete Approximation

In this section we shall briefly study the semidiscrete approximation u_h of u defined by (1.8). If $u_h(t)$ exists for $0 \le t \le T$, putting $\varphi = u_h$ in (1.8) and taking real parts leads easily to

$$\|u_h(t)\| = \|u_h^0\|, \qquad 0 \le t \le T, \tag{2.1}$$

which is the semidiscrete counterpart of (1.3). It may also easily be seen, if f is given by (1.2), that putting $\varphi = u_{ht}$ in (1.8) and taking imaginary parts yields that u_h satisfies the counterpart of (1.4) as well.

Since f is locally Lipschitz, the O.D.E. system (1.8) has a unique solution, at least locally. Fix h and assume that $[0, t_h)$, $0 < t_h \le T$, is the maximal interval of existence-uniqueness of $u_h(t)$. For $t \in [0, t_h)$ (2.1) and (1.6) yield that $|u_h(t)|_\infty \le c(h) < \infty$; we conclude by continuity that $t_h = T$, i.e. that u_h exists uniquely on $[0, T]$.

To find a bound for the error $\|u(t) - u_h(t)\|$ we use the following well-known device. Fix $\delta > 0$ and let $M_\delta = \{z \in \mathbb{C} : \exists (x, t) \in \bar{\Omega} \times [0, T] \; |z - u(x, t)| < \delta\}$. Let $f_\delta : \mathbb{C} \to \mathbb{C}$ be a globally Lipschitz continuous function that coincides with f on M_δ and let L be its Lipschitz constant; it is *not* assumed that $\mathrm{Im}(f_\delta(v), v) = 0$ for $v \in H_0^1$. We consider next the auxiliary function $v_h : [0, T] \to S_h$, defined as the unique solution of the system of O.D.E.'s

$$\begin{cases} (v_{ht}, \varphi) + \mathrm{i}(\nabla v_h, \nabla \varphi) = \mathrm{i}(f_\delta(v_h), \varphi) \quad \forall \varphi \in S_h, \quad 0 \le t \le T, \\ v_h(0) = u_h^0. \end{cases} \tag{2.2}$$

First, we shall estimate the error $\|u(t) - v_h(t)\|$ by comparing in the customary way v_h with the *elliptic projection* $P_I u$ of u. In general, given $v \in H_0^1$, define its elliptic projection $P_I v \in S_h$ by

$$(\nabla(P_I v), \nabla \varphi) = (\nabla v, \nabla \varphi) \qquad \forall \varphi \in S_h. \tag{2.3}$$

Then, it may be shown that $P_I v$ satisfies

$$\|v - P_I v\| + h\|v - P_I v\|_1 \le c h^r \|v\|_r \qquad \forall v \in H^r \cap H_0^1. \tag{2.4}$$

Lemma 2.1. *Let v_h be defined by (2.2). Then, if u is sufficiently smooth,*

$$\max_{0 \le t \le T} \|u(t) - v_h(t)\| \le c(\|u^0 - u_h^0\| + h^r). \tag{2.5}$$

Proof. Write $u - v_h = (u - P_I u) + (P_I u - v_h) = \rho + \theta$. Since f and f_δ coincide on M_δ, (2.2), (1.1) and (2.3) give for $\varphi \in S_h$

$$(\theta_t, \varphi) + i(\nabla \theta, \nabla \varphi) = -(\rho_t, \varphi) + i(f_\delta(v_h) - f_\delta(u), \varphi)\,, \qquad 0 \le t \le T.$$

Putting $\varphi = \theta$ and taking real parts yields $\frac{d}{dt}\frac{\|\theta(t)\|^2}{2} \le (\|f_\delta(v_h) - f_\delta(u)\| + \|\rho_t\|)\,\|\theta(t)\|$. Hence,

$$\begin{aligned} \frac{d}{dt}\|\theta(t)\| &\le L\|v_h - u\| + \|\rho_t\| \\ &\le C(\|\theta(t)\| + \|\rho_t(t)\| + \|\rho(t)\|), \quad 0 \le t \le T. \end{aligned} \tag{2.6}$$

Gronwall's Lemma, (2.3) and (2.4) yield now (2.5). □

We now proceed to bound $\|u-u_h\|$. In the following result and in the sequel we shall omit, in general, to state hypotheses or the type "let h (or k) be sufficiently small" or "let u be sufficiently smooth".

Theorem 2.1. *Let u_h be the solution of* (1.8) *and suppose that u_h^0 satisfies* (1.9). *Then*

$$\max_{0\le t\le T} \|u(t)-u_h(t)\| \le ch^r\,. \tag{2.7}$$

Proof. (1.9) and (2.5) give

$$\max_{0\le t\le T} \|u(t)-v_h(t)\| \le ch^r. \tag{2.8}$$

Defining ρ,θ as in the proof of Lemma 2.1 and using (1.6), (2.8) and (2.4) yields, for $0\le t\le T$ and any $\varphi\in S_h$:

$$\begin{aligned}
|u(t)-v_h(t)|_\infty &\le |\rho(t)|_\infty + |\theta(t)|_\infty\\
&\le |u(t)-\varphi|_\infty + |\varphi - P_I u(t)|_\infty + |\theta(t)|_\infty\\
&\le |u(t)-\varphi|_\infty + Ch^{-d/2}(\|u(t)-\varphi\| + \|\rho(t)\| + \|\theta(t)\|)\\
&\le |u(t)-\varphi|_\infty + Ch^{-d/2}\|u(t)-\varphi\| + Ch^{r-d/2}.
\end{aligned}$$

We conclude, by (1.7), that there exists $h_0>0$ such that for $h\le h_0$, $v_h(x,t)\in M_\delta$ for $(x,t)\in\bar{\Omega}\times[0,T]$. For such h , obviously $u_h=v_h$ and (2.7) follows from (2.8). □

Remark 2.1. Suppose that $d=1$, f is given by (1.2) and let $\|u_h^0\|_1\le C$. Then, using the Sobolev inequality (which may be easily established on $[0,1]$)

$$|v|_4^4 \le 2\|v\|^3\,\|v_x\|\,, \qquad \forall v\in H_0^1 \tag{2.9}$$

we obtain from (2.1) and the semidiscrete version of (1.4) that $\|u_{hx}(t)\|$ and $|u_h(t)|_4$ are uniformly bounded for $h\in(0,1)$, $t\in[0,T]$, by a constant independent of h. Hence, by Sobolev's theorem, a similar bound holds for $|u_h(t)|_\infty$ and the error estimate (2.7) follows with no recourse to (1.6), (1.7) or f_δ. □

3. Fully Discrete Approximations

In this section we shall study the existence, uniqueness and convergence to the exact solution of (1.1) of the solutions of the fully discrete schemes (1.10) and (1.13).

We start with (1.10) To prove existence of solutions we shall use the following complex-valued version of a well-known Brouwer-type fixed-point result, cf. [2].

Lemma 3.1. *Let $(H,(\cdot,\cdot))$ be a finite-dimensional inner product space and $\|\cdot\|$ the associated norm. Let $g:H\to H$ be continuous and assume that there exists $\alpha>0$ such that for every $z\in H$ with $\|z\|=\alpha$ there holds* $\mathrm{Re}(g(z),z)\ge 0$. *Then, there exists a $z^*\in H$ such that $g(z^*)=0$ and $\|z^*\|\le\alpha$.*

Proof. Assume that for every $z\in H$ with $\|z\|\le\alpha$ we have $g(z)\ne 0$. Let $B=\{z\in H:\ \|z\|\le\alpha\}$ and define $p:B\to B$ by $p(z)=-\alpha g(z)/\|g(z)\|$. Since p is continuous, by Brouwer's fixed-point theorem, there is a $z_0\in B$ such that $p(z_0)=z_0$; but this would yield $\|z_0\| = \|p(z_0)\| = \alpha$ and $\|z_0\|^2 = (p(z_0), z_0) = -\alpha(g(z_0), z_0)/\|g(z_0)\| \le 0$, a contradiction. $\square$

Put now $U^{n+1/2} = \frac{U^n+U^{n+1}}{2}$ and defining $\Phi : S_h \to S_h$ by

$$(\Phi(v), \chi) = \frac{1}{2}[-(\nabla v, \nabla \chi) + (f(v), \chi)]\,, \qquad v, \chi \in S_h,$$

rewrite (1.10) with $U^0 = u_h^0$ as

$$U^{n+1/2} = U^n + \mathrm{i}k\Phi(U^{n+1/2})\,, \qquad 0 \le n \le J-1. \tag{3.1}$$

Given U^n, let $\Pi : S_h \to S_h$ be defined for $v \in S_h$ by $\Pi(v) = v - U^n - \mathrm{i}k\Phi(v)$. Then $\mathrm{Re}(\Pi(v), v) = \|v\|^2 - \mathrm{Re}(U^n, v) \ge \|v\|\,(\|v\| - \|U^n\|)$. Hence, for every $v \in S_h$ such that $\|v\| = \|U^n\| + 1$, there holds $\mathrm{Re}(\Pi(v), v) > 0$; existence of a $v^* \in S_h$ such that $\Pi(v^*) = 0$, i.e. of a U^{n+1} satisfying (1.10), follows from Lemma 3.1. Setting now $\varphi = U^n + U^{n+1}$ in (1.10) and taking real parts yields (1.11).

We next investigate the uniqueness of solutions of (1.10) in the case that f is given by (1.2), i.e. when $f(u) = \lambda|u|^2u$, $\lambda \in \mathbb{R}$. Given $U^n \in S_h$ let $V, W \in S_h$ satisfy (3.1), i.e. let

$$V = U^n + \mathrm{i}k\Phi(V), \qquad W = U^n + \mathrm{i}k\Phi(W). \tag{3.2}$$

Then $\|V-W\|^2 = -\frac{\mathrm{i}k}{2}\|\nabla(V-W)\|^2 + \frac{\mathrm{i}k}{2}(f(V)-f(W), V-W)$ from which

$$\|V-W\|^2 = -\frac{k}{2}\,\mathrm{Im}(f(V)-f(W), V-W), \tag{3.3a}$$

$$\|\nabla(V-W)\|^2 = \mathrm{Re}(f(V)-f(W), V-W). \tag{3.3b}$$

Hence, by Hölder's inequality we obtain

$$\|V-W\|^2 \le \frac{k}{2}|f(V)-f(W)|_{4/3}\,|V-W|_4, \tag{3.4a}$$

$$\|\nabla(V-W)\|^2 \le |f(V)-f(W)|_{4/3}\,|V-W|_4. \tag{3.4b}$$

Since $f(z) = \lambda|z|^2z$, we have $|f(z_1)-f(z_2)| \le |\lambda|\,(|z_1|+|z_2|)^2|z_1-z_2|$, for $z_1, z_2 \in \mathbb{C}$. Therefore, by Hölder's inequality

$$|f(V)-f(W)|_{4/3} \le |\lambda|\,\big||V|+|W|\big|_4^2|V-W|_4 \;\le 4|\lambda|\,|V,W|_4^2\,|V-W|_4, \tag{3.5}$$

where we denote $|V,W|_p = \max(|V|_p, |W|_p)$. Note also that taking in the first equation of (3.2) the inner product with V and then real parts yields for V (and ditto for W):

$$k\|\nabla V\|^2 - \lambda k|V|_4^4 = 2\,\mathrm{Im}(U^n, V) \le 2\|U^0\|^2, \tag{3.6}$$

where we have used the fact that, by (3.2), (1.11),

$$\|V, W\| = \max(\|V\|, \|W\|) \le \|U^0\|.$$

The estimates (3.3)–(3.6) are used below to show that, under suitable hypotheses, $V = W$, a fact that implies uniqueness of U^n.

If $d=1$, using the Sobolev-type inequality (2.9), (3.4) and (3.5) we obtain $|V-W|_4^4 \leq c\,k^{3/2}\lambda^2|V,W|_4^4\,|V-W|_4^4$, from which, if $V \neq W$, we would have

$$1 \leq ck^{3/2}\lambda^2|V,W|_4^4. \tag{3.7}$$

Assume now that there exists c independent of h such that $\|U^0\| \leq c$ (e.g. take U^0 as the L^2 projection of $u^0 \in L^2$ onto S_h). First let $\lambda \leq 0$. Then (3.6) yields

$$\|V_x\| \leq ck^{-1/2}, \tag{3.8}$$

which by (2.9) implies in turn that

$$|V|_4^4 \leq ck^{-1/2} \tag{3.9}$$

and two analogous estimates for W. Hence by (3.7) $1 \leq ck\lambda^2$, a contradiction if k is sufficiently small. Let now $\lambda > 0$. (2.9) gives $|V|_4^4 \leq c_1\|V_x\|$, which in view of (3.6) yields $k\|V_x\|^2 - c_1k\lambda\|V_x\| \leq k\|V_x\|^2 - k\lambda|V|_4^4 \leq C$. Therefore $\|V_x\| \leq \lambda c_1 + C^{1/2}k^{-1/2}$ and consequently, if k is sufficiently small, (3.8) and (3.9) hold in this case as well; uniqueness follows again.

If $d=2$ (2.9) is replaced by the Gagliardo–Nirenberg inequality, [1], [7]:

$$v|_4^4 \leq c_0\|v\|^2\|\nabla v\|^2\,, \qquad \forall v \in H_0^1, \tag{3.10}$$

where c_0 is no greater than π^{-1}, cf. [7]. Using now (3.10) in conjunction with (3.4) and (3.5) yields $|V-W|_4^4 \leq 8c_0k\lambda^2|V,W|_4^4\,|V-W|_4^4$, i.e. if $V \neq W$ that

$$1 \leq 8c_0k\lambda^2|V,W|_4^4. \tag{3.11}$$

If $\lambda \leq 0$, then (3.6) yields that $\|\nabla V\|^2 \leq 2k^{-1}\|U^0\|^2$ and, in turn, (3.10) gives $|V|_4^4 \leq 2c_0k^{-1}\|U^0\|^4$. This (which holds for W as well), inserted in (3.11) results in a contradiction if $c_0|\lambda|\,\|U_0\|^2 < \frac{1}{4}$. If $\lambda > 0$ (3.10) substituted in (3.6) yields $\|\nabla V\|^2 \leq 4k^{-1}\|U_0\|^2/(2-\lambda\|U_0\|^2)$ provided that $\lambda\|U_0\|^2 < 2$. Hence, by (3.10), $|V|_4^4 \leq 2c_0k^{-1}\|U_0\|^4/(1-\lambda c_0\|U_0\|^2)$. As a consequence, (3.11) gives a contradiction if $c_0\lambda\|U_0\|^2 < \frac{\sqrt{65}-1}{32} = .22069\ldots$. As pointed out in the Introduction this is a qualitatively 'correct' restriction if $\lambda > 0$. (3.11) of course shows that if the estimate $|U^n|_4^4 = o(k^{-1})$, $k \to 0$, $0 \leq n \leq J$, can be established, then the U^n are unique in two space dimensions. If $d=3$, (3.10) should be replaced by the inequality $|v|_4^4 \leq c\|v\|\,\|\nabla v\|^3$, valid for $v \in H_0^1$. Then (3.11) becomes $1 \leq ck^{1/2}\lambda^2|V,W|_4^4$ and uniqueness holds therefore if $|U^n|_4^4 = o(k^{-1/2})$, $k \to 0$, $0 \leq n \leq J$.

In another direction note that in any dimension, it follows from the definition of f that

$$\|f(V)-f(W)\| \leq |\lambda|\Big(\int_\Omega (|V|+|W|)^4\,|V-W|^2dx\Big)^{\frac{1}{2}} \leq \sqrt{2}\,|\lambda|\,|V,W|_\infty^2\|V-W\|.$$

Hence (3.3a) and the Cauchy–Schwarz inequality would give if $V \neq W$, that

$$1 \leq \frac{k}{\sqrt{2}}|\lambda|\,|V,W|_\infty^2.$$

Therefore, use of (1.6) yields uniqueness if the mesh condition $kh^{-d}|\lambda|\,\|U^0\|^2 < \sqrt{2}c_I^{-2}$ is imposed.

We collect all these observations in

Proposition 3.1. *For $0 \le n \le J$, there exists a solution $U^n \in S_h$ of the scheme* (1.10) *that satisfies* (1.11). *If f is given by* (1.2) *this solution is unique provided one of the following holds:*

(i) $d = 1$, $\|U^0\| \le c$ *for some constant c independent of h , and k is sufficiently small.*

(ii) $d = 2$ *and* $c_0|\lambda|\,\|U^0\|^2 < \frac{1}{4}$ *if* $\lambda \le 0$ *or* $c_0\lambda\|U^0\|^2 < \frac{\sqrt{65}-1}{32}$ *if* $\lambda > 0$.

(iii) $d = 2$, $|U^n|_4^4 = o(k^{-1})$ *as* $k \to 0$ *for* $0 \le n \le J$ *and k is sufficiently small.*

(iv) $d = 3$, $|U^n|_4^4 = o(k^{-1/2})$ *as* $k \to 0$ *for* $0 \le n \le J$ *and k is sufficiently small.*

(v) $1 \le d \le 3$ *and* $|\lambda|\,\|U^0\|^2 k h^{-d} < \sqrt{2} c_I^{-2}$, *where c_I is the constant of* (1.6). □

We proceed now to prove an L^2 error estimate for (1.10). Let $\delta, M_\delta, f_\delta, L$ be defined as in section 2. Then define V^n by

$$\text{(3.12)} \qquad \begin{cases} \frac{1}{k}(V^{n+1} - V^n, \chi) + \frac{\mathrm{i}}{2}(\nabla(V^{n+1} + V^n), \nabla\chi) = i(f_\delta(\frac{1}{2}(V^{n+1} + V^n)), \chi) \\ \qquad\qquad\qquad\qquad \forall\chi \in S_h, \quad 0 \le n \le J-1, \\ V^0 = u_h^0. \end{cases}$$

The existence of V^{n+1} follows from a slight modification of the argument for the existence of U^{n+1} since $\mathrm{Im}(f_\delta(v), v)$ is not necessarily zero for $v \in H_0^1$. We use instead the boundedness of f_δ on $\mathbb{C}$, something that we can always arrange. Uniqueness of V^{n+1} is trivial: (3.3a) is replaced now by the fact that

$$\|V - W\|^2 = -\frac{k}{2}\,\mathrm{Im}(f_\delta(V) - f_\delta(W), V - W) \le \frac{kL}{2}\|V - W\|^2$$

implying $V = W$ if $k < 2/L$. Estimating the error $\|u^n - V^n\|$ is also straightforward by the standard energy argument for Crank–Nicolson–Galerkin methods, cf. e.g. [16]:

Lemma 3.2. *If V^n satisfy* (3.12) *and u is sufficiently smooth then*

$$\text{(3.13)} \qquad \max_{0 \le n \le J} \|u^n - V^n\| \le c(u,\delta)(\|u^0 - u_h^0\| + k^2 + h^r).$$

Proof. Let $\theta^n = V^n - P_I u^n$, $\rho^n = P_I u^n - u^n$. By (2.4)

$$\text{(3.14)} \qquad \|\rho^n\| \le c(u) h^r.$$

To estimate θ^n note that (3.12), (2.3) and (1.1) yield for $0 \le n \le J-1$, $\chi \in S_h$

$$\text{(3.15)} \qquad (\theta^{n+1} - \theta^n, \chi) + \frac{\mathrm{i}k}{2}(\nabla(\theta^{n+1} + \theta^n), \nabla\chi) = -k(\omega^n, \chi),$$

where $\omega^n = \omega_1^n + \omega_2^n + \omega_3^n + \omega_4^n$ and

$$\omega_1^n = k^{-1}[(P_I - I)(u^{n+1} - u^n)]$$
$$\omega_2^n = k^{-1}(u^{n+1} - u^n) - u_t^{n+1/2}$$
$$\omega_3^n = \mathrm{i}\{\Delta u^{n+1/2} - \frac{1}{2}\Delta(u^n + u^{n+1})\}$$
$$\omega_4^n = \mathrm{i}\{f_\delta(u^{n+1/2}) - f_\delta(\frac{1}{2}(V^n + V^{n+1}))\},$$

where we put $v^{n+1/2} = v(t^{n+1/2}) = v(t^n + \frac{k}{2})$. Now it is straightforward to check that for constants $c = c(u)$, $\|\omega_1^n\| \le ch^r$, $\|\omega_i^n\| \le ck^2$, $i = 2, 3$, and, using the Lipschitz condition of f_δ and (3.14), that

$$\|\omega_4^n\| \le \frac{L}{2}(\|\theta^n\| + \|\theta^{n+1}\|) + c(u,\delta)(k^2 + h^r).$$

Taking $\chi = \frac{1}{2}(\theta^n + \theta^{n+1})$ in (3.15) and then real parts yields $\|\theta^{n+1}\| \le \|\theta^n\| + k\|\omega^n\|$, which, in view of the above estimates for the ω_i^n and (3.14), yields (3.13) for k sufficiently small. □

The proof of an L^2 estimate for $u^n - U^n$ follows:

Theorem 3.1. *Suppose that u is sufficiently smooth,* (1.9) *holds and* $k = o(h^{d/4})$. *Then, there exists a unique solution U^n of* (1.10) *that satisfies*

$$\max_{0 \le n \le J} \|u^n - U^n\| \le c(u)(k^2 + h^r). \tag{3.16}$$

Proof. Fix $\delta > 0$. Then (1.9) and (3.13) give

$$\max_{0 \le n \le J} \|u^n - V^n\| \le c(k^2 + h^r). \tag{3.17}$$

For an arbitrary $\chi \in S_h$ and θ^n as in the proof of Lemma 3.2 we have, using (1.6), (2.4), (3.13) that for $0 \le n \le J$

$$\begin{aligned} |u^n - V^n|_\infty &\le |u^n - \chi|_\infty + |\chi - P_I u^n|_\infty + |\theta^n|_\infty \\ &\le |u^n - \chi|_\infty + ch^{-d/2}(\|u^n - \chi\| + \|\rho^n\|) + |\theta^n|_\infty \\ &\le (|u^n - \chi|_\infty + ch^{-d/2}\|u^n - \chi\|) + ch^{r-d/2} + ch^{-d/2}k^2. \end{aligned}$$

It is seen then, using (1.7) and our hypotheses, that $|u^n - V^n|_\infty < \frac{\delta}{2}$, $0 \le n \le J$, for k, h sufficiently small. Since, for k sufficiently small, $|u^{n+1/2} - \frac{1}{2}(u^n + u^{n+1})|_\infty < \frac{\delta}{2}$, $0 \le n \le J-1$, we conclude that $\frac{1}{2}(V^n + V^{n+1})(x) \in M_\delta$ for $x \in \bar{\Omega}, 0 \le n \le J-1$. But then (3.12) gives that for $0 \le n \le J$, $V^n = U^n$, where U^n is a solution of (1.10). Moreover U^n satisfies (3.16) in view of (3.17). In addition, solutions of (1.10) that are close to the exact solution u^n in the sense of e.g. (3.16) are necessarily unique. To see this, note that (1.6), (1.7), (3.16) and (2.4) give for $\chi \in S_h$, $0 \le n \le J$

$$\begin{aligned} |u^n - U^n|_\infty &\le |U^n - \chi|_\infty + |u^n - \chi|_\infty \\ &\le ch^{-d/2}\|U^n - u^n\| + (ch^{-d/2}\|u^n - \chi\| + |u^n - \chi|_\infty) \to 0, \quad \textit{as} \quad k, h \to 0. \end{aligned}$$

Therefore $\max_n |U^n|_\infty \le c$ for some constant c independent of k and h. Such solutions are unique by Proposition 3.1. □

We now proceed to the scheme (1.13). To establish existence of solutions let $U^{n+1/2} = \frac{1}{2}(U^n + U^{n+1})$, define $\Psi : S_h \to S_h$, given $U^n \in S_h$, by

$$(\Psi(v), \chi) = \frac{1}{2}\big[-(\nabla v, \nabla \chi) + \frac{\lambda}{2}((|2v - U^n|^2 + |U^n|^2)v, \chi)\big], \qquad v, \chi \in S_h,$$

and rewrite (1.13) as

$$U^{n+1/2} = U^n + \mathrm{i}k\Psi(U^{n+1/2})\,. \tag{3.18}$$

Defining now $\Pi : S_h \to S_h$ as $\Pi(v) = v - U^n - \mathrm{i}k\Psi(v)$ we may easily see that $\mathrm{Re}(\Pi(v), v) > 0$ for $v \in S_h$ such that $\|v\| = \|U^n\| + 1$. Existence of a solution of $\Pi(v) = 0$, i.e. of U^{n+1} , follows from Lemma 3.1. Setting now $\varphi = U^n + U^{n+1}$ in (1.13) and taking real parts yields (1.11), whereas putting $\varphi = U^{n+1} - U^n$ and taking imaginary parts yields (1.14). The a priori estimates that (1.14) provides are crucial in the study of uniqueness of solutions of (1.13). Indeed, given $U^n \in S_h$, let V, W satisfy (3.18), i.e. suppose that

$$V = U^n + \mathrm{i}k\Psi(V)\,, \quad W = U^n + \mathrm{i}k\Psi(W); \tag{3.19}$$

recall that by (1.11) $\|V, W\| = \max(\|V\|, \|W\|) \le \|U_0\|$. Denoting now $G(V, W) = |2V - U^n|^2 V - |2W - U^n|^2 W$, we see from (3.19) that

$$\|V - W\|^2 = -\frac{\mathrm{i}k}{2}\|\nabla(V - W)\|^2 + \frac{\mathrm{i}k\lambda}{2}(G(V, W) + |U^n|^2(V - W), V - W).$$

Consequently, taking real and imaginary parts in the above and using Hölder's inequality in the right-hand sides of the resulting identities, we obtain the following analogs of (3.4a,b) in the case of (1.13):

$$\|V - W\|^2 \le \frac{|\lambda| k}{2}|G(V, W)|_{4/3}\,|V - W|_4, \tag{3.20a}$$

$$\|\nabla(V - W)\|^2 \le |\lambda|\,|G(V, W)|_{4/3}|V - W|_4 + |\lambda|\,(|U^n|^2(V - W), V - W). \tag{3.20b}$$

Now, since $\big||2z_1 - z|^2 z_1 - |2z_2 - z|^2 z_2\big| \le 4(|z_1| + |z_2| + \frac{1}{2}|z|)^2 |z_1 - z_2|$ for $z_1, z_2, z \in \mathbb{C}$, a straightforward application of Hölder's inequality yields that

$$|G(V, W)|_{4/3} \le c\,|V, W, U^n|_4^2\,|V - W|_4,$$

where $|V, W, U^n|_4 = \max(|V|_4, |W|_4, |U^n|_4)$ and c is a numerical constant. This estimate, inserted in (3.20a,b), yields, respectively,

$$\|V - W\|^2 \le c_1|\lambda|\; k\,|V, W, U^n|_4^2\,|V - W|_4^2, \tag{3.21a}$$

$$\|\nabla(V - W)\|^2 \le c_2|\lambda|\,|V, W, U^n|_4^2\,|V - W|_4^2, \tag{3.21b}$$

where c_1, c_2 are numerical constants. Suppose finally that the initial condition U^0 of (1.13) is chosen so that

$$\|U^0\|_1 \le c, \quad c \text{ independent of } h. \tag{3.22}$$

(This would be the case e.g. if $u^0 \in H_0^1$ and $U^0 = P_I u^0$ implying $\|U^0\|_1 \le c\|u^0\|_1$.)

If $d = 1$, it follows from (2.9) and (3.22) that $|U^n|_4^4 \le c\|\nabla U^n\|$, $0 \le n \le J$. Then (1.14) yields $\|\nabla U^n\|^2 - \lambda c\|\nabla U^n\| \le c'$; we conclude

$$\|\nabla U^n\| + |U^n|_4 \le c\,, \qquad 0 \le n \le J, \tag{3.23}$$

which implies $|V, W, U^n|_4 \le c$. Then, by (2.9), (3.21a,b) we have

$$|V - W|_4^4 \le c\lambda^2 k^{3/2} |V - W|_4^4,$$

i.e. uniqueness for k sufficiently small.

If $d = 2$ and $\lambda \le 0$, use of (3.10), (3.22) and (1.14) gives (3.23) again. It follows, by (3.10), (3.21a,b) that $|V - W|_4^4 \le c\lambda^2 k |V - W|_4^4$. If $d = 3$ and $\lambda \le 0$, the same argument goes through, since now the Sobolev-type inequality $|v|_4^4 \le c\|v\|\,\|\nabla v\|^3$, $v \in H_0^1$, (3.22) and (1.14) imply (3.23); as a consequence, (3.21a,b) yield now that $|V - W|_4^4 \le c\lambda^2 k^{1/2} |V - W|_4^4$. In both cases we have uniqueness for k sufficiently small. Finally, if $d = 2$ and $\lambda > 0$, (3.10), (3.22) and (1.14) yield $\|\nabla U^n\|^2 (1 - \frac{c_0\lambda}{2}\|U^0\|^2) \le c$ and therefore, in the same manner as above, uniqueness for k sufficiently small, provided $c_0\lambda\|U^0\|^2 < 2$. We summarize in the following

Proposition 3.2. *For $0 \le n \le J$ there exists a solution $U^n \in S_h$ of the scheme* (1.13)*; U^n satisfies* (1.11) *and* (1.14)*. Suppose U^0 is chosen so that* (3.22) *holds and that k is sufficiently small. Then U^n is unique if $d = 1$ or $d = 2$ and $\lambda \le 0$ or $d = 3$ and $\lambda \le 0$ or $d = 2$, $\lambda > 0$ and $c_0\lambda\|U^0\|^2 < 2$.* □

To complete the study of these schemes we finally prove an L^2 error estimate for (1.13).

Theorem 3.2. *Suppose that u is sufficiently smooth,* (1.9) *holds and $k = o(h^{d/4})$. Then, there exists a unique solution U^n of* (1.13) *that satisfies*

$$\max_{0 \le n \le J} \|u^n - U^n\| \le c(k^2 + h^r). \tag{3.24}$$

Proof. We shall only outline the proof as many of the estimates are analogs of similar ones in the proofs of Lemma 3.2 and Theorem 3.1. Let $F : \mathbb{C} \times \mathbb{C} \to \mathbb{C}$ be defined by $F(w, z) = \frac{\lambda}{4}(|w|^2 + |z|^2)(w + z)$. Fix $\delta > 0$ and let $\tilde{M}_\delta = \{(z, w) \in \mathbb{C} \times \mathbb{C} : \exists (x,t), (y,s) \in \bar{v}ar \times [0,T] \quad |z - u(x,t)|, |w - u(y,s)| < \delta\}$ and $F_\delta : \mathbb{C} \times \mathbb{C} \to \mathbb{C}$ be a (globally) Lipschitz continuous function that coincides with F on $\tilde{M}_\delta$. Define V^n, $0 \le n \le J$, in S_h by

$$\begin{cases} \frac{1}{k}(V^{n+1} - V^n, \chi) + \frac{\mathrm{i}}{2}\big(\nabla(V^{n+1} + V^n), \nabla\chi\big) = \mathrm{i}\big(F_\delta(V^{n+1}, V^n), \chi\big) \\ \qquad\qquad\qquad\qquad \forall \chi \in S_h, \quad 0 \le n \le J-1, \\ V^0 = u_h^0. \end{cases} \tag{3.25}$$

That the V^n exist uniquely in S_h follows in a straightforward manner from Lemma 3.1 and the Lipschitz continuity of F_δ, if k is sufficiently small. In addition, V^n satisfies

$$\max_{0 \le n \le J} \|u^n - V^n\| \le c(k^2 + h^r)\,. \tag{3.26}$$

To see this, let $\theta^n = V^n - P_I u^n$. Then it follows from (1.1), (3.25) that (3.15) holds again, mutatis mutandis, with $\omega^n = \sum_{i=1}^4 \omega_i^n$, where, for $1 \le i \le 3$, the ω_i^n are defined as in the proof of Lemma 3.2 and $\omega_4^n = i\{f(u^{n+1/2}) - F_\delta(V^{n+1}, V^n)\}$, $u^{n+1/2} = \frac{1}{2}(u^n + u^{n+1})$. (Here f is given by (1.2).) This last term is estimated as follows, in view of (3.14)

$$\begin{aligned}\|\omega_4^n\| &\le \||u^{n+1/2}|^2(u^{n+1/2} - \frac{1}{2}(u^n + u^{n+1}))\| \\ &+\|(|u^{n+1/2}|^2 - \frac{1}{2}(|u^n|^2 + |u^{n+1}|^2))(u^n + u^{n+1})\| + \|F_\delta(u^{n+1}, u^n) - F_\delta(V^{n+1}, V^n)\| \\ &\le c(u)k^2 + \tilde{L}(\|u^{n+1} - V^{n+1}\| + \|u^n - V^n\|) \\ &\le c(u,\delta)(\|\theta^n\| + \|\theta^{n+1}\| + k^2 + h^r),\end{aligned}$$

where $\tilde{L}$ is the Lipschitz constant of F_δ. (3.26) follows now exactly as in the proof of Lemma 3.2. Finally, repeating the argument of the proof of Theorem 3.1 it is seen, since $k = o(h^{d/4})$, that for k and h sufficiently small, $|u^n - V^n|_\infty < \frac{\delta}{2}, \quad 0 \le n \le J$. Hence $(V^n(x), V^{n-1}(x)) \in \tilde{M}_\delta \quad \forall x \in \bar{\Omega}$, i.e. V^n coincides with U^n, a solution of (1.13), and (3.24) holds. As before, we may argue that solutions of (1.13) satisfying (3.24) are unique. □

4. Newton's Method

In this section we shall study the fully discrete scheme that results when, at each time step, the nonlinear system represented by (1.10) is approximated by one iteration of Newton's method with suitable starting conditions. In the sequel we suppose that f is given by (1.2) and let RS_h denote the space of the real-valued elements of S_h. Hence, given $\varphi \in S_h$, there exist $\chi, \psi \in RS_h$ such that $\varphi = \chi + i\psi$.

For $n \ge 1$, let in (1.10) $U^n = V^n + iW^n, \quad V^n, W^n \in RS_h$. It is straightforward to check that applying one step of Newton's method to the nonlinear system (1.10) yields the following time stepping scheme, that, for $0 \le n \le J-1$, given initial approximations V_0^{n+1}, W_0^{n+1} to $V^{n+1}, W^{n+1} \in RS_h$, determines the (final) approximations V_1^{n+1}, $W_1^{n+1} \in RS_h$ to V^{n+1}, W^{n+1} as solutions of the linear system

$$\begin{aligned}&(V_1^{n+1},\chi) - \frac{k}{2}(\nabla W_1^{n+1},\nabla\chi) + \frac{\lambda k}{4}\big((V_0^{n+1}+V_1^n)(W_0^{n+1}+W_1^n)(V_1^{n+1}-V_0^{n+1}),\chi\big) \\ &\quad + \frac{\lambda k}{8}\big([(V_0^{n+1}+V_1^n)^2 + 3(W_0^{n+1}+W_1^n)^2]\,(W_1^{n+1}-W_0^{n+1}),\chi\big) \\ &= (V_1^n,\chi) + \frac{k}{2}(\nabla W_1^n,\nabla\chi) - \frac{\lambda k}{8}\big([(V_0^{n+1}+V_1^n)^2 + (W_0^{n+1}+W_1^n)^2] \\ &\quad \cdot (W_0^{n+1}+W_1^n),\chi\big) \quad \forall \chi \in RS_h,\end{aligned} \tag{4.1a}$$

$$(4.1b)\quad \begin{aligned}&(W_1^{n+1},\chi)+\frac{k}{2}(\nabla V_1^{n+1},\nabla\chi)-\frac{\lambda k}{4}\big((V_0^{n+1}+V_1^n)(W_0^{n+1}+W_1^n)(W_1^{n+1}-W_0^{n+1}),\chi\big)\\ &\qquad -\frac{\lambda k}{8}\big([3(V_0^{n+1}+V_1^n)^2+(W_0^{n+1}+W_1^n)^2](V_1^{n+1}-V_0^{n+1}),\chi\big)\\ &=(W_1^n,\chi)-\frac{k}{2}(\nabla V_1^n,\nabla\chi)+\frac{\lambda k}{8}\big([(V_0^{n+1}+V_1^n)^2+(W_0^{n+1}+W_1^n)^2]\\ &\qquad \cdot(V_0^{n+1}+V_1^n),\chi\big)\quad \forall\chi\in RS_h.\end{aligned}$$

To provide initial values for the scheme, define $V_1^0, W_1^0 \in RS_h$ by

$$(4.2)\qquad V_1^0+\mathrm{i}W_1^0=U_1^0=U^0=Pu^0,$$

where P is the L^2-projection operator onto S_h. Then, at each time step $n, 0\le n\le J-1$, compute the starting values $V_0^{n+1}+\mathrm{i}W_0^{n+1}=U_0^{n+1}$ needed in (4.1a,b) by

$$(4.3)\qquad U_0^{n+1}=2U_1^n-U_1^{n-1}\quad \text{if}\quad n=1,\dots,J-1,$$

$$(4.4)\qquad (U_0^1-U_1^0,\chi)+\frac{\mathrm{i}k}{2}\big(\nabla(U_0^1+U_1^0),\nabla\chi\big)=\mathrm{i}k\lambda\big(|U_1^0|^2\,U_1^0,\chi\big)\qquad \forall\chi\in S_h.$$

In the theorem that follows we shall show that these approximations exist uniquely and satisfy an L^2 optimal-order error estimate. To this effect we fix $\delta>0$ and, denoting by v, resp. w, the real, resp. imaginary, parts of u, the solution of (1.1), define the intervals I_δ, J_δ as

$$(4.5)\qquad \begin{aligned}I_\delta&=\big[-\delta+\inf\ v(x,t)\ ,\ \delta+\sup\ v(x,t)\big],\\ J_\delta&=\big[-\delta+\inf\ w(x,t)\ ,\ \delta+\sup\ w(x,t)\big],\end{aligned}$$

where the inf and sup are taken over $\bar{\Omega}\times[0,T]$. We also suppose that k and h are sufficiently small, and the hypotheses of Theorem 3.1 (with $U^0=Pu^0$) hold so that there exists a unique solution U^n , $0\le n\le J$, of (1.10) satisfying

$$(4.6)\qquad \max_{0\le n\le J}|u^n-U^n|_\infty<\frac{\delta}{2}\,.$$

Theorem 4.1. *Suppose u is sufficiently smooth, $k=o(h^{d/4})$ and let U^n, $0\le n\le J$, satisfy* (1.10) *and* (4.6). *Then, $U_1^n=V_1^n+\mathrm{i}W_1^n$, $n=0,\dots,J$, are uniquely defined by* (4.1)–(4.4) *and satisfy*

$$(4.7)\qquad \max_{0\le n\le J}\|U_1^n-U^n\|\le C^*(k^2+h^r),$$

for some constant $C^*=C^*(u)$, independent of k and h.

Proof. (4.4) defines U_0^1 uniquely as solution of an invertible linear system. Moreover, using techniques of section 3, we may easily see that

$$(4.8)\qquad \|U_0^1-U^1\|\le\tilde{C}(k^2+h^r).$$

To establish (4.7) we shall prove that U_1^ℓ exists uniquely for $0\le\ell\le J$ and that

$$(4.9)\qquad \|U_1^\ell-U^\ell\|\le C_\ell(k^2+h^r)$$

for constants C_ℓ independent of k, h, that are given for $2 \le \ell \le J$ by

$$C_\ell = Dk + (1 + Dk)C_{\ell-1} + DkC_{\ell-2}, \tag{4.10}$$

where $C_0 = 0$, C_1 will be specified below and the constant D is defined (with 20/20 hindsight) as follows: Let c_1 be the maximum of the two constants (both denoted by $c(u)$) occurring in (3.16) and in

$$\max_{1\le n\le J-1} \|u^{n+1} - 2u^n + u^{n-1}\| \le c(u)k^2. \tag{4.11}$$

Define L_δ so that for $g : \mathbb{R}^2 \to \mathbb{R}, \quad g(x, y) = (x^2 + y^2)y$ there holds

$$\max_{x,y\in I_\delta\cup J_\delta} |\partial_1 g(x, y)| + \max_{x,y\in I_\delta\cup J_\delta} |\partial_2 g(x, y)| \le L_\delta, \tag{4.12}$$

where we denote $\partial_1 g = g_x$, $\partial_2 g = g_y$ etc. Moreover, for fixed $0 < \gamma < 1$ define c_2 so that

$$\frac{1 + 2L_\delta|\lambda|k}{1 - 2L_\delta|\lambda|k} \le 1 + c_2 k \qquad \text{for} \quad k \le \frac{\gamma}{2L_\delta|\lambda|}. \tag{4.13}$$

Using this notation define finally D as

$$D = \max(5c_1, 2c_2 + 3). \tag{4.14}$$

Given C_1, it may be easily seen that if the C_ℓ are given by (4.10), then there exists a constant C^*, independent of k and h, such that

$$\max_{0\le n\le J} C_n \le C^*. \tag{4.15}$$

In the sequel we shall also suppose that k, h will be eventually taken to be sufficiently small; in particular, so small that inequalities of the type $c\,C^* h^{-d/2}(k^2 + h^r) < \frac{\delta}{2}$ are satisfied. This of course can always be achieved since $k = o(h^{d/4})$ and $r \ge 2$.

The proof of (4.9)–(4.10) will be done inductively. (4.9) holds trivially for $\ell = 0$ (with $C_0 = 0$) in view of the choice (4.2). Assume that given $0 \le n \le J-1$, U_1^ℓ exist uniquely and (4.9) holds for $0 \le \ell \le n$. We shall show that U_1^{n+1} exists uniquely and that (4.9) is true if $\ell = n + 1$.

It is straightforward to check first that V_1^{n+1}, W_1^{n+1} exist uniquely in RS_h (and hence U_1^{n+1} in S_h) as solution of the $2\dim S_h \times 2\dim S_h$ invertible linear system represented by (4.1a,b). To this end, consider the associated homogeneous system (given V_0^{n+1}, W_0^{n+1}, V_1^n, W_1^n). Note that (1.6), (4.9) and (4.6) yield the a priori estimates $|V_1^\ell|_\infty + |W_1^\ell|_\infty \le c$, $0 \le \ell \le n$, and that (1.6), (4.8) and (4.3) also yield then that $|V_0^1|_\infty + |W_0^1|_\infty \le c$, $|V_0^{n+1}|_\infty + |W_0^{n+1}|_\infty \le c$. Conclude then, by putting $\chi = V_1^{n+1}$, resp. $\chi = W_1^{n+1}$, in (4.1a), resp. (4.1b), and adding, that the homogeneous system has only the trivial solution.

The basic idea in the inductive step is to compare U_1^{n+1} with $\tilde{U}^{n+1}$, where

$$\begin{aligned}(\tilde{U}^{\ell+1} - U_1^\ell, \chi) + \frac{\mathrm{i}k}{2}\big(\nabla(\tilde{U}^{\ell+1} + U_1^\ell), \nabla\chi\big) = \mathrm{i}k\big(f(\tfrac{1}{2}(\tilde{U}^{\ell+1} + U_1^\ell)), \chi\big)\\ \forall\chi \in S_h, \quad 0 \le \ell \le n.\end{aligned} \tag{4.16}$$

Using techniques of section 3 it may be easily inferred from (4.9) that, for k, h sufficiently small, (4.16) has a solution satisfying (since $\tilde{U}^1 = U^1$)

$$|\tilde{U}^{\ell+1} - u^{\ell+1}|_\infty < \frac{\delta}{2}, \quad 0 \le \ell \le n. \tag{4.17}$$

In particular $\frac{1}{2}(\tilde{V}^{\ell+1} + V_1^\ell)(x) \in I_\delta$, $\frac{1}{2}(\tilde{W}^{\ell+1} + W_1^\ell)(x) \in J_\delta$, for $0 \le \ell \le n$, $x \in \bar{\Omega}$, where $\tilde{U}^{\ell+1} = \tilde{V}^{\ell+1} + i\tilde{W}^{\ell+1}$. We also note that by (4.16), (1.10) and (4.6), (4.17), (4.12), (4.13) there follows the stability estimate

$$\|U^{\ell+1} - \tilde{U}^{\ell+1}\| \le (1 + c_2 k)\, \|U^\ell - U_1^\ell\|, \quad 0 \le \ell \le n. \tag{4.18}$$

Write now (4.16) as a system of two equations for $\tilde{V}^{\ell+1}$ and $\tilde{W}^{\ell+1}$, and subtract the first of the two resulting equations from (4.1a). Expand the nonlinear expressions in the terms of the equation by Taylor's theorem up to second-order terms about the point $\big(\frac{1}{2}(V_0^{n+1} + V_1^n),\ \frac{1}{2}(W_0^{n+1} + W_1^n)\big)$ to obtain

$$\begin{aligned}
&(V_1^{n+1} - \tilde{V}^{n+1}, \chi) - \frac{k}{2}\big(\nabla(W_1^{n+1} - \tilde{W}^{n+1}), \nabla\chi\big)\\
&+ \frac{\lambda k}{2}\big(\partial_1 g\big(\frac{1}{2}(V_0^{n+1} + V_1^n), \frac{1}{2}(W_0^{n+1} + W_1^n)\big)(V_1^{n+1} - \tilde{V}^{n+1}), \chi\big)\\
&+ \frac{\lambda k}{2}\big(\partial_2 g\big(\frac{1}{2}(V_0^{n+1} + V_1^n), \frac{1}{2}(W_0^{n+1} + W_1^n)\big)(W_1^{n+1} - \tilde{W}^{n+1}), \chi\big)\\
&- \frac{\lambda k}{8}\big(\partial_1^2 g(A,B)(\tilde{V}^{n+1} - V_0^{n+1})^2 + \partial_2^2 g(A,B)(\tilde{W}^{n+1} - W_0^{n+1})^2\\
&\qquad 2\partial_1\partial_2 g(A,B)(\tilde{V}^{n+1} - V_0^{n+1})(\tilde{W}^{n+1} - W_0^{n+1}), \chi\big) = 0 \qquad \forall \chi \in RS_h,
\end{aligned} \tag{4.19}$$

where

$$\begin{aligned}
A &= \frac{1}{2}\big[\xi(\tilde{V}^{n+1} + V_1^n) + (1-\xi)(V_0^{n+1} + V_1^n)\big],\\
B &= \frac{1}{2}\big[\xi(\tilde{W}^{n+1} + W_1^n) + (1-\xi)(W_0^{n+1} + W_1^n)\big],
\end{aligned}$$

and $\xi = \xi_n : \bar{\Omega} \to [0,1]$. Denoting $\mu_{ij} = \max_{x,y \in I_\delta \cup J_\delta} |\partial_i\partial_j\, g(x,y)|$, $c_g = \mu_{11} + 2\mu_{12} + \mu_{22}$, taking in (4.19) $\chi = \tilde{V}^{n+1} - V^{n+1}$ and using (1.6), we see that

$$\begin{aligned}
\|V_1^{n+1} - \tilde{V}^{n+1}\|^2 &- \frac{k}{2}\big(\nabla(W_1^{n+1} - \tilde{W}^{n+1}), \nabla(V_1^{n+1} - \tilde{V}^{n+1})\big)\\
&\le \frac{1}{2}|\lambda| L_\delta k\big(\|V_1^{n+1} - \tilde{V}^{n+1}\|^2 + \|W_1^{n+1} - \tilde{W}^{n+1}\|\,\|V_1^{n+1} - \tilde{V}^{n+1}\|\big)\\
&\quad + \frac{1}{8}|\lambda| c_g\, c_I\, k h^{-d/2}\big(\|\tilde{V}^{n+1} - V_0^{n+1}\|^2 + \|\tilde{W}^{n+1} - W_0^{n+1}\|^2\\
&\qquad + \|\tilde{V}^{n+1} - V_0^{n+1}\|\,\|\tilde{W}^{n+1} - W_0^{n+1}\|\big)\|V_1^{n+1} - \tilde{V}^{n+1}\|.
\end{aligned}$$

In an entirely analogous manner a similar estimate may be obtained for $\|W_1^{n+1} - \tilde{W}^{n+1}\|^2$. Adding the two inequalities gives

$$\begin{aligned}
\|U_1^{n+1} - \tilde{U}^{n+1}\|^2 \le\, & L_\delta |\lambda| k \|U_1^{n+1} - \tilde{U}^{n+1}\|^2\\
&+ \frac{3\sqrt{2}}{16}\,|\lambda| c_g\, c_I\, k h^{-d/2} \|\tilde{U}_0^{n+1} - U_0^{n+1}\|^2\, \|U_1^{n+1} - \tilde{U}^{n+1}\|.
\end{aligned}$$

Hence taking $L_\delta|\lambda|k < \frac{1}{2}$ and putting $\alpha = \frac{3}{8}\sqrt{2}|\lambda|c_g c_I$ gives

$$\|U_1^{n+1} - \tilde{U}^{n+1}\| \le \alpha k h^{-d/2} \|U_0^{n+1} - \tilde{U}^{n+1}\|^2. \tag{4.20}$$

(It is straightforward to check that (4.20) also holds if $n = 0$. This yields, in view of (4.8), since $\tilde{U}^1 = U^1$ and $k = o(h^{d/4})$

$$\begin{aligned} \|U_1^1 - U^1\| &\le \alpha \tilde{C}^2 k h^{-d/2} (k^2 + h^r)^2 \\ &\le C_1 (k^2 + h^r), \end{aligned}$$

where C_1 is a constant independent of k and h. This inequality defines then C_1 and verifies (4.9) if $\ell = 1$.) Finally, for $n \ge 1$, since

$$\begin{aligned} \tilde{U}^{n+1} - U_0^{n+1} = (\tilde{U}^{n+1} - U^{n+1}) + (U^{n+1} - u^{n+1}) - 2(U^n - u^n) + (U^{n-1} - u^{n-1}) \\ + (u^{n+1} - 2u^n + u^{n-1}) + 2(U^n - U_1^n) - (U^{n-1} - U_1^{n-1}), \end{aligned}$$

using (4.18), (3.16), (4.11), (4.9) for $\ell = n, n-1$ and the notation for constants introduced in the beginning of the proof, we have

$$\|\tilde{U}^{n+1} - U_0^{n+1}\| \le \big(5c_1 + (3 + c_2 k) C_n + C_{n-1}\big)(k^2 + h^r) = d_{n+1}(k^2 + h^r).$$

It follows by (4.20), since $d_{n+1} \le (4 + c_2)C^* + 5c_1, \quad k = o(h^{d/4})$, by taking k and h sufficiently small, that $\|U_1^{n+1} - \tilde{U}^{n+1}\| \le d_{n+1} k (k^2 + h^r)$, i.e. the basic estimate sought. This, together with (4.18), (4.9) for $\ell = n$ yields easily that

$$\begin{aligned} \|U^{n+1} - U_1^{n+1}\| &\le \|U^{n+1} - \tilde{U}^{n+1}\| + \|\tilde{U}^{n+1} - U_1^{n+1}\| \\ &\le \big(Dk + (1 + Dk)C_n + DkC_{n-1}\big)(k^2 + h^r) \\ &= C_{n+1}(k^2 + h^r), \end{aligned}$$

which completes the inductive step. □

5. Implementation of Newton's Method

To avoid having to solve the $2\dim S_h \times 2\dim S_h$ real linear system of equations represented by (4.1a,b) whose matrix changes with n, we shall devise, as stated in the Introduction, an iterative method for solving for each n (4.1a,b) approximately. We shall refer to it as the *inner* iteration, the 'outer' being the single step of Newton's method. This inner iteration requires solving, at each time step n, $0 \le n \le J$, $j_n \ge 1$ linear sparse complex systems of size $\dim S_h \times \dim S_h$ and computes approximations $U^{n,j} = V^{n,j} + \mathrm{i}W^{n,j}$, $j = 0, 1, \dots, j_n$, to u^n as follows:

$$U^{0,j_0} = U^0 = Pu^0. \tag{5.1}$$

Using then starting values $U^{n,0}$ computed by

$$(U^{1,0} - U^0, \chi) + \frac{\mathrm{i}k}{2}\big(\nabla(U^{1,0} + U^0), \nabla\chi\big) = \mathrm{i}k\big(f(U^0), \chi\big) \qquad \forall \chi \in S_h, \tag{5.2}$$

$$U^{n+1,0} = 2U^{n,j_n} - U^{n-1,j_{n-1}} \qquad \text{if} \quad n = 1, 2, \dots, J-1, \tag{5.3}$$

the inner iteration is, for $n = 0, \dots, J-1$:

$$
\begin{aligned}
&(V^{n+1,j+1}, \chi) - \frac{k}{2}(\nabla W^{n+1,j+1}, \nabla\chi) \\
&\quad + \frac{\lambda k}{4}\big((V^{n+1,0} + V^{n,j_n})(W^{n+1,0} + W^{n,j_n})(V^{n+1,j} - V^{n+1,0}), \chi\big) \\
&\quad + \frac{\lambda k}{8}\big([(V^{n+1,0} + V^{n,j_n})^2 + 3(W^{n+1,0} + W^{n,j_n})^2]\,(W^{n+1,j} - W^{n+1,0}), \chi\big) \\
&= (V^{n,j_n}, \chi) + \frac{k}{2}(\nabla W^{n,j_n}, \nabla\chi) \\
&\quad - \frac{\lambda k}{8}\big([(V^{n+1,0} + V^{n,j_n})^2 + (W^{n+1,0} + W^{n,j_n})^2](W^{n+1,0} + W^{n,j_n}), \chi\big) \\
&\qquad\qquad\qquad\qquad \forall \chi \in RS_h\,, \qquad j = 0, \dots, j_{n+1} - 1,
\end{aligned} \tag{5.4a}
$$

$$
\begin{aligned}
&(W^{n+1,j+1}, \psi) + \frac{k}{2}(\nabla V^{n+1,j+1}, \nabla\psi) \\
&\quad - \frac{\lambda k}{4}\big((V^{n+1,0} + V^{n,j_n})(W^{n+1,0} + W^{n,j_n})(W^{n+1,j} - W^{n+1,0}), \psi\big) \\
&\quad - \frac{\lambda k}{8}\big([3(V^{n+1,0} + V^{n,j_n})^2 + (W^{n+1,0} + W^{n,j_n})^2](V^{n+1,j} - V^{n+1,0}), \psi\big) \\
&= (W^{n,j_n}, \psi) - \frac{k}{2}(\nabla V^{n,j_n}, \nabla\psi) \\
&\quad + \frac{\lambda k}{8}\big([(V^{n+1,0} + V^{n,j_n})^2 + (W^{n+1,0} + W^{n,j_n})^2](V^{n+1,0} + V^{n,j_n}), \psi\big) \\
&\qquad\qquad\qquad\qquad \forall \psi \in RS_h\,, \qquad j = 0, \dots, j_{n+1} - 1.
\end{aligned} \tag{5.4b}
$$

The inner iteration may be written compactly in the form

$$
\mathcal{A}\begin{pmatrix} V^{n+1,j+1} \\ W^{n+1,j+1} \end{pmatrix} + \mathcal{B}_n \begin{pmatrix} V^{n+1,j} \\ W^{n+1,j} \end{pmatrix} = F_n, \quad j = 0, \dots, j_{n+1} - 1, \tag{5.4$'$}
$$

where the real linear operators $\mathcal{A}, \mathcal{B}_n$ on $(RS_h)^2$ and the vector $F_n \in (RS_h)^2$ are easily discernible from (5.4a,b). In computations we implement the scheme in complex form, i.e. seek $U^{n+1,j+1} \in S_h, \quad 0 \le n \le J-1, \quad 0 \le j \le j_{n+1} - 1$, such that

$$
\begin{aligned}
&(U^{n+1,j+1}, \varphi) + \frac{\mathrm{i}k}{2}(\nabla U^{n+1,j+1}, \nabla\varphi) \\
&= (U^{n,j_n}, \varphi) - \frac{\mathrm{i}k}{2}(\nabla U^{n,j_n}, \nabla\varphi) + (\eta^{n,j}, \varphi)\,, \qquad \forall \varphi \in S_h,
\end{aligned} \tag{5.4$''$}
$$

where the complex-valued $\eta^{n,j}$ depends on the real and imaginary parts of $U^{n+1,j}$ (linearly) and on those of $U^{n+1,0}$, U^{n,j_n}.

We shall estimate now the error $\|U^{n,j_n} - U^n\|$, where U^n is the solution of (1.10). Since the plan and most of the computations of the proof are very similar to those of the proof of Theorem 4.1 we shall omit many details.

Theorem 5.1. *Under the hypotheses of Theorem 4.1 and given integers* $j_n \geq 1, U^{n,j_n} = V^{n,j_n} + \mathrm{i}W^{n,j_n}$ *are defined uniquely in* S_h *by the scheme* (5.1)–(5.4*a,b*) *and satisfy*

$$\max_{0\leq n\leq J} \|U^{n,j_n} - U^n\| \leq \hat{C}^*(k^2 + h^r), \tag{5.5}$$

where $\hat{C}^*$ *is a constant that depends on* u *and* j_n *but is independent of* k *and* h.

Proof. It is obvious from (5.2) and (5.4″) that $U^{n,j}, 0 \leq n \leq J-1, 0 \leq j \leq j_n$, are defined uniquely. Suppose that the conclusions of Theorem 3.1 and (4.6) hold given $\delta > 0$. We shall prove inductively that, for $0 \leq \ell \leq J$:

$$\|U^{\ell,j_\ell} - U^\ell\| \leq \hat{C}_\ell\,(k^2 + h^r), \tag{5.6}$$

where, if $2 \leq \ell \leq J$,

$$\begin{aligned} \hat{C}_\ell =&(\tilde{C}k)^{j_\ell}\big\{5c_1 + Dk + (3+Dk)\hat{C}_{\ell-1} + (1+Dk)\hat{C}_{\ell-2}\big\} \\ &+ Dk + (1+Dk)\hat{C}_{\ell-1} + Dk\hat{C}_{\ell-2}, \end{aligned} \tag{5.7}$$

with c_1, D as in the proof of Theorem 4.1 and $\tilde{C}$ a constant, that will be computed below and depends on $|\lambda|$, $\max|u(x,t)|$ and δ. Given $\hat{C}_0$, $\hat{C}_1$, (5.7) implies the existence of a constant $\hat{C}^*$, independent of k and h, such that $\max_{0\leq n\leq J}\hat{C}_n \leq \hat{C}^*$.

Now (5.6) is trivial for $\ell = 0$ and $\hat{C}_0 = 0$. Assume that (5.6) holds for $0 \leq \ell \leq n$ and let $\tilde{U}_1^{\ell+1} = \tilde{V}_1^{\ell+1} + i\tilde{W}_1^{\ell+1}$ be defined by

$$\mathcal{A}\begin{pmatrix}\tilde{V}_1^{\ell+1}\\ \tilde{W}_1^{\ell+1}\end{pmatrix} + \mathcal{B}_n\begin{pmatrix}\tilde{V}_1^{\ell+1}\\ \tilde{W}_1^{\ell+1}\end{pmatrix} = F_\ell, \quad 0 \leq \ell \leq n. \tag{5.8}$$

As in section 4 it is easily seen that, for k, h sufficiently small, $\tilde{U}_1^{\ell+1}$, $0 \leq \ell \leq n$, exist uniquely and

$$\|\tilde{U}_1^1 - U^1\| \leq C(k^2 + h^r), \tag{5.9a}$$

$$\|\tilde{U}_1^{\ell+1} - U^{\ell+1}\| \leq \big[Dk + (1+Dk)\hat{C}_\ell + Dk\hat{C}_{\ell-1}\big](k^2+h^r), \qquad 1 \leq \ell \leq n+1. \tag{5.9b}$$

Subtracting (5.8) for $\ell = n$ from (5.4′) we obtain, after routine by now estimations, that there exists $\tilde{C} = \tilde{C}(|\lambda|, |u|_\infty, \delta)$ such that

$$\|U^{n+1,j+1} - \tilde{U}_1^{n+1}\| \leq \tilde{C}k\|U^{n+1,j} - \tilde{U}_1^{n+1}\|, \qquad 0 \leq j \leq j_{n+1}-1. \tag{5.10}$$

Also, (4.4), (5.2), (5.9a) and (5.10) give

$$\|U^{1,j_1} - U^1\| \leq \hat{C}_1\,(k^2 + h^r),$$

thus defining $\hat{C}_1$ and verifying (5.6) for $\ell = 1$. The rest of the proof follows now that of Theorem 4.1. Using e.g. an analogous decomposition for $\tilde{U}_1^{n+1} - U^{n+1,0}$, the induction hypotheses, (5.9b) and (5.10) yield

$$\|U^{n+1,j_{n+1}} - \tilde{U}_1^{n+1}\| \leq (\tilde{C}k)^{j_{n+1}}\big\{5c_1 + Dk + (3+Dk)\hat{C}_n + (1+Dk)\hat{C}_{n-1}\big\}(k^2+h^r), \tag{5.11}$$

which together with (5.9b) implies $\|U^{n+1,j_{n+1}} - U^{n+1}\| \leq \hat{C}_{n+1}(k^2+h^r)$. □

This result tells us that, under our hypotheses, performing for each n, $j_n \geq 1$ inner iterations guarantees the stability and the $O(k^2 + h^r)$ asymptotic L^2-error bound of the scheme (5.1)–(5.4). (In fact, if $j_n = 1$ for all n, and we write the scheme directly in terms of $U^{n,1}$, we get, for $n \geq 1$, $\chi \in S_h$

$$(U^{n+1,1} - U^{n,1}, \chi) + \frac{\mathrm{i}k}{2}\big(\nabla(U^{n+1,1} + U^{n,1}), \nabla\chi\big) = \mathrm{i}k\big(f(\frac{3}{2}U^{n,1} - \frac{1}{2}U^{n-1,1}), \chi\big),$$

which we recognize as a standard linearization of the Crank–Nicolson method obtained by extrapolating to $O(k^2)$ from previous values in the nonlinear term. In particular, this scheme is stable and has an L^2 error bound of $O(k^2 + h^r)$.)

From e.g. (5.11) it is evident that taking j_n larger than one for each n should improve the error constant and the conservation properties of the method. To get an idea of what j_n should be in practice for this purpose, we performed some numerical experiments.

We first computed the numerical solution of an easy problem, namely of

$$\begin{cases} u_t = \mathrm{i}u_{xx} + \mathrm{i}|u|^2u, & (x,t) \in [0,1] \times [0,5], \\ u(0,t) = u(1,t) = 0, 0 \leq t \leq 5, & \\ u(x,0) = \sin \pi x, & 0 \leq x \leq 1, \end{cases} \tag{5.12}$$

using piecewise linear, continuous elements in space, i.e. $r = 2$. (All of the experiments reported in the sequel were performed in double precision using complex arithmetic and the VAX Fortran compiler on a VAX 8600 at the University of Crete.) The integrals involved in the nonlinear term, the projection of the initial condition etc. were computed exactly. We computed the quantities

$$I_1^n = I_1(t^n) = \|U^{n,j_n}\|^2 \tag{5.13}$$

$$I_2^n = I_2(t^n) = \|U_x^{n,j_n}\|^2 - \tfrac{1}{2}|U^{n,j_n}|_4^4, \tag{5.14}$$

i.e. the discrete analogs for (5.12) of the invariants (1.3) and (1.4). (U^{n,j_n} was computed by (5.1), (5.2), (5.3), (5.4″).) We took, for safety $j_1 = 4$ at the first step and for $n > 1$ we experimented with values of j_n equal to 1 or 2 or 3 or 4 for all n. In Table 1 we show the values of I_1 and I_2 to 8 decimal digits at $t = i$, $i = 0, 1, \ldots, 5$, from a run with $h = k = 0.01$.

We deduce from this table (the evidence is corroborated by similar runs with smaller h and k) that for the equation and time scale of (5.12) there is practically no difference between the values of I_1 and I_2 corresponding to $j_n = 3$ or 4. However there is a distinct difference between taking $j_n = 2$ or $j_n = 3$. It appears that both I_1 and I_2 are conserved well for $j_n = 3$. In fact it is evident that taking $j_n = 3$ we have practically achieved the values that the *exact* Newton's method with one step would give.

We next computed the numerical solution of a harder to integrate problem with periodic boundary conditions at the endpoints of the spatial interval. Although the formulation and analysis of our schemes was done for homogeneous Dirichlet boundary conditions, it is not hard to see that under minor technical modifications (that include e.g. defining the elliptic projection $P_I u$ as the projection of u onto S_h in the H^1

$I_1(t^n)$				
t^n \ j_n	1	2	3	4
0	.50000000	.50000000	.50000000	.50000000
1	.49985254	.49996255	.50000116	.50000122
2	.49971053	.49992489	.50000231	.50000243
3	.49957087	.49988710	.50000339	.50000358
4	.49942461	.49984926	.50000454	.50000478
5	.49928157	.49981157	.50000572	.50000602

$I_2(t^n)$				
t^n \ j_n	1	2	3	4
0	4.74770808	4.74770808	4.74770808	4.74770808
1	4.74628698	4.74736425	4.74771766	4.74771822
2	4.74492662	4.74701892	4.74772734	4.74772845
3	4.74359035	4.74667620	4.74774045	4.74774213
4	4.74221954	4.74633128	4.74775244	4.74775468
5	4.74088659	4.74598470	4.74776153	4.74777643

TABLE 5.1. Effect of j_n on $I_1(t^n)$ and $I_2(t^n)$; Problem (5.12), $r = 2$, $h = k = 0.01$.

norm and not in H_0^1 etc.), and assuming a smooth periodic solution of the continuous problem gives again our error estimates. As S_h we can take for example the space of smooth periodic splines of order r on a uniform mesh if $d = 1$, etc. We consider the test problem, cf. [15]:

$$\begin{cases} u_t = -iu_{xx} - 2i|u|^2u, & (x,t) \in [-5,5] \times [0,1], \\ u(0,t) = u(1,t), & t \in [0,1], \\ u(x,0) = 4e^{-i(6x+\frac{\pi}{2})}\mathrm{sech}(4x), & x \in [-5,5]. \end{cases} \tag{5.15}$$

The modulus of the initial condition is a solitary wave of amplitude 4, centered at $x = 0$, and of support essentially in [-2,2]. For $t > 0$ this moves to the right without change of form with speed 12 and has completed 1.2 revolutions at $t = 1$. We computed again with the scheme (5.1)–(5.4) in its complex formulation, adapted of course to the equation (5.15) which has $-u_{xx}$ instead of u_{xx}. We monitored the quantities $I_1^n = I_1(t^n)$ given again by (5.13) and $I_2'(t^n)$, the discrete analog of the second invariant appropriate for (5.15), given by

$$I_2'^{\,n} = I_2'(t^n) = \|U_x^{n,j_n}\|^2 - |U^{n,j_n}|_4^4. \tag{5.16}$$

$I_1(t^n)$			
t^n \ j_n	1	2	3
0	8.00000000	8.00000000	8.00000000
0.5	7.99240064	7.98710572	7.99995621
1	7.98491813	7.97431174	7.99991233

$I_2'(t^n)$			
t^n \ j_n	1	2	3
0	245.504539	245.504539	245.504539
0.5	244.547135	245.168987	245.503916
1	243.607008	244.835513	245.503399

TABLE 5.2. Effect of j_n on $I_1(t^n)$ and $I_2'(t^n)$; Problem (5.15), $r = 2$, $h = .01$, $k = .00125$.

We computed with piecewise linear, continuous periodic splines on a uniform mesh with meshlength h on $[-5, 5]$ and evaluated the integrals in the inner products using the three-point Gauss rule on each subinterval of the spatial discretization so that the nonlinear term is computed exactly. In Table 2 we show I_1 and I_2' at $t = 0$, 0.5 and 1 with j_n taken to be equal to 1, 2 or 3 for all $n > 1$ (again $j_n = 4$ gives results practically identical to those of $j_n = 3$) and $h = 0.01$, $k = 0.00125$ (i.e. with 1000 space intervals in [-5,5] and 800 time steps to reach $T = 1$).

Again we see that $j_n = 3$ gives better approximations at $t^n = 1$. Numerical results with other values of h and k and also with cubic periodic splines yielded entirely analogous results.

References

1. H. Brezis and T. Gallouet, *Nonlinear Schrödinger evolution equations*, Nonlinear Analysis **4** (1980) 677–681.
2. F.E.: Browder, *Existence and uniqueness theorems for solutions of nonlinear boundary value problems*, In: Applications of Nonlinear Partial Differential Equations (R. Finn ed.), Proc. Symp. Appl. Math. v. 17, pp. 24–49. Providence: American Mathematical Society 1965.
3. M. Delfour, M. Fortin and G. Payre, *Finite-difference solutions of a non-linear Schrödin- ger equation*, J. Comp. Phys. **44** (1981) 277–288.
4. D.F. Griffiths, A.R. Mitchell and J.Ll. Morris, *A numerical study of the nonlinear Schrödinger equation*, Comp. Methds Appl. Mech. Engrg. **45** (1984) 177–215.
5. B.M. Herbst, J. Ll. Morris and A.R. Mitchell, *Numerical experience with the nonlinear Schrödinger equation*, J. Comp. Phys. **60** (1985) 282–305.

6. B. Le Mesurier, G., Papanicolaou, C. Sulem and P.–L. Sulem, *The focusing singularity of the nonlinear Schrödinger equation*, In: Directions in Partial Differential Equations (M. G. Crandall, P. H. Rabinowitz and R. E. Turner, eds.), pp. 159–201. New York: Academic Press 1987.
7. T. Ogawa, *A proof of Trudinger's inequality and its application to nonlinear Schrödinger equations*, Nonl. Anal. **14** (1990) 765–769.
8. A. Pazy, *Semigroups of Linear Operators and Applications to Partial Differential Equations*, New York: Springer–Verlag, 1983.
9. J.J. Rasmussen and K. Rypdal, *Blow-up in Nonlinear Schrödinger equations–I. A general review*, Phys. Scr. **33** (1986) 481–497.
10. J.M. Sanz-Serna, *Methods for the numerical solution of the nonlinear Schrödinger equation*, Math. Comp. **43** (1984) 21–27.
11. J.M. Sanz-Serna and J.G. Verwer, *Conservative and nonconservative schemes for the solution of the nonlinear Schrödinger equation*, IMA J. Numer. Anal. **6** (1986) 25–42.
12. W.A. Strauss, *The Nonlinear Schrödinger equation*, In: Contemporary Developments in Continuum Mechanics and Partial Differential Equations (G. M. de la Penha and L. A. J. Medeiros, eds.), pp. 452–465. New York: North–Holland 1978.
13. W.A. Strauss and L. Vazquez, *Numerical solution of a nonlinear Klein–Gordon equation*, J. Comp. Phys. **28** (1978) 271–278.
14. P.L. Sulem, C. Sulem and A. Patera, *Numerical simulation of singular solutions to the two-dimensional cubic Schrödinger equation*, Comm. Pure Appl. Math. **37** (1984) 755–778.
15. T.R. Taha and M.J. Ablowitz, *Analytical and numerical aspects of certain nonlinear evolution equations II. Numerical, nonlinear Schrödinger equation*, J. Comp. Phys. **55** (1984) 203–230.
16. V. Thomée, *Galerkin finite element methods for parabolic problems*, Lecture Notes in Mathematics v. 1054. Berlin-Heidelberg: Springer-Verlag, 1984.
17. Y. Tourigny and J.Ll. Morris, *An investigation into the effect of product approximation in the numerical solution of the cubic nonlinear Schrödinger equation*, J. Comp. Phys. **76** (1988) 103–130.
18. J.G. Verwer and J.M. Sanz-Serna, *Convergence of method of lines approximations to partial differential equations*, Computing **33** (1984) 297–313.
19. J.A.C. Weideman and B.M. Herbst, *Split-step methods for the solution of the nonlinear Schrödinger equation*, SIAM J. Numer. Anal. **23** (1986) 485–507.

Note added in proof: In a recent paper, which appeared in *Nonlinear Analysis* **14**, 765–769 (1990), Ogawa has improved the constant that appears in the right–hand side of the Gagliardo–Nirenberg inequality (3.10) by replacing 1/2 by a positive number c_0, no greater than π^{-1}. It follows that if $d = 2$ and $\lambda > 0$ the continuous problem (1.1) has unique global solutions in H^2 provided $u^0 \in H^2 \cap H_0^1$ is chosen so that $c_0\lambda\|u^0\|^2 < 2$. Analogously, we may slightly improve the constants in the uniqueness results of the discrete schemes in Sect. 3. Specifically, it is easily seen that the conclusion of Proposition 3.1 holds if the hypothesis (ii) is weakened to

$$(ii) \qquad d = 2 \ \text{ and } \ c_0|\lambda|\,\|U^0\|^2 < 1/4 \ \text{ if } \ \lambda \le 0 \quad \text{or} \quad c_0\lambda\|U^0\|^2 < \frac{\sqrt{65}-1}{32} \ \text{ if } \ \lambda > 0,$$

and that the hypothesis of the last line of Proposition 3.2 just requires that $c_0\lambda\|U^0\|^2 < 2$ if $d = 2, \lambda > 0$.

Mathematics Department, University of Crete, 714 09 Heraklion, Crete, Greece

Mathematics Department, University of Crete, 714 09 Heraklion, Crete, Greece

Mathematics Department, University of Tennessee, Knoxville, Tenn. 37996, USA