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Finite difference approximation for nonlinear Schrödinger equations with application to blow-up computation

by

Norikazu SAITO and Takiko SASAKI

UNIVERSITY OF TOKYO

GRADUATE SCHOOL OF MATHEMATICAL SCIENCES

KOMABA, TOKYO, JAPAN

Finite difference approximation for nonlinear Schrödinger equations with application to blow-up computation

Norikazu Saito* and Takiko Sasaki†

Graduate School of Mathematical Sciences, The University of Tokyo

3-8-1 Komaba, Meguro, Tokyo 153-8914, Japan

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This paper presents a coherent analysis of the finite difference method to nonlinear Schrödinger (NLS) equations in one spatial dimension. We use the discrete H^1 framework to establish well-posedness and error estimates in the L^∞ norm. The nonlinearity $f(u)$ of a NLS equation is assumed to satisfy only a growth condition. We apply our results to computation of blow-up solutions for a NLS equation with the nonlinearity $f(u) = -|u|^{2p}$, p being a positive real number. Particularly, we offer the numerical blow-up time $T(h,\tau)$, h and τ as discretization parameters of space and time variables. We prove that $T(h,\tau)$ converges to the blow-up time T_∞ of the solution of the original NLS equation. Several numerical examples are presented to confirm the validity of theoretical results. Furthermore, we infer from numerical investigation that the convergence of $T(h,\tau)$ is at a second order rate in τ if the Crank–Nicolson scheme is applied to time discretization.

Key words: nonlinear Schrödinger equation, blow-up, finite difference method

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1. Introduction

The blow-up of solutions is a central concern in the theory of nonlinear partial differential equations. However, it is often the case that we cannot obtain analytic evidence or predictions related to blow-up solutions. Therefore, numerical methods are actually an important approach for the study of blow-up phenomena.

For example, Akrivis et al. [2] studied the blow-up phenomenon for the nonlinear Schrödinger (NLS) equation with cubic nonlinearity, in 2 and 3 spatial dimensions.

*norikazu@ms.u-tokyo.ac.jp

†tsasaki@ms.u-tokyo.ac.jp

They derived the blow-up rate numerically. For the two dimensional case, this corresponds to a critical case. Then they calculated the blow-up rate numerically as

$$\ln\left[\left(\ln\frac{1}{T_\infty - t}\right)\frac{1}{T_\infty - t}\right]^{1/2}.$$

Since the appearance of that paper, Merle and Raphael [13] have demonstrated analytically that the appropriate blow-up rate in the critical case is lower than numerical predictions suggest.

Furthermore, Besse et al. [4] also considered the blow-up problem for NLS equations. They presented numerical investigations related to the dependence of the blow-up time on factors such as the properties of the initial data, the nonlinearity in the equation, and the damping term in the equation.

In this way, numerical results have illuminated many meaningful properties of blow-up solutions that are difficult to prove analytically. Moreover, some numerical results have contributed to derivations of analytical evidence.

However, such results are based on numerical blow-up experiments. No mathematical proof exists that connects analytical blow-ups and numerical blow-ups. To bridge that gap, some results have been proposed related to the convergence of the numerical blow-up time for some heat and wave equations. The pioneering study of this topic was produced by Nakagawa [14] in 1976. He considered a finite difference scheme for a semilinear heat equation

$$\partial_t u - \partial_x^2 u = u^2 \quad (t > 0,\ x \in I = (0,1)) \tag{1}$$

with the Dirichlet boundary condition $u(t,0) = u(t,1) = 0$. Hereinafter, we write $\partial_t = \partial/\partial t$, and so on. If the initial data $u(0,x) = u_0(x)$ are sufficiently large, the unique solution blows up in finite time T_∞ in the sense that

$$\lim_{t\to T_\infty} \|u(t,\cdot)\|_{L^\infty(I)} = \infty.$$

He proposed a numerical blow-up time, and proved that it converges to the exact blow-up time. His strategy is summarized as follows:

Step A. He considers the explicit finite difference approximation for (1) with a (fixed) spatial grid size h and variable time increments Δt_n for $n \geq 0$. Discrete time variables are defined as $t_{n+1} = t_n + \Delta t_n$ for $n \geq 0$. Let $u_h^n(x)$ be the piece-wise constant interpolation of the finite difference solution to $u(t_n, x)$. The time increment Δt_n is defined in terms of u_h^n by

$$\Delta t_n = \tau \min\left\{1, \frac{1}{\|u_h^n\|_{L^2(I)}}\right\},$$

where $\tau = ch^2$ with some $0 < c \leq 1/2$. We have $\Delta t_n \leq \tau$. Then, the numerical blow-up time is defined as

$$T(\tau) = \lim_{n\to\infty} t_n = \lim_{n\to\infty} \sum_{k=0}^{n-1} \Delta t_k \leq \infty. \tag{2}$$

By the definition, $T(\tau) < \infty$ implies that $\|u_h^n\|_{L^2(I)} \to \infty$ as $n \to \infty$.

Step B. Blow-up of u is characterized by a differential inequality for a functional $J(u(t,\cdot))$. Then, by *considering the discrete analogue of the differential inequality*, blow up of the discrete analogue $J_h(u_h(t_n,\cdot))$ of $J(u(t,\cdot))$ is characterized.

Step C. Using the fact

$$\lim_{\tau\to 0}\max_{t_n\in[0,T]}|J_h(u_h(t_n,\cdot)) - J(u(t_n,\cdot))| = 0 \tag{3}$$

for any $T < T_\infty$, he concluded the convergence of the numerical blow up time

$$\lim_{\tau\to 0} T(\tau) = T_\infty. \tag{4}$$

Following Nakagawa's study, many other studies have been produced with the aim of computing numerical blow-up solutions for heat equations. For examples, see [6], [8], and [15]. Recently, similar studies have examined nonlinear wave equations; see [7] and [17].

Apparently, little is known for NLS equations. As a matter of fact, conservative quantities play a crucial role in theory of Schrödinger equations. For example, for the solution of a cubic NLS equation

$$i\partial_t u + \partial_x^2 u = u|u|^2 \quad (t>0,\ x\in\mathbb{R}),$$

its L^2 norm is preserved:

$$\|u(t,\cdot)\|_{L^2(\mathbb{R})} = \|u(0,\cdot)\|_{L^2(\mathbb{R})} \quad (t\ge 0).$$

Hereinafter, $i=\sqrt{-1}$ denotes the imaginary unit. In the design of numerical schemes, the analytic property of the solutions must not be spoiled. Consequently, we prefer conservative numerical schemes. However, the reproduction of blow-up is difficult using conservative schemes because all norms are equivalent in a finite dimensional space. A similar issue for the Keller–Segel system of chemotaxis was discussed and numerical blow-up analysis was reported in [24].

Zhang [23] presented the following interesting result. Consider a special NLS equation

$$i\partial_t u + \partial_x^2 u = -|u|^{2p} \qquad (t>0,\ x\in I=(0,1)), \tag{5a}$$

$$u(t,0)=u(t,1)=0 \qquad (t>0), \tag{5b}$$

$$u(0,x)=u_0(x) \qquad (x\in \bar{I}=[0,1]), \tag{5c}$$

where $p\ge 1$ is a given real number. In contrast to the standard NLS equation, the problem (5) admits no conservation properties. Nevertheless, we are interested in (5) because the finite-time behavior of the solution is controlled by the inequality for a certain functional. To state it more precisely, we set

$$J(t,v) = \frac{\pi}{4}\int_0^1 \mathrm{Im}(e^{i\pi^2 t}v(x))\sin(\pi x)\ dx \tag{6}$$

for $t\ge 0$ and $v\in L^\infty(I)$. Furthermore, we set

$$\lambda_p(u_0) = \frac{2p-1}{\pi^2}|J(0,u_0)|^{2p-1} \tag{7}$$

and

$$T_* = \begin{cases} 1/(2\pi) & \text{if } \lambda_p(u_0) < 1, \\ t_* & \text{if } \lambda_p(u_0) \ge 1, \end{cases} \tag{8}$$

where $0 < t_* \le 1/(2\pi)$ is the unique solution of the equation

$$\sin(\pi^2 t) = \frac{1}{\lambda_p(u_0)} \qquad \left(0 < t \le \frac{1}{2\pi}\right). \tag{9}$$

Zhang then proved the following result.

Proposition 1.1 ([23, Theorem 3.1, case 2])**.** *Let $J(0,u_0) > 0$ and let $0 < T < T_*$ be an arbitrary. Then, if a smooth solution*

$$u \in C^1([0,T]; L^2(I)) \cap C^0([0,T]; H^2(I) \cap H^1_0(I))$$

of (5) exists in $0 \le t \le T$, we have

$$|J(t,u(t))| \ge C_* J(0,u_0) \left[1 - \frac{2p-1}{\pi^2} J(0,u_0)^{2p-1} \sin(\pi^2 t)\right]^{-1/(2p-1)}, \tag{10}$$

for $0 \le t \le T$, where C_* denotes the absolute positive constant depending only on p.

Inequality (10) itself does not appear in the statement of [23, Theorem 3.1, case 2]. However, we first derive (10) and then obtain the main conclusion. As a consequence of (10), there exists a constant $0 < T_J \le T_*$ such that

$$\lim_{t \to T_J} |J(t,u(t))| = 0. \tag{11}$$

Moreover, we have $|J(t,u(t,\cdot))| \le C\|\partial_x u(t,\cdot)\|_{L^2(I)} \le C\|u(t,\cdot)\|_{L^\infty(I)}$. Therefore, we conclude that $u(t,x)$ blows up at finite time $t = T_\infty \le T_J$ in the sense of (2).

This observation indicates the possibility that we can apply Nakagawa's strategy to the NLS equation (5).

This paper has dual purposes. The first is to prove that the implicit θ finite difference (FD) scheme can reproduce the blow-up phenomenon for the NLS equation (5) if $1/2 \le \theta \le 1$. Particularly, we show that the numerical blow-up time $T(h,\tau)$, which converges to the exact blow-up time T_∞, can be introduced by Nakagawa's strategy. To this end, we first establish well-posedness and convergence for the FD scheme. Then, we readily deduce (3) (see Step C above). To consider a discrete version J_h of J (see Step B above), we must define a numerical blow-up time $T(h,\tau)$ as

$$T(h,\tau) \le \frac{1}{4\pi}$$

for technical reasons. Consequently, the time increment Δt_n should be defined as (see (34))

$$\Delta t_n = \tau \cdot \min\left\{1,\ \frac{1}{\|u_h^n\|^q_{L^\infty(I)}},\ a_n\right\} \qquad (n \ge 0), \tag{12}$$

where $q \ge 1$ and $\{a_n\}$ denotes a certain sequence such that $T(h,\tau) \le 1/(4\pi)$ (see (35)). Consequently, $T(h,\tau) < \infty$ does not imply $\|u_h^n\|_{L^\infty(I)} \to \infty$ as $n \to \infty$. Therefore, the original strategy of Nakagawa cannot be applied directly (see Step

A above). To surmount this difficulty, we propose an abstract generalization of results obtained from previous studies [6], [7], [8], [15], [17] and [21]. We introduce a certain abstract setting (I)–(VIII) and consider assumptions (H1)–(H6) (see Section 4). Then, we prove

$$\begin{aligned}
&\text{(H1)–(H4) and (H5)} \quad \Rightarrow \quad T_\infty \geq \limsup_{h,\tau\to 0} T(h,\tau) \quad \text{(see Proposition 4.2);}\\
&\text{(H1)–(H4) and (H6)} \quad \Rightarrow \quad T_\infty \leq \liminf_{h,\tau\to 0} T(h,\tau) \quad \text{(see Proposition 4.3).}
\end{aligned}$$

Subsequently we show that the FD scheme with (12) satisfies assumptions (H1)–(H4) and (H5). Then, we prove that (H6) is actually satisfied by Proposition 4.2. Therefore, we can apply Proposition 4.3 and obtain $\lim_{h,\tau\to 0} T(h,\tau) = T_\infty$.

The second purpose of the study presented in this paper is to state well-posedness and convergence results for the finite difference schemes for NLS equations in a coherent manner. Numerous studies have examined the finite difference method for linear and nonlinear Schrödinger equations. Particularly, [9] is useful to review those subjects. Whereas discrete conservation properties and computational efficiency are well discussed, only a few reports describe convergence and error analysis. For example, we consider a linear Schrödinger equation and the implicit θ scheme for time discretization. Then, the case $1/2 \leq \theta \leq 1$ is well-known to be stable in the sense that $\|G_n\|_2 \leq 1$ holds, where G_n is the finite difference matrix of the FD scheme (see (15)) and $\|\cdot\|_2$ the matrix 2-norm. In contrast, the case for which $\theta = 0$ is not stable in this sense (see also Remark 3.2). However, we cannot find the explicit proof (except for the case $\theta = 1/2$) in the literature. Moreover, when $\theta = 1/2$, G_n becomes a unitary operator in the sense that $\|G_n\|_2 = 1$ holds. Because G_n is a discrete analogue of the Schrödinger semigroup $S(t)$ (see Appendix A), it is a discrete counterpart of the unitarity of $S(t)$. However, the (vector) 2-norm is useless to address nonlinear terms, for example, $-|u|^{2p}$. The ∞-norm is of great use to treat nonlinear terms, but no estimates are available for $\|G_n\|_\infty$. This dilemma complicates error analysis for NLS equations. In fact, if considering a nonlinear heat equation, then we can overcome this issue using the (discrete) smoothing property of the heat semigroup.

Fortunately, our targets are problems have one spatial dimension, such that the discrete H^1 norm $|||\cdot|||_h$ is available (see (48) for the definition). Particularly, we can use a discrete Sobolev inequality $\|\boldsymbol{v}\|_\infty \leq C|||\boldsymbol{v}|||_h$ for $\boldsymbol{v} \in \mathbb{C}^N$, where $\|\cdot\|_\infty$ denotes the vector ∞-norm (see Proposition 2.1 (i)). Moreover, we obtain the discrete unitarity $|||G_n|||_h = 1$ for $\theta = 1/2$ and the discrete contraction property $|||G_n|||_h < 1$ for $1/2 < \theta \leq 1$ (see Proposition 3.1). Combining these facts, we can establish well-posedness and error estimates in the ∞-norm (see Theorems I and II). In other words, we carry out a coherent analysis in the discrete H^1 framework to deduce error estimates in the ∞-norm. L^∞ error estimates for several systems of NLS equations are found, for example, in [3] and [19]. However, those works lack the operator theoretical perspective that we study in this paper.

Our results are valid for quite general NLS equations $i\partial_t u + \partial_x^2 u = f(u) + g(t,x)$. More specifically, on the nonlinerity $f(u)$ we assume only the growth condition, say Condition (f), defined in Section 2. For example, $f(u) = u|u|^{2p}$ and $f(u) = -|u|^{2p}$ for $p \geq 1$ satisfy Condition (f) (see Example 2.4). We use no conservation properties to establish well-posedness and error estimates. Furthermore, our error estimates are valid as long as the smooth solution of the NLS equation exists.

This paper comprises six sections and three appendices. In Section 2, we introduce the notation used for this study, NLS equation in a general form and implicit θ finite difference scheme. Particularly, we introduce the growth condition, say Condition (f), on $f(u)$ and state a useful criterion of Condition (f) to hold (Proposition 2.3). Our main theorems related to the well-posedness (Theorem I), error estimates (Theorem II) and numerical blow-up result (Theorem III) are also stated there. We describe the proof of Theorems I and II in Section 3. Theorem III is proved in Section 5 using an abstract theory developed in Section 4. We confirm the validity of Theorem III by numerical examples in Section 6. We review the well-posedness and regularity of solutions for NLS equations in a bounded interval in Appendix A. In Appendix B, we describe the proof of Proposition 2.3. In numerical experiments, we solve the resulting nonlinear equations using a modified Newton method introduced into Appendix C.

2. Main results

We consider the following initial-boundary value problem

$$i\partial_t u + \partial_x^2 u = f(u) + g(t,x) \qquad (t > 0,\ x \in (0,L)), \tag{13a}$$

$$u(t,0) = 0,\ u(t,L) = 0 \qquad (t > 0), \tag{13b}$$

$$u(0,x) = u_0(x) \qquad (x \in [0,L]), \tag{13c}$$

where $u = u(t,x)$ denotes a complex-valued function to be find, $f = f(s)$, $g = g(t,x)$, and $u_0 = u_0(x)$ are prescribed continuous functions. We assume that $u_0(0) = u_0(L) = 0$ and $g(t,0) = g(t,L) = 0$ for all $t \geq 0$.

The unique existence of a solution of (13) is well-known. For example, there exists a smooth classical solution of (13), if $f(x+iy)$ is a smooth function of x, y, $g(t,x)$ is a smooth function of t, x, and $u_0(x)$ is a smooth function of x satisfying the compatibility condition with the boundary condition. More specific statements will be recalled in Appendix A.

To state the finite difference scheme, we introduce $0 < N \in \mathbb{Z}$ and let

$$h = L/(N+1), \quad x_j = jh \qquad (0 \leq i \leq N+1).$$

As a discretization of time variable, we take positive constants $\Delta t_1, \Delta t_2, \ldots$ and set

$$t_0 = 0, \quad t_n = t_{n-1} + \Delta t_{n-1} \quad (n \geq 1).$$

We denote by u_i^n the finite difference approximation of $u(t_n, x_j)$ and set

$$\begin{aligned}
u_j^{n+\theta} &= (1-\theta)u_j^n + \theta u_j^{n+1},\\
g_j^{n+\theta} &= (1-\theta)g(t_n, x_j) + \theta g(t_{n+1}, x_j),\\
D_k u_j^n &= \frac{u_j^{n+1} - u_j^n}{k},\\
\delta_h^2 u_j^n &= \frac{u_{j-1}^n - 2u_j^n + u_{i+1}^n}{h^2}.
\end{aligned}$$

Let $0 \le \theta \le 1$. Then, we consider the standard implicit θ scheme

$$
\begin{aligned}
& iD_{\Delta t_n} u_j^n + \delta_h^2 u_j^{n+\theta} \\
& \qquad = (1-\theta) f(u_j^n) + \theta f(u_j^{n+1}) + g_j^{n+\theta} && (1 \le j \le N,\ n \ge 0), && \text{(14a)} \\
& u_0^n = 0,\ u_{N+1}^n = 0 && (n \ge 1), && \text{(14b)} \\
& u_j^0 = u^0(x_j) && (0 \le j \le N+1). && \text{(14c)}
\end{aligned}
$$

It is convenient to rewrite (14) to the vector and matrix form. To this end, we let

$$
\lambda_n = \frac{\Delta t_n}{h^2}
$$

and introduce $H_n, K_n \in \mathbb{C}^{N\times N}$ defined as

$$
H_n = I_N + i\theta\lambda_n A, \quad K_n = I_N - i(1-\theta)\lambda_n A,
$$

where $I_N \in \mathbb{R}^{N\times N}$ denotes the identity matrix and

$$
A = \begin{pmatrix} 2 & -1 & & 0 \\ -1 & 2 & -1 & \\ & \ddots & \ddots & \\ 0 & & -1 & 2 \end{pmatrix} \in \mathbb{R}^{N\times N}.
$$

Actually, A is well-known as a positive-definite symmetric matrix so that H_n is non-singular. Therefore, we can set

$$
G_n = H_n^{-1} K_n. \tag{15}
$$

Introducing

$$
\boldsymbol{u}^n = \begin{pmatrix} u_1^n \\ \vdots \\ u_N^n \end{pmatrix} \quad (n \ge 1), \quad \boldsymbol{u}^0 = \begin{pmatrix} u_0(x_1) \\ \vdots \\ u_0(x_N) \end{pmatrix}, \quad \boldsymbol{g}^{n+\theta} = \begin{pmatrix} g_1^{n+\theta} \\ \vdots \\ g_N^{n+\theta} \end{pmatrix},
$$

we can rewrite (14) equivalently as

$$
\begin{aligned}
\boldsymbol{u}^n = G_{n-1}\boldsymbol{u}^{n-1} - i\Delta t_{n-1} H_{n-1}^{-1}[(1-\theta)\boldsymbol{f}(\boldsymbol{u}^{n-1}) + \theta \boldsymbol{f}(\boldsymbol{u}^n)] \\
- i\Delta t_{n-1} H_{n-1}^{-1} \boldsymbol{g}^{n-1+\theta} \qquad (n \ge 1).
\end{aligned} \tag{16}
$$

To state conditions on f, well-posedness and error estimates, we must introduce some norms. As usual, we use

$$
\|\boldsymbol{v}\|_\infty = \max_{1\le j\le N} |v_j|, \quad \|\boldsymbol{v}\|_2 = \left(\sum_{j=1}^N |v_j|^2 h \right)^{1/2} \qquad (\boldsymbol{v} = (v_1, \ldots, v_N)^{\mathrm{T}} \in \mathbb{C}^N)
$$

and

$$
(\boldsymbol{v}, \boldsymbol{w})_2 = \sum_{i=1}^N v_j \overline{w_j} h \qquad (\boldsymbol{v} = (v_1, \ldots, v_N)^{\mathrm{T}},\ \boldsymbol{w} = (w_1, \ldots, w_N)^{\mathrm{T}} \in \mathbb{C}^N),
$$

where $\overline{w_j}$ denotes the complex conjugate of w_j and $\cdot^{\mathrm{T}}$ the transpose of a matrix (vector). We have $\|\boldsymbol{v}\|_2^2 = (\boldsymbol{v}, \boldsymbol{v})_2$. The matrix

$$A_h = \frac{1}{h^2} A \in \mathbb{R}^{N \times N}$$

is a positive-definite symmetric matrix so that its square root $A_h^{\frac{1}{2}}$ is defined in a natural way. We introduce the discrete $H_0^1(0, L)$ norm as

$$|||\boldsymbol{v}|||_h = \|A_h^{\frac{1}{2}} \boldsymbol{v}\|_2 \qquad (\boldsymbol{v} \in \mathbb{C}^N). \tag{17}$$

We can calculate as

$$\|A_h^{\frac{1}{2}} \boldsymbol{v}\|_2^2 = (A_h \boldsymbol{v}, \boldsymbol{v})_2 = \sum_{j=1}^{N+1} \left| \frac{v_j - v_{j-1}}{h} \right|^2 h \quad (\boldsymbol{v} \in \mathbb{C}^N, v_0 = v_{N+1} = 0). \tag{18}$$

Therefore, we can express the following.

$$|||\boldsymbol{v}|||_h = \left[\left(\frac{|v_1|^2}{h^2} + \sum_{j=2}^{N} \left| \frac{v_j - v_{j-1}}{h} \right|^2 + \frac{|v_N|^2}{h^2} \right) h \right]^{1/2} \qquad (\boldsymbol{v} \in \mathbb{C}^N). \tag{19}$$

With $|||\cdot|||_h$, a discrete Sobolev and inverse inequalities are available.

Proposition 2.1. (i) $\|\boldsymbol{v}\|_\infty \le \sqrt{L}\ |||\boldsymbol{v}|||_h$ *for* $\boldsymbol{v} \in \mathbb{C}^N$.

(ii) $|||\boldsymbol{v}|||_h \le 2h^{-1} \|\boldsymbol{v}\|_2$ *for* $\boldsymbol{v} \in \mathbb{C}^N$.

Proof. (i) Let $\boldsymbol{v} = (v_1, \ldots, v_N)^{\mathrm{T}} \in \mathbb{C}^N$ and set $v_0 = v_{N+1} = 0$. Let $1 \le j \le N$. We can write it as $v_j = \displaystyle\sum_{i=0}^{j} (v_i - v_{i-1})$. Therefore, by (19) and the Cauchy–Schwarz inequality,

$$|v_j| \le \sum_{i=1}^{N+1} \left| \frac{v_i - v_{i-1}}{h} \right| h^{1/2} h^{1/2} \le \sqrt{L}\ \|A_h^{\frac{1}{2}} \boldsymbol{v}\|_2.$$

(ii) Again using (18) and (19),

$$|||\boldsymbol{v}|||_h^2 = \|A_h^{\frac{1}{2}} \boldsymbol{v}\|_2^2 \le 2 \sum_{i=1}^{N+1} \frac{|v_i|^2 + |v_{j-1}|^2}{h^2} h \le \frac{4}{h^2} \|\boldsymbol{v}\|_2^2,$$

which completes the proof. □

Proposition 2.2. *For a smooth function* v *in* $[0, L]$ *satisfying* $v(0) = v(L) = 0$*, we have*

$$|||\boldsymbol{v}|||_h \le \sqrt{L}\ \|\partial_x v\|_{L^\infty(0,L)}, \tag{20}$$

where $\boldsymbol{v} = (v(x_1), \ldots, v(x_N))^{\mathrm{T}} \in \mathbb{C}^N$.

Proof. It is a consequence of the fundamental theorem of calculus. □

We make the following assumption related to f:

Condition (f). There exist positive, continuous and non-decreasing functions $C_{1f}(\eta)$ and $C_{2f}(\eta)$ of $\eta \geq 0$ such that

$$|||\boldsymbol{f}(\boldsymbol{u})|||_h \leq C_{1f}(|||\boldsymbol{u}|||_h) \qquad (\boldsymbol{u} \in \mathbb{C}^N), \tag{21a}$$

$$|||\boldsymbol{f}(\boldsymbol{u}) - \boldsymbol{f}(\boldsymbol{v})|||_h \leq C_{2f}\,(\boldsymbol{u} \wedge \boldsymbol{v})\, |||\boldsymbol{u} - \boldsymbol{v}|||_h \qquad (\boldsymbol{u}, \boldsymbol{v} \in \mathbb{C}^N), \tag{21b}$$

where $\boldsymbol{u} \wedge \boldsymbol{v} = \max\{|||\boldsymbol{u}|||_h, |||\boldsymbol{v}|||_h\}$.

The following proposition provides a useful criterion of Condition (f) to hold. The proof will be presented in Appendix B.

Proposition 2.3. *If $\phi(x,y) = \operatorname{Re} f(z)$ and $\psi(x,y) = \operatorname{Im} f(z)$, $z = x + iy$, are both C^1 functions of $\mathbb{R}_x \times \mathbb{R}_y \to \mathbb{R}$ with $f(0) = 0$, then Condition (f) is satisfied. Particularly, we can take*

$$C_{1f}(\eta) = c_0(\eta)\eta, \qquad C_{2f}(\eta) = c_0(\eta) \qquad (\eta \geq 0),$$

where

$$c_0(\eta) = c_L \max_{|z| \leq \sqrt{L}\eta} \left(\phi_x(x,y)^2 + \phi_y(x,y)^2 + \psi_x(x,y)^2 + \psi_y(x,y)^2\right)^{1/2}$$

with $c_L = \sqrt{2 + 4L^2}$. The value of c_L might not be the best possible.

Example 2.4. Let $\alpha \in \mathbb{C}$ and $m \geq 2$. Then, $f(u) = \alpha u|u|^m$ satisfies Condition (f). We have

$$C_{1f}(\eta) = c_1\eta^{m+1}, \quad C_{2f}(\eta) = c_1\eta^m,$$

where $c_1 = |\alpha|(m+1)c_L$. Furthermore, $f(u) = \alpha|u|^m$ also satisfies Condition (f) and

$$C_{1f}(\eta) = c_2\eta^{m+1}, \quad C_{2f}(\eta) = c_2\eta^m,$$

where $c_2 = |\alpha| m c_L$.

We are now in a position to state the main results presented in this paper. First, we describe the well-posedness of the scheme (14).

Theorem I (Well-posedness)**.** *Let $1/2 \leq \theta \leq 1$ and let J be a positive integer. Let $R > 0$ and assume*

$$|||\boldsymbol{u}^0|||_h \leq R, \quad \sup_{0 \leq n \leq J} |||\boldsymbol{g}^{n-1+\theta}|||_h \leq R. \tag{22}$$

Assume, moreover, that Condition (f) is satisfied. Take $\Delta t_1, \Delta t_2, \ldots, \Delta t_J$ satisfying $\Delta t_n \leq \tau$ with some $\tau > 0$. Then, there exists a constant $\gamma_{R,J} > 0$ depending only on J, R, $C_{1f}(2R)$, and $C_{2f}(2R)$ such that, if $\tau \leq \gamma_{R,J}$, the scheme (14) *admits a solution $\boldsymbol{u}^n$ for any $1 \leq n \leq J$ with*

$$\sup_{1 \leq n \leq J} |||\boldsymbol{u}^n|||_h \leq 2R. \tag{23}$$

The solution $\boldsymbol{u}^n$ satisfying (23) *is unique (for a given partition $\Delta t_1, \Delta t_2, \ldots, \Delta t_J$).*

Remark 2.5. Theorems I and II described below remain valid for $0 \le \theta < 1/2$, if $\tau = ch^4$ is assumed with some $c > 0$. See Remark 3.2. However, the condition $\tau = ch^4$ is unreasonable in actual computations. Therefore, we do not study the case $0 \le \theta < 1/2$ further.

Our next results are error estimates. Let u and $\boldsymbol{u}^n$ respectively denote the solutions of (13) and (14). We set $\boldsymbol{U}^n = (U_1^n, \ldots, U_N^n)^{\mathrm{T}}$, where $U_j^n = u(t_n, x_j)$ $(j = 1, \ldots, N)$. The error is defined as

$$\boldsymbol{e}^n = \boldsymbol{U}^n - \boldsymbol{u}^n.$$

If posing appropriate assumptions on $f(u)$, g and u_0, we obtain a smooth solution u of (13) (see Proposition A.2). However, we directly assume the regularity of u in Theorem II below. Let $Q = [0, T] \times [0, L]$ and assume

$$u,\ \partial_x \partial_t^l u,\ \partial_x^m u \in C^0(Q) \quad (1 \le l \le \sigma,\ 1 \le m \le 5), \tag{24}$$

where

$$\sigma = \begin{cases} 2 & \text{for } \theta = 1/2, \\ 1 & \text{for } 1/2 < \theta \le 1. \end{cases} \tag{25}$$

Moreover, set

$$M_0 = M_0(u) = \|u\|_{L^\infty(Q)} + \|\partial_x \partial_t^\sigma u\|_{L^\infty(Q)} + \|\partial_x^5 u\|_{L^\infty(Q)},$$
$$M_1 = M_1(u) = \sqrt{L}\|\partial_x u\|_{L^\infty(Q)},$$

and

$$\kappa = \kappa(u) = C_{2f}(6M_1).$$

If u further has a fine extension property, then we can obtain better error estimates. Introducing an extension operator $\mathcal{E}$ from $C^0([0, L]) \cap H_0^1(0, L)$ to $C([-L, 2L])$ by

$$(\mathcal{E}v)(x) = \begin{cases} -v(x) & (x \in [-L, 0]) \\ v(x) & (x \in [0, L]) \\ -v(2L - x) & (x \in [L, 2L]) \end{cases} \qquad (v \in C^0([0, L]) \cap H_0^1(0, L)).$$

We consider the following assumption:

$$\partial_x^m (\mathcal{E}u) \in C^0([0, T] \times [-L, 2L]) \quad (1 \le m \le 5); \tag{26a}$$
$$f(0) = 0. \tag{26b}$$

Theorem II (Error estimates)**.** *Let* $1/2 \le \theta \le 1$. *Let* $T > 0$. *Assume that Condition (f) is satisfied. Assume moreover that the unique solution* u *of* (13) *satisfies* (24) *and the solution* $\boldsymbol{u}^n$ *of* (14) *is unique. Then there exist positive constants* C_0, τ_0 *and* h_0 *such that, if* $\tau \le \tau_0$ *and* $h \le h_0$*, then we have*

$$\sup_{0 \le t_n \le T} |||\boldsymbol{e}^n|||_h \le C_0 M_0 T \exp(2\kappa T)(\tau^\sigma + h^s) \tag{27}$$

and

$$\sup_{0 \le t_n \le T} \|\boldsymbol{e}^n\|_\infty \le C_0 M_0 T \sqrt{L} \exp(2\kappa T)(\tau^\sigma + h^s), \tag{28}$$

where

$$s = \begin{cases} 2 & \textit{if (26) is satisfied,} \\ 3/2 & \textit{otherwise.} \end{cases} \tag{29}$$

Several remarks must be made at this point.

Remark 2.6. In Theorem II, the constant C_0 is an absolute constant, whereas τ_0 and h_0 depend on T, M_0 and M_1.

Remark 2.7. The L^∞ error estimate (28) is a readily obtainable consequence of (27) by virtue of Proposition 2.1 (i). However, it provides only a sub-optimal error estimate for space discretization without assuming (26). We observe the optimal order (second order) convergence using numerical experiments (see Examples 2.11 and 2.12), but we are unable to remove (26) by our method of analysis at present.

Remark 2.8. If we pose the periodic boundary condition instead of the Dirichlet condition, then we can remove the assumption (26) and obtain the optimal order convergence in $|||\cdot|||_h$ and $\|\cdot\|_\infty$. Herein, $|||\cdot|||_h$ should be redefined suitably.

Remark 2.9. Some error estimates in $L^\infty(0,T;L^2(\Omega))$ and $L^\infty(Q)$ for the Crank–Nicolson/finite element approximation for NLS equations were presented in an earlier report [1]. Here, Ω is a polyhedral domain in $\mathbb{R}^d$. Akrivis et al. [1] first introduced the truncated NLS equation where $f(s)$ is replaced by a global Lipschitz continuous function $\tilde{f}(s)$ such that $f(s) = \tilde{f}(s)$ for $|s| \le M$ with a given $M > 0$. Then, an error estimate in $L^\infty(Q)$ of the approximation $\tilde{u}_h^n$ of the truncated problem was derived under the assumption $\tau = ch^{\frac{d}{4}+\varepsilon}$ with $c, \varepsilon > 0$. From this result, they derive the optimal order error estimate in $L^\infty(0,T;L^2(\Omega))$. However, we cannot avoid $\tau = ch^{\frac{d}{4}+\varepsilon}$. An attempt to remove this restriction has been reported (see [22]). Their method is applicable to our scheme in the case of $\theta = 1/2$. Consequently, we obtain

$$\sup_{0\le t_n\le T} \|\boldsymbol{e}^n\|_\infty \le (\text{Const.}) h^{-\frac{1}{2}}(\tau^2 + h^2)$$

if we choose as $\tau = ch^{\frac{1}{4}+\varepsilon}$. This error estimate is sub-optimal both for time and space. However, by following the argument of [1] and using (28), we can deduce the optimal order error estimate in $\|\cdot\|_2$ without assuming any condition on τ and h.

Remark 2.10. It is readily apparent that our problems and results include the linear case ($f(s) = 0$). It would be interesting to compare (27) with corresponding results for the finite difference method to a one-dimensional linear heat equation presented in [20, theorem 10.2]. Thomée actually derived the second order (in space) error estimate in $|||\cdot|||_h$. He applied the smoothing property of a discrete (finite difference) heat equation. However, as described before, no smoothing property is available for the Schrödinger equation in a bounded domain.

Example 2.11. One can confirm the validity of error estimates (27) and (28) using simple numerical examples. First, we consider

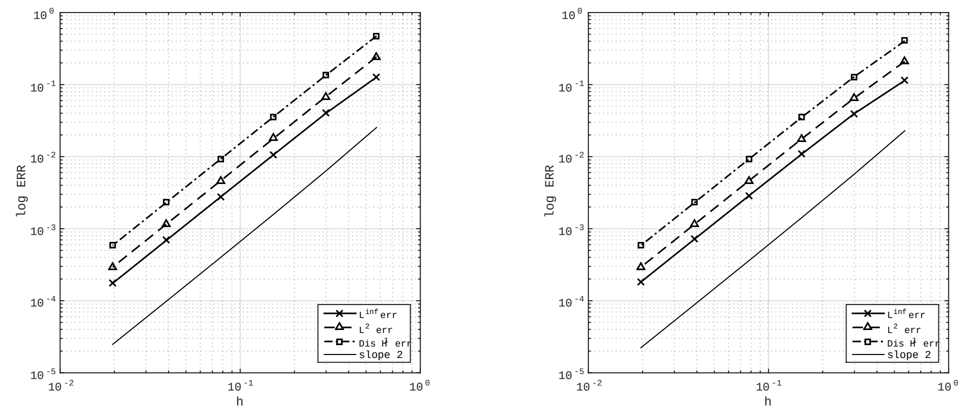
$$u(t,x) = e^t(\sin x + i\sin(2x)) \quad (t \ge 0,\ 0 \le x \le L = 2\pi) \tag{30}$$

and define $g(t,x)$ as $g(t,x) = i\partial_t u - \partial_x^2 u - u|u|^2$. The assumption (26) is satisfied. We let $T = 1$ and use a modified Newton method to solve nonlinear equations at each time step t_n (see Appendix C). In Fig. 1, we present $(\log h, \log \|\boldsymbol{e}^n\|_\infty)$, $(\log h, \log \|\boldsymbol{e}^n\|_2)$ and $(\log h, \log |||\boldsymbol{e}^n|||_h)$ for $\theta = 1/2$ ($\tau = h/10$) and $\theta = 1$ ($\tau = h^2/100$). Results show that the second-order convergence actually occurs in $\|\cdot\|_\infty$, $\|\cdot\|_2$ and $|||\cdot|||_h$.

Example 2.12. We consider the case in which $f(u) = -|u|^2$, $L = 1$ and $u_0(x) = -5i\sin(\pi x)$. In this case, the assumption (26) can not be expected to hold. The exact solution is not available. Therefore, we employ the following technique. Letting $\boldsymbol{u}^n(h)$ be the solution of (14) for h, we define

$$E_\infty(h) = \sup_{0 \le t_n \le T} \|\boldsymbol{u}^n(2h) - \boldsymbol{u}^n(h)\|_\infty.$$

Then, assuming $\sup_{0\le t_n \le T} \|\boldsymbol{e}^n\|_\infty = Ch^\alpha$, we have $E_\infty(h) \le C(1+2^\alpha)h^\alpha$. Similarly, $E_2(h)$ and $E_{1h}(h)$ are defined in terms of $\|\cdot\|_2$ and $|||\cdot|||_h$. Figure 2 shows $(\log h, \log E_\infty(h))$, $(\log h, \log E_2(h))$ and $(\log h, \log E_{1h}(h))$ for $\theta = 1/2$ ($\tau = h/10$) and $\theta = 1$ ($\tau = h^2/100$). The result demonstrates that the second order convergence also occurs in this case.



(a) $\theta = 1/2$ (b) $\theta = 1$

Figure 1: $\log h$ versus log ERR: $i\partial_t u = \partial_x^2 u + u|u|^2 + g(t,x)$, ERROR $= \|\boldsymbol{e}^n\|_\infty, \|\boldsymbol{e}^n\|_2, |||\boldsymbol{e}^n|||_h$. See Example 2.11 for additional details.

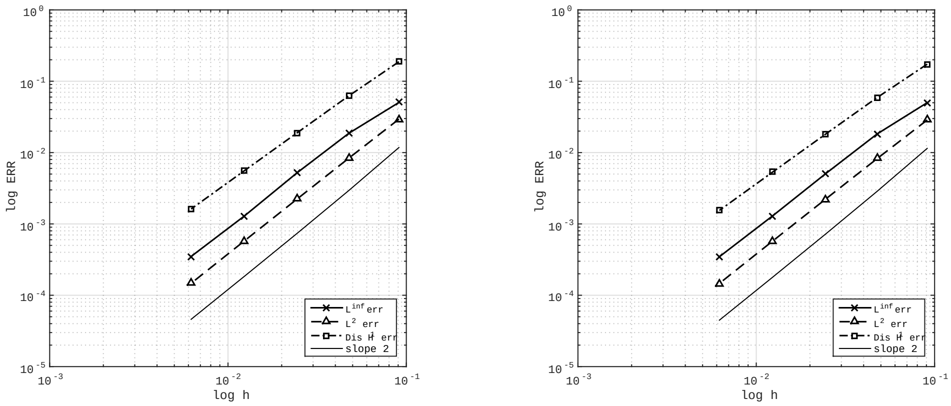
Remark 2.13. The function $f(u) = u|u|^{\frac{1}{2}}$ does not satisfy Condition (f). However, we obtain the second-order convergence by numerical experiments. Therefore, Condition (f) is a sufficient condition to deduce error estimates.

Finally, we describe the numerical blow-up result. We consider (5). Consequently, we deal with the case $f(u) = -|u|^{2p}$ with a positive real number p and $L = 1$ in (13).

One might recall that we are interested in the reproduction of the blow-up of solutions of (5). Therefore, to avoid technical difficulties, we suppose that u_0 is large (in a certain sense) in addition to the basic assumptions on the smoothness. We assume

$$J(0, u_0) > \mu_p \equiv \left(\frac{\sqrt{2}\pi^2}{2p-1}\right)^{2p-1}. \tag{31}$$

Then, in view of (10), we have $T_J < 1/(4\pi)$ and $T_\infty < 1/(4\pi)$. From this, we can set the numerical blow-up time $T(h,\tau)$, that will be defined below, as $T(h,\tau) < 1/(4\pi)$.



(a) $\theta = 1/2$ (b) $\theta = 1$

Figure 2: $\log h$ versus log ERR: $i\partial_t u = \partial_x^2 u - |u|^2$, ERR $= E_\infty(h), E_2(h), E_{1h}(h)$. See Example 2.12 for additional details.

This enables us to avoid numerous unnecessary difficulties. Moreover, we assume $J(0, u_0) > 2$ to ensure (83) used below.

We recall that our finite difference scheme is given as

$$
\begin{aligned}
& iD_{\Delta t_n} u_j^{n+1} + \delta_h^2 u_j^{n+\theta} \\
& \qquad = -\left[(1-\theta)|u_j^{n+1}|^{2p} + \theta |u_j^n|^{2p}\right] && (1 \le j \le N,\ n \ge 0), && \text{(32a)} \\
& u_0^n = u_{N+1}^n = 0 && (n \ge 1), && \text{(32b)} \\
& u_j^0 = u_0(x_j) && (0 \le j \le N+1). && \text{(32c)}
\end{aligned}
$$

At this stage, we state our choose of Δt_n for $n \ge 0$. Let

$$0 < \tau < \frac{1}{4\pi}, \qquad q > 0 \tag{33}$$

be arbitrary. Then, we define Δt_n as

$$\Delta t_n = \tau \cdot \min\left\{1,\ \frac{1}{\|\boldsymbol{u}^n\|_\infty^q},\ a_n\right\} \qquad (n \ge 0). \tag{34}$$

Hereinafter, we set

$$a_0 = 1, \quad a_n = \frac{1}{2}\left(\frac{1}{4\pi} - t_{n-1}\right) \quad (n \ge 1). \tag{35}$$

In fact, $a_n \ge 0$ for $n \ge 1$. Furthermore, we can introduce the numerical blow-up time

$$T(h, \tau) = \lim_{n\to\infty} t_n = \lim_{n\to\infty} \sum_{k=0}^{n-1} \Delta t_k \le \frac{1}{4\pi}. \tag{36}$$

Theorem III (Approximation of the blow-up time)**.** *Assume that the unique solution u of* (5) *satisfies* (24) *and that*

$$J(0, u_0) > \min\{2,\ \mu_p\}. \tag{37}$$

Then, u and $J(t, u(t,\cdot))$ blow up, respectively, in $T_\infty < 1/(4\pi)$ and $T_J < 1/(4\pi)$ with $T_\infty \le T_J$. Assume, furthermore, $T_\infty = T_J$, i.e.,

$$\lim_{t\to T_\infty} J(t, u(t,\cdot)) = \infty. \tag{38}$$

Consider the finite difference scheme (32) *for $1/2 \le \theta \le 1$ and the numerical blow-up time $T(h,\tau)$ defined by* (36)*. Then, we have*

$$\lim_{h,\tau\to 0} T(h,\tau) = T_\infty. \tag{39}$$

Remark 2.14. Theorem III is somewhat restrictive because we have assumed $T_J = T_\infty$. However, we have not succeeded in removing it at present. It is noteworthy that the same assumptions are (sometimes implicitly) assumed in all related earlier studies (see [6], [7], [8], [14], [15] and [17]).

Remark 2.15. We have no information related to the rate of convergence. However, from numerical experiments in Section 6, we infer that $|T(h,\tau) - T_\infty| \le C\tau^\sigma$ if $\tau/h = \text{Const}$, where σ is defined as (25).

3. Well-posedness and error estimates (Proofs of Theorems I and II)

This section is devoted to proofs of Theorems I and II. For any matrix $B \in \mathbb{C}^{N\times N}$ and any norm of $\mathbb{C}^N$, we set

$$\|B\| = \sup_{\boldsymbol{v}\in\mathbb{C}^N} \frac{\|B\boldsymbol{v}\|}{\|\boldsymbol{v}\|}.$$

The following proposition plays a crucial role in what follows.

Proposition 3.1. *For any $n \ge 0$,*

$$|||H_n|||_h < 1, \tag{40a}$$

$$|||G_n|||_h = 1 \quad \left(\theta = \frac{1}{2}\right), \qquad |||G_n|||_h < 1 \quad \left(\frac{1}{2} < \theta \le 1\right). \tag{40b}$$

Proof. Because $|||\cdot|||_h$ is defined in terms of $A_h^{\frac{1}{2}}$, we obviously have

$$|||H_n|||_h = \|H_n\|_2, \qquad |||G_n|||_h = \|G_n\|_2.$$

Therefore, (40) is a consequence of the following inequalities and equality:

$$\|H_n\|_2 \le 1, \tag{41a}$$

$$\|G_n\|_2 = 1 \quad \left(\theta = \frac{1}{2}\right), \qquad \|G_n\|_2 < 1 \quad \left(\frac{1}{2} < \theta \le 1\right). \tag{41b}$$

Although those results seem not to be new, we state their proofs for the reader's convenience. Recall that $\|G_n\|_2 = \sqrt{r(G_n^* G_n)}$, where $r(B)$ and B^* respectively denote the spectral radius and conjugate transpose of a matrix B. Setting

$$\phi(\mu) = \frac{1 - i(1-\theta)\lambda_n\mu}{1 + i\theta\lambda_n\mu}, \quad \psi(\mu) = \frac{1 + i(1-\theta)\lambda_n\mu}{1 - i\theta\lambda_n\mu}$$

for $\mu \geq 0$, the eigenvalues of $G_n^* G_n$ are given explicitly as

$$\psi(\mu_1)\psi(\mu_1), \quad \psi(\mu_2)\phi(\mu_2), \quad \ldots, \quad \psi(\mu_N)\phi(\mu_N)$$

in terms of the eigenvalues $0 < \mu_1 < \mu_2 < \cdots < \mu_N$ of A. Moreover, by direct calculation, we deduce

$$0 < \psi(\mu)\phi(\mu) \begin{cases} < 1 & (1/2 < \theta \leq 1) \\ = 1 & (\theta = 1/2) \\ > 1 & (0 \leq \theta < 1/2) \end{cases} \tag{42}$$

for $\mu \geq 0$. Combining those results, we obtain (41b). Inequality (41a) is proved similarly. □

Remark 3.2. We consider the case for which $0 \leq \theta < 1/2$. According to (42), we have $\|G_n\|_2 > 1$ and $|||G_n|||_h > 1$. However, if assuming $\tau = ch^4$ with some $c > 0$, then we have

$$\|G_{k-1}G_{k-2}\cdots G_0\|_2 \leq C_T \quad (0 \leq t_k \leq T), \tag{43}$$

where $C_T > 0$ is a constant depending on $T > 0$. In fact, because

$$\psi(\mu)\phi(\mu) \leq 1 + (1-2\theta)\frac{\Delta t_n^2}{h^4}\mu^2 \leq 1 + c(1-2\theta)\tau\mu^2$$

for $\mu > 0$, we can perform an estimation as

$$\|G_{k-1}G_{k-2}\cdots G_0\|_2 \leq \sqrt{(1+c'\tau)^k} \leq \exp\left(\frac{1}{2}c'T\right) \quad (0 \leq t_k \leq T)$$

with a suitable constant $c' > 0$. Theorems I and II in the case $0 \leq \theta < 1/2$ are proved using (43) instead of (40b) in the following proof.

Proof of Theorem I. Let $\Lambda_n = \{1, \ldots, n\}$ for $n \in \mathbb{N}$. Set

$$\mathcal{B}_R = \left\{ \{\boldsymbol{v}^n\}_{n \in \Lambda_J} \subset \mathbb{C}^N \mid \sup_{n \in \Lambda_J} |||\boldsymbol{v}^n|||_h \leq R \right\} \tag{44}$$

for $R > 0$.

Furthermore, we have by (16)

$$\begin{aligned} \boldsymbol{u}^n = G_{n-1}\cdots G_0\boldsymbol{u}^0 - i\sum_{k=1}^{n-1}\Delta t_{k-1}G_{n-1}\cdots G_k H_{k-1}^{-1}[\boldsymbol{F}(\boldsymbol{u}^{k-1+\theta}) + \boldsymbol{g}^{k-1+\theta}] \\ - i\Delta t_{n-1}H_{n-1}^{-1}[\boldsymbol{F}(\boldsymbol{u}^{n-1+\theta}) + \boldsymbol{g}^{n-1+\theta}], \end{aligned} \tag{45}$$

where we have used the following abbreviation

$$\boldsymbol{F}(\boldsymbol{u}^{k-1+\theta}) = (1-\theta)\boldsymbol{f}(\boldsymbol{u}^{k-1}) + \theta\boldsymbol{f}(\boldsymbol{u}^k) \quad (1 \leq k \leq n). \tag{46}$$

We introduce a Banach space

$$\mathcal{X}_J = \{\boldsymbol{W} = \{\boldsymbol{w}^n\}_{n \in \Lambda_J} \mid \boldsymbol{w}^n \in \mathbb{C}^N \ (n \in \Lambda_J)\} \tag{47}$$

with the norm

$$\|\boldsymbol{W}\|_{\mathcal{X}_J} = \sup_{n\in\Lambda_J} |||\boldsymbol{w}^n|||_h \tag{48}$$

for $\boldsymbol{W} = \{\boldsymbol{w}^n\}_{n\in\Lambda_J} \in \mathcal{X}_J$. Then, $\mathcal{B}_{2R}$ is a closed ball in $\mathcal{X}_J$.

We introduce the operator $\mathcal{T} : \mathcal{X}_J \to \mathcal{X}_J$ by setting

$$\tilde{\boldsymbol{U}} = \mathcal{T}\boldsymbol{U},$$

where $\tilde{\boldsymbol{U}} = \{\tilde{\boldsymbol{u}}^n\}_{n\in\Lambda_J}$, $\boldsymbol{U} = \{\boldsymbol{u}^n\}_{n\in\Lambda_J}$ and

$$\begin{aligned}\tilde{\boldsymbol{u}}^n = G_{n-1}\cdots G_0\boldsymbol{u}^0 - i\sum_{k=1}^{n-1}\Delta t_{k-1}G_{n-1}\cdots G_k H_{k-1}^{-1}[\boldsymbol{F}(\boldsymbol{u}^{k-1+\theta}) + \boldsymbol{g}^{k-1+\theta}]\\ - i\Delta t_{n-1}H_{n-1}^{-1}[\boldsymbol{F}(\boldsymbol{u}^{n-1+\theta}) + \boldsymbol{g}^{n-1+\theta}],\end{aligned}$$

with (46).

We show that $\mathcal{T}$ is a contraction operator from $\mathcal{B}_{2R}$ into itself with a suitably chosen τ.

First, let $\boldsymbol{U} \in \mathcal{B}_{2R}$ and set $\tilde{\boldsymbol{U}} = \mathcal{T}\boldsymbol{U}$. We have by (21a) and (40)

$$\begin{aligned}|||\tilde{\boldsymbol{u}}^n|||_h &\le |||\boldsymbol{u}^0|||_h + \sum_{k=1}^{n}\Delta t_{k-1}|||\boldsymbol{F}(\boldsymbol{u}^{k-1+\theta})|||_h + \sum_{k=1}^{n}\Delta t_{k-1}|||\boldsymbol{g}^{k-1+\theta}|||_h\\ &\le R + \sum_{k=1}^{n}\Delta t_{k-1}[(1-\theta)C_{1f}(|||\boldsymbol{u}^{k-1}|||_h) + \theta C_{1f}(|||\boldsymbol{u}^k|||_h)] + \Delta t_n R\\ &\le R + \tau J[C_{1f}(2R) + R].\end{aligned}$$

Next, let $\boldsymbol{U}, \boldsymbol{V} \in \mathcal{B}_{2R}$ and set $\tilde{\boldsymbol{U}} = \mathcal{T}\boldsymbol{U}$, $\tilde{\boldsymbol{V}} = \mathcal{T}\boldsymbol{V}$. Then, by using (21b) and (40), we can conduct an estimation as

$$\begin{aligned}|||\tilde{\boldsymbol{u}}^n - \tilde{\boldsymbol{v}}^n|||_h &\le \sum_{k=1}^{n}\Delta t_{k-1}|||\boldsymbol{F}(\boldsymbol{u}^{k-1+\theta}) - \boldsymbol{F}(\boldsymbol{v}^{k-1+\theta})|||_h\\ &\le C_{2f}(2R)\sum_{k=1}^{n}\Delta t_{k-1}|||\boldsymbol{u}^{k+1-\theta} - \boldsymbol{v}^{k+1-\theta}|||_h\\ &\le C_{2f}(2R)\tau J\|\boldsymbol{U} - \boldsymbol{V}\|_{\mathcal{X}_J}.\end{aligned}$$

Putting together those estimates, it is apparent that, if

$$0 < \tau \le \gamma_{R,J} = \min\left\{\frac{R}{J[C_{1f}(2R) + R]},\ \frac{1}{2JC_{2f}(2R)}\right\},$$

then $\mathcal{T}$ becomes a contraction mapping of $\mathcal{B}_{2R} \to \mathcal{B}_{2R}$.

Results show that $\mathcal{T}$ has a unique fixed point $\boldsymbol{U}$ that satisfies (45) and $\|\boldsymbol{U}\|_{\mathcal{X}_J} \le 2R$. This completes the proof of Theorem I. $\square$

We proceed to the proof of Theorem II. We use a version of the well-known discrete Gronwall inequality.

Proposition 3.3. *Let* $\{x_n\}_{n\geq 0}$, $\{y_n\}_{n\geq 1}$, $\{a_n\}_{n\geq 1}$, $\{b_n\}_{n\geq 1}$ *and* $\{\Delta t_n\}_{n\geq 0}$ *satisfy*

$$x_n \geq 0,\ y_n \geq 0,\ a_n \geq 0,\ b_n \geq 0,$$
$$x_n + \sum_{j=1}^{n} \Delta t_{j-1} y_j \leq x_0 + \sum_{j=1}^{n} \Delta t_{j-1} a_j x_j + \sum_{j=1}^{n} \Delta t_{j-1} b_j.$$

Assume that $1 - \Delta t_{n-1} a_n > 0$ *for all* $n \geq 1$. *Then, setting* $\gamma_n = (1 - \Delta t_{n-1} a_n)^{-1}$, *we have*

$$x_n + \sum_{j=1}^{n} \Delta t_{j-1} y_j \leq \left(x_0 + \sum_{j=1}^{n} \Delta t_{j-1} b_j \right) \exp\left(\sum_{j=1}^{n} \Delta t_{j-1} \gamma_j a_j \right) \qquad (n \geq 1). \quad (49)$$

Proof. That is fundamentally the same as that of [10, Lemma 5.1]. □

Proof of Theorem II. It is divided into three steps.
Step 1. We derive several useful estimates. According to (45), we obtain the following expression of the error:

$$\boldsymbol{e}^n = -i \sum_{k=1}^{n-1} \Delta t_{k-1} G_{n-1} \cdots G_k H_{k-1}^{-1} (\boldsymbol{r}^k + \boldsymbol{R}_1^k + \boldsymbol{R}_2^k + \boldsymbol{\phi}^k)$$
$$- i \Delta t_{n-1} H_{n-1}^{-1} (\boldsymbol{r}^n + \boldsymbol{R}_1^n + \boldsymbol{R}_2^n + \boldsymbol{\phi}^n) \quad (50)$$

with $\boldsymbol{e}^0 = \boldsymbol{0}$, where

$$\begin{aligned} r_j^n &= i D_{\Delta t_n} U_j^n - i[(1-\theta)\partial_t u(t_{n-1}, x_j) + \theta \partial_t u(t_n, x_j)], \\ R_{1,j}^n &= (1-\theta)[\delta_h^2 U_j^{n-1} - \partial_x^2 u(t_{n-1}, x_j)], \\ R_{2,j}^n &= \theta[\delta_h^2 U_j^n - \partial_x^2 u(t_n, x_j)], \\ \phi_j^n &= (1-\theta)[f(U_j^{n-1}) - f(u_j^{n-1})] + \theta[f(U_j^n) - f(u_j^n)]. \end{aligned}$$

Therefore, again using (40),

$$|||\boldsymbol{e}^n|||_h \leq \sum_{k=1}^{n} \Delta t_{k-1} (|||\boldsymbol{r}^k|||_h + |||\boldsymbol{R}_1^k|||_h + |||\boldsymbol{R}_2^k|||_h + |||\boldsymbol{\phi}^k|||_h) \qquad (n \geq 1). \qquad (51)$$

By virtue of Condition (f), we obtain

$$|||\boldsymbol{\phi}^n|||_h \leq (1-\theta) C_{2f}(\boldsymbol{u}^{n-1} \wedge \boldsymbol{U}^{n-1}) |||\boldsymbol{e}^{n-1}|||_h + \theta C_{2f}(\boldsymbol{u}^n \wedge \boldsymbol{U}^n) |||\boldsymbol{e}^n|||_h. \qquad (52)$$

We state an estimation of $|||\boldsymbol{r}^n|||_h$ only for the case $\theta = \frac{1}{2}$. It is noteworthy that $r_0^n = r_{N+1}^n = 0$. Because

$$\begin{aligned} & D_{\Delta t_{n-1}} U_j^n - \frac{1}{2} [\partial_t u(t_{n-1}, x_j) + \partial_t u(t_n, x_j)] \\ &= -\frac{\Delta t_{n-1}}{4} \int_{t_{n-1}}^{t_n} \partial_t^3 u(s, x_j)\, ds + \frac{1}{4} \int_0^1 (1-s) \Delta t_{n-1}^2 \partial_t^3 u(t_{n-1} + s\Delta t_{n-1}, x_j)\, ds \\ &\qquad + \frac{1}{4} \int_0^1 (1-s) \Delta t_{n-1}^2 \partial_t^3 u(t_n - s\Delta t_{n-1}, x_j)\, ds, \end{aligned}$$

we can calculate as

$$\frac{r_j^n - r_{j-1}^n}{h} = -\frac{\Delta t_{n-1}}{4h}\int_{x_{j-1}}^{x_j}\int_{t_{n-1}}^{t_n} \partial_x\partial_t^3 u(s,\xi)\ dsd\xi$$
$$+\frac{1}{4h}\int_{x_{j-1}}^{x_j}\int_0^1 (1-s)\Delta t_{n-1}^2 u[\partial_x\partial_t^3 u(t_{n-1}+s\Delta t_{n-1},\xi)+\partial_x\partial_t^3 u(t_n - s\Delta t_{n-1},\xi)]\ dsd\xi.$$

Therefore,

$$\left|\frac{r_j^n - r_{j-1}^n}{h}\right| \le C\Delta t_{n-1}^2 \|\partial_x\partial_t^3 u\|_{L^\infty(Q)}.$$

Hereinafter, C denotes various absolute positive constants. This inequality is valid for $1 \le j \le N+1$. Therefore, in view of (19)

$$|||\boldsymbol{r}^n|||_h \le C\tau^2\|\partial_x\partial_t^3 u\|_{L^\infty(Q)}.$$

Next we present estimations of $|||\boldsymbol{R}_1^n|||_h$ and $|||\boldsymbol{R}_2^n|||_h$. Set $\rho_j^n = \delta_h^2 U_j^n - \partial_x^2 u(t_n, x_j)$. First, we derive estimations without assuming (26). Similar to the manner presented above, we have

$$\frac{\rho_j^n - \rho_{j-1}^n}{h} = \frac{h^2}{6h}\int_{x_{j-1}}^{x_j}\int_0^1 (1-s)^3[\partial_x^5 u(t_n,\xi+sh) + \partial_x^5 u(t_n,\xi-sh)]\ dsd\xi \tag{53}$$

for $2 \le j \le N$. However, we have

$$|\rho_1^n|,\ |\rho_N^n| \le Ch^2\|\partial_x^4 u\|_{L^\infty(Q)}.$$

Therefore, by (19)

$$\begin{aligned}
|||\boldsymbol{R}_1^n|||_h^2 &\le C(1-\theta)^2\left(2\frac{h^4\|\partial_x^4 u\|_{L^\infty(Q)}^2}{h^2} + \sum_{j=2}^N h^4\|\partial_x^5 u\|_{L^\infty(Q)}^2\right)h \\
&\le C(1-\theta)^2\left(h^3\|\partial_x^4 u\|_{L^\infty(Q)}^2 + h^4\|\partial_x^5 u\|_{L^\infty(Q)}^2\right) \\
&\le C(1-\theta)^2(h^3+h^4)(\|\partial_x^4 u\|_{L^\infty(Q)}^2 + \|\partial_x^5 u\|_{L^\infty(Q)}^2).
\end{aligned}$$

Consequently, we obtain

$$|||\boldsymbol{R}_1^n|||_h + |||\boldsymbol{R}_2^n|||_h \le Ch^{\frac{3}{2}}(\|\partial_x^4 u\|_{L^\infty(Q)} + \|\partial_x^5 u\|_{L^\infty(Q)}). \tag{54}$$

Now we assume (26). We use the same symbol u to express the extension $\mathcal{E}u$ of u. Moreover, we set $U_{-1}^n = -U_1^n$ and $U_{N+2}^n = -U_N^n$. Then, because $\delta_h^2 U_0^n = 0$ and $\partial_x^2 u(t_n, 0) = i\partial_t u(t_n,0) - f(u(t_n,0)) - g(t_n,0) = 0$ for example, we have $\rho_0^n = 0$ and $\rho_{N+1}^n = 0$. Moreover, the expression (53) is valid for $i=1$ and $i=N+1$. Consequently, we deduce

$$|||\boldsymbol{R}_1^n|||_h + |||\boldsymbol{R}_2^n|||_h \le Ch^2(\|\partial_x^4 u\|_{L^\infty(Q)} + \|\partial_x^5 u\|_{L^\infty(Q)})$$

instead of (54).

Putting those estimates together, we obtain

$$|||\boldsymbol{r}^n|||_h + |||\boldsymbol{R}_1^n|||_h + |||\boldsymbol{R}_2^n|||_h \le C_0 M_0(\tau^\sigma + h^s), \tag{55}$$

where C_0 denotes an absolute positive constant.

Step 2. We choose $\tau_0' > 0$ and $h_0 > 0$ such that

$$1 - \tau\kappa \geq \frac{1}{2}, \quad T\exp(2\kappa T)C_0 M_0(\tau^\sigma + h^s) \leq \frac{1}{2}M_1 \tag{56}$$

for $\tau \leq \tau_0'$ and $h \leq h_0$. Below, we always suppose that $\tau \leq \tau_0'$ and $h \leq h_0$.

We prove (27) under the assumption that

$$|||\boldsymbol{u}^n|||_h \leq R = 6M_1 \qquad (0 \leq t_n \leq T). \tag{57}$$

As a consequence of (51), (52) and (55), we have

$$|||\boldsymbol{e}^n|||_h \leq \sum_{k=1}^{n} \Delta t_{k-1}\kappa |||\boldsymbol{e}^k|||_h + \sum_{k=1}^{n} \Delta t_{k-1} C_0 M_0(\tau^\sigma + h^s).$$

Because $1 - \Delta t_{k-1}\kappa \geq 1 - \tau\kappa > 1/2$ and $(1 - \Delta t_{k-1}\kappa)^{-1} \leq 2$, we can apply Proposition 3.3 to obtain

$$\begin{aligned} |||\boldsymbol{e}^n|||_h &\leq \sum_{k=1}^{n} \Delta t_{k-1} C_0 M_0(\tau^\sigma + h^s) \cdot \exp\left(\sum_{k=1}^{n} \Delta t_{k-1}(1 - \Delta t_{k-1}\kappa)^{-1}\kappa\right) \\ &\leq (\tau^\sigma + h^s) \cdot T C_0 M_0 \exp(2\kappa T). \end{aligned} \tag{58}$$

Step 3. We prove (27) without assuming (57). Assume that there exists $0 < n \in \mathbb{Z}$ such that

$$|||\boldsymbol{u}^{n-1}|||_h \leq R, \quad |||\boldsymbol{u}^n|||_h > R, \quad t_n \leq T. \tag{59}$$

It is readily apparent that we have $|||\boldsymbol{U}^{n-1}|||_h \leq M_1$ by Proposition 2.2. In view of (58) in Step 2,

$$\begin{aligned} |||\boldsymbol{u}^{n-1}|||_h &\leq |||\boldsymbol{U}^{n-1}|||_h + T C_0 M_0 \exp(2\kappa T)(\tau^\sigma + h^s) \\ &\leq |||\boldsymbol{U}^{n-1}|||_h + T C_0 M_0 \exp(2\kappa T)(\tau^\sigma + h^s) \leq \frac{3}{2}M_1. \end{aligned}$$

At this stage, we apply Theorem I with the initial value $\boldsymbol{u}^{n-1}$, $J = 2$ and $R_1 = \frac{3}{2}M_1$. Then, $\gamma_{2,R_1} > 0$ exists such that, if $\tau \leq \tau_0 = \min\{\tau_0', \gamma_{2,R_1}\}$, then

$$|||\boldsymbol{u}^n|||_h \leq 2R_1 = 3M_1 < R,$$

which contradicts (59). Therefore, as long as $\tau \leq \tau_0$ and $h \leq h_0$, we have (57). Consequently, we obtain (27). □

4. Abstract convergence result for the blow-up time

In this section, we develop an abstract theory for approximating the blow-up time. We first state a problem setting (I)–(VIII). Then we describe conditions that imply the reproduction of the blow-up. The proof of Theorem III is an application of Propositions 4.1–4.3 given below.

Let X be a (real or complex valued) normed vector space equipped with the norm $\|\cdot\|_X$. Assume that a function

$$u \in C([0, T_\infty); X) \tag{I}$$

is given for some $T_\infty > 0$. (We might imagine that u is the solution of a partial differential equation.) Our main assumption is that

$$\lim_{t \to T_\infty} \|u(t)\|_X = \infty. \tag{II}$$

We introduce non-uniform time-grid points

$$0 = t_0 < t_1 < \cdots < t_n < \cdots$$

and assume that

$$\Delta t_n = t_{n+1} - t_n \le \tau \qquad (n \ge 0) \tag{III}$$

for a given $\tau > 0$. Let X_h be a closed subspace of X with a parameter $h > 0$. Then, suppose that we are given

$$u_{\tau,h}^n = u_\rho^n \in X_h \quad (n \ge 0) \tag{IV}$$

where

$$\rho = (\tau, h).$$

We further assume that

$$\lim_{\rho \to 0} \max_{t_n \in [0,T]} \|u_\rho^n - u(t_n)\|_X = 0 \text{ for any } T \in (0, T_\infty). \tag{V}$$

Hereinafter, by $\rho \to 0$, we mean that $|\tau| + |h| \to 0$. Consequently, u_ρ^n might be an approximation of $u(t_n)$ by, for example, the finite difference method. There, h denotes the granularity parameter of spatial discretization.

We let

$$T(\rho) = T(\tau, h) = \sum_{n=0}^{\infty} \Delta t_n \le \infty. \tag{60}$$

Then, we want to find some conditions that imply

$$T(\rho) < \infty;$$
$$\lim_{t_n \to T(\rho)} \|u_\rho^n\|_X = \lim_{n \to \infty} \|u_\rho^n\|_X = \infty;$$
$$\lim_{\rho \to 0} T(\rho) = T_\infty.$$

To achieve this purpose, we provide an auxiliary observation. In many applications, (II) is a consequence of

$$\frac{d}{dt} J(t, u(t)) \ge G_0(|J(t, u(t))|) \quad (t > 0), \tag{61}$$

where $J : (0, \infty) \times X \to \mathbb{R}$ is a functional satisfying

$$|J(t, v)| \le C_J \|v\|_X \qquad (t \ge 0, v \in X), \tag{VI}$$

with $C_J > 0$ and $G : [0, \infty) \to [0, \infty)$ is a function of class (G) defined below.

Condition (G). $G : [0, \infty) \to [0, \infty)$ is called a function of class (G) if the following conditions (62a)–(62c) are satisfied:

$$G \text{ is continuously differentiable and is strictly monotone increasing;} \tag{62a}$$

$$G(s) > 0 \text{ for } s > 0; \tag{62b}$$

$$\int_\beta^\infty \frac{ds}{G(s)} < \infty \qquad (\beta\text{: a positive constant}). \tag{62c}$$

Actually, if $J(0, u(0)) \geq \alpha > 0$ for some $\alpha > 0$, then (61) implies that $J(t, u(t))$ is a strictly increasing function of $t > 0$. Furthermore, there exists $T_J > 0$ such that $J(t, u(t)) \to \infty$ as $t \to T_J$, where

$$0 < T_J \leq \int_\alpha^\infty \frac{dz}{G(z)} < \infty. \tag{63}$$

Therefore, we deduce (II) for $T_\infty < T_J$.

Based on this observation, we assume directly that

$$J(t, u(t)) \to \infty \quad \text{as} \quad t \to T_\infty \tag{VII}$$

instead of (61). Moreover, we introduce a functional $J_h : (0, \infty) \times X_h \to \mathbb{R}$ which satisfies

$$|J_h(t, v)| \leq C'_J \|v\|_X \qquad (t \geq 0,\ v \in X_h), \tag{VIII}$$

where C'_J is a positive constant that is independent of $t \geq 0$. Assume that

$$J_h(0, u_\rho^0) \geq \alpha \text{ with some } \alpha > 0; \tag{H1}$$

$$\frac{J_h(t_{n+1}, u_\rho^{n+1}) - J_h(t_n, u_\rho^n)}{\Delta t_n} \geq G(J_h(t_n, u_\rho^n)) \quad (n \geq 0), \tag{H2}$$

where G is a function of class (G). As a consequence of (H1) and (H2), we have $J_h(t_n, u_\rho^n) \geq \alpha$ and $J_h(t_n, u_\rho^n)$ is monotone increasing on $n \in \mathbb{N}$. We remark that (H2) should be understood recurrently. That is, first, we have (H2) for $n = 0$ under (H1). Therefore $J_h(t_1, u_\rho^1) \geq \alpha$. Then, we have (H2) for $n = 1$ and so on.

Furthermore, suppose the following:

$$\Delta t_n \leq \frac{\tau}{H(J_h(t_n, u_\rho^n))} \qquad (n \geq 0); \tag{H3}$$

$$\frac{1}{H(J_h(0, u_\rho^0))} \leq 1; \tag{H4}$$

$$\lim_{\rho \to 0} \max_{t_n \in [0,T]} \left| J_h(t_n, u_\rho^n) - J(t_n, u(t_n)) \right| = 0 \text{ for any } T \in (0, T_\infty); \tag{H5}$$

$$\|u_\rho^n\|_X \to \infty \text{ as } n \to \infty \text{ if } T(\rho) \leq M \text{ with some } 0 < M \leq T_\infty. \tag{H6}$$

Hereinafter, $H : [0, \infty) \to [0, \infty)$ is a function satisfying the following (64a)–(64d):

$$H \text{ is continuous and monotone increasing;} \tag{64a}$$

$$\lim_{s \to \infty} H(s) = \infty; \tag{64b}$$

$$\text{the mapping } s \mapsto s + \tau \frac{G(s)}{H(s)} \text{ is monotone increasing;} \tag{64c}$$

$$\int_\gamma^\infty \frac{G'(z)}{G(z)H(z)} dz < \infty \quad (\gamma\text{: a positive constant}). \tag{64d}$$

We designate such H a function of class (H) associated with G.

We are now in a position to state our main results in this section.

Proposition 4.1. *Let (I)–(VIII) be given. Assuming that (H1)–(H4) are satisfied, then we have*

$$T(\rho) \leq 2\left(\int_{\alpha}^{\infty} \frac{dz}{G(z)} + C\tau\right), \tag{65}$$

where G is the function appearing in (H2). Particularly $T(\rho) < \infty$.

Proposition 4.2. *Let (I)–(VIII) be given. Assuming that (H1)–(H4) and (H5) are satisfied, then we have*

$$\limsup_{\rho \to 0} T(\rho) \leq T_\infty$$

and

$$\lim_{t_n \to T(\rho)} \|u_\rho^n\|_X = \lim_{n \to \infty} \|u_\rho^n\|_X = \infty.$$

Proposition 4.3. *Let (I)–(VIII) be given. Assuming that (H1)–(H4) and (H6) are satisfied, then we have*

$$T_\infty \leq \liminf_{\rho \to 0} T(\rho).$$

Remark 4.4. In previous works, we defined

$$\Delta t_n = \tau \min\left\{1,\ \frac{1}{\|u_\rho^n\|_X^q}\right\} \tag{66}$$

with some $q > 0$. Therefore, setting $H(s) = (s/C'_J)^q$, we have (III), (H3) and (H6).

Proof of Proposition 4.1. Consider the finite difference scheme

$$\frac{v^{n+1} - v^n}{\Delta s_n} = G(v^n) \quad (n = 0, 1, 2, \cdots), \quad v^0 = J_h(u_\rho^0), \tag{67}$$

where Δs_n is defined as

$$\Delta s_n = \frac{\tau}{H(v^n)}.$$

It follows from (H4), (62b) and (64a) that

$$\Delta s_n \leq \tau \qquad \text{for} \quad (n \geq 0).$$

Moreover, it was shown in [8, Theorem 2.1] that $\lim_{n\to\infty} v^n = \infty$ and

$$\sum_{k=0}^{\infty} \Delta s_k \leq \int_{\alpha}^{\infty} \frac{dz}{G(z)} + C\tau < \infty, \tag{68}$$

where C is a constant that is independent of τ.

To prove (65), it is sufficient to show that

$$\sum_{k=0}^{\infty} \Delta t_k \leq 2 \sum_{k=0}^{\infty} \Delta s_k.$$

We recall that $J_h(u_\rho^n) \geq \alpha$ for $n \geq 0$ and $J_h(u_\rho^n)$ is a strictly monotone increasing sequence in n in view of (H1) and (H2), as described previously.

First, from (H3), one obtains

$$\Delta t_0 \leq \frac{\tau}{H(J_h(0, u_\rho^0))} = \frac{\tau}{H(v^0)} = \Delta s_0.$$

If

$$\sum_{n=0}^{\infty} \Delta t_n \leq \Delta s_0$$

takes place, the proof is finished. Otherwise, there exists an $n_1 \geq 0$ such that

$$\sum_{n=0}^{n_1} \Delta t_n \leq \Delta s_0 \quad \text{and} \quad \Delta s_0 < \sum_{n=0}^{n_1+1} \Delta t_n. \tag{69}$$

Consequently, we can estimate the following:

$$\begin{aligned}
\sum_{n=0}^{n_1+1} \Delta t_n &= \sum_{n=0}^{n_1} \Delta t_n + \Delta t_{n_1+1} \\
&\leq \Delta s_0 + \frac{\tau}{H(t_{n_1+1}, J_h(u_\rho^{n_1+1}))} \leq \Delta s_0 + \frac{\tau}{H(J_h(0, u_\rho^0))} = 2\Delta s_0.
\end{aligned}$$

Moreover, it follows from (H2) that

$$\begin{aligned}
J_h(t_{n_1+2}, u_\rho^{n_1+2}) &\geq J_h(t_{n_1+1}, u_\rho^{n_1+1}) + \Delta t_{n_1+1} G(J_h(t_{n_1+1}, u_\rho^{n_1+1})) \\
&\geq J_h(t_{n_1}, u_\rho^{n_1}) + \Delta t_{n_1} G(J_h(t_{n_1}, u_\rho^{n_1})) + \Delta t_{n_1+1} G(J_h(t_{n_1+1}, u_\rho^{n_1+1})) \\
&\geq J_h(t_{n_1}, u_\rho^{n_1}) + (\Delta t_{n_1} + \Delta t_{n_1+1}) G(J_h(t_{n_1}, u_\rho^{n_1})) \geq \cdots \\
&\geq J_h(0, u_\rho^0) + \left(\sum_{n=0}^{n_1+1} \Delta t_k \right) G(J_h(0, u_\rho^0)) \\
&\geq v^0 + \Delta s_0 G(v^0) = v^1.
\end{aligned} \tag{70}$$

Based on that result, we obtain that

$$\Delta t_{n_1+2} \leq \frac{\tau}{H(J_h(t_{n_1+2}, u_\rho^{n_1+2}))} \leq \frac{\tau}{H(v^1)} = \Delta s_1. \tag{71}$$

Therefore, either (71) or (72) holds:

$$\sum_{n=n_1+2}^{\infty} \Delta t_n \leq \Delta s_1. \tag{72}$$

At this stage, if

$$\sum_{n=n_1+2}^{n_2} \Delta t_n \leq \Delta s_1 \quad \text{and} \quad \Delta s_1 < \sum_{n=n_1}^{n_2+1} \Delta t_n.$$

takes place, the proof is completed. Otherwise, in exactly the same manner as shown above, we deduce

$$\sum_{n=n_1+2}^{n_2+1} \Delta t_n \leq 2\Delta s_1$$

and $J_h(t_{n_2+2}, u_\rho^{n_2+2}) \geq v^2$.

Consequently,

$$\Delta t_{n_2+2} \leq \frac{\tau}{H(J_h(u_\rho^{n_2+2}))} \leq \frac{\tau}{H(v^2)} = \Delta s_2.$$

Repeating this argument, we find a sequence $\{n_j\}_{j=1}^\infty$ such that $J_h(t_{n_j+2}, u_\rho^{n_j+2}) \geq v^j$ and

$$\sum_{n=n_j+2}^{n_{j+1}+1} \Delta t_n \leq 2\Delta s_j,$$

for all $j \geq 1$. Consequently,

$$\begin{aligned}\sum_{n=0}^{\infty} \Delta t_n &= \lim_{r\to\infty} \left(\sum_{n=0}^{n_1+1} \Delta t_n + \sum_{n=n_1+2}^{n_2+1} \Delta t_n + \cdots + \sum_{n=n_{r-1}+2}^{n_r+1} \Delta t_n \right) \\ &\leq 2 \lim_{r\to\infty} \sum_{n=0}^{r-1} \Delta s_n \leq 2 \left(\int_\alpha^\infty \frac{dz}{G(z)} + C\tau \right),\end{aligned}$$

which completes the proof. □

Proof of Proposition 4.2. We show

$$T^* \equiv \limsup_{\rho\to 0} T(\rho) \leq T_\infty \tag{73}$$

by contradiction. Let

$$T_\infty < T^* \tag{74}$$

and set $\varepsilon = (T^* - T_\infty)/4$. There exist $R > 0$ and $\hat{\tau} > 0$ such that

$$2 \left(\int_R^\infty \frac{dz}{G(z)} + C\hat{\tau} \right) < \varepsilon.$$

Below we fix such R and $\hat{\tau}$. Then, by (H5), there exists $\tau_\# > 0$ and $h_\# > 0$ such that

$$|J(t_n, u(t_n)) - J_h(t_n, u_\rho^n)| \leq R$$

for $\tau \in (0, \tau_\#]$ and $h \in (0, h_\#]$. Moreover, in view of (VII), there exists $t' = t'_R < T_\infty$ such that $J(u(t')) > 2R$. Set

$$\tau_* = \min \left\{ \hat{\tau},\ \tau_\#,\ T_\infty - t', \right\}$$

and assume $\tau \in (0, \tau_*]$ below. Consequently, we obtain $\tau \leq T_\infty - t'$ and

$$J_h(t_n, u_\rho^n) \geq J(t_n, u(t_n)) - R.$$

There exists $k \in \mathbb{N}$ satisfying $t' \leq t_k < T_\infty$ because $\tau < T_\infty - t'$. Therefore,

$$J_h(t_k, u_\rho^k) \geq J(t_k, u(t_k)) - R > R. \tag{75}$$

It follows from (74) that we can take a sub-sequence $\{\rho_i = (\tau_i, h_i)\}_{i=1}^\infty$ with $\rho_i \to 0$ as $i \to \infty$ such that

$$T_\infty + \varepsilon < T(\rho_i).$$

However, as a consequence of Proposition 4.1 and (75), we obtain

$$T(\rho_i) = \sum_{n=0}^{\infty} \Delta t_n = \sum_{n=0}^{k} \Delta t_n + \sum_{n=k+1}^{\infty} \Delta t_n \leq t_k + 2\left(\int_R^\infty \frac{dz}{G(z)} + C\hat{\tau} \right) < T_\infty + \varepsilon.$$

This result presents a contradiction. Therefore, we obtain (73). □

Proof of Proposition 4.3. As a consequence of Proposition 4.1, we know that $T(\rho) < \infty$. We will show that

$$T_\infty \leq \liminf_{\rho\to 0} T(\rho) \equiv T_* \tag{76}$$

by contradiction. In addition, we assume that

$$T_* < T_\infty.$$

Then, there exists a sub-sequence $\{\rho_i = (\tau_i, h_i)\}_{i=1}^\infty$ such that $\rho_i \to 0$ as $i \to \infty$ and

$$T(\rho_i) \leq T_* + \delta < T_\infty,$$

where $\delta = (T_\infty - T_*)/2$. Therefore, (H6) can be applied to obtain $\|u_\rho^n\|_X \to \infty$ as $t \to T(\rho)$.

We have

$$\max_{0\leq t\leq T_*+\delta} \|u(t)\|_X < \infty. \tag{77}$$

However, the solution $u_{h_i}^n$ satisfies

$$\lim_{n\to\infty} \|u_{\rho_i}^n\|_X = \lim_{t_n\to T(\rho_i)} \|u_{\rho_i}^n\|_X = \infty. \tag{78}$$

Those (77) and (78) contradict to (V). Therefore, (76) is proved. □

Remark 4.5. Main results established in other studies reported in the literature [6], [7], [8], [14], [15], and [17] can be obtained by application of Propositions 4.1, 4.2 and 4.3.

5. Approximation of the blow-up time (Proof of Theorem III)

This section is dedicated to the proof of Theorem III. It would be interesting to derive a discrete version of (10). However, we do not attempt to proceed in this direction. Instead, we shall apply Propositions 4.1–4.3 with

$$X = L^\infty(0,1), \quad \|\cdot\|_X = \|\cdot\|_{L^\infty(0,1)}.$$

Below, we assume that the unique solution u of (5) is sufficiently smooth and that (37) is satisfied. Then, as described before, u and $J(t, u(t,\cdot))$ blow up, respectively, in $T_\infty < 1/(4\pi)$ and $T_J < 1/(4\pi)$. It must be recalled that we are assuming $T_\infty = T_J$ (see (38)). Let $\boldsymbol{u}^n = (u_1^n, \ldots, u_N^n)^{\mathrm{T}}$ be the unique solution of (32) and set $u_0^n = u_{N+1}^n = 0$. Recall moreover that the numerical blow-up time $T(h,\tau)$ defined by (36).

We set

$$I_j = \begin{cases} \left[0, \frac{h}{2}\right] & (j = 0) \\ \left(x_j - \frac{h}{2}, x_j + \frac{h}{2}\right] & (j = 1, 2, \ldots, N) \\ \left(1 - \frac{h}{2}, 1\right] & (j = N + 1) \end{cases}$$

and introduce

$$X_h = \{v_h \in X \mid v_h \text{ is a constant function on each } I_j \ (j = 0, 1, \cdots, N + 1)\}.$$

We define $u_\rho^n \in X_h$, $\rho = (\tau, h)$, for $n = 0, 1, \ldots$ by

$$u_\rho^n(x) = u_j^n \qquad (x \in I_j,\ j = 0, 1, \ldots, N + 1). \tag{79}$$

Now we introduce $J_h : [0, \infty) \times X_h \to \mathbb{R}$, which is a discrete version of J, as

$$J_h(t_n, v) = \frac{1}{2\beta(h)} \sum_{j=1}^{N} \mathrm{Im}(\eta^n v(x_j)) \sin(\pi x_j) h$$

for $n \in \mathbb{N}$ and $v \in X_h$, where $\beta(h) = \displaystyle\sum_{j=1}^{N} \sin(\pi x_j) h$ and η^n is a unique solution of

$$\frac{\eta^{n+1} - \eta^n}{\Delta t_n} = i\pi^2 \left[\theta\eta^n + (1 - \theta)\eta^{n+1}\right] \quad (n \geq 0), \qquad \eta^0 = 1. \tag{80}$$

It is readily apparent that η^n is an approximation of $e^{i\pi^2 t_n}$. Particularly, we have positive constants C' and $\hat{\tau}$ such that

$$|\eta^n - e^{i\pi^2 t_n}| \leq C'\tau^\sigma, \quad |\eta^n| \leq 2 \tag{81}$$

for $n \geq 1$ and $\tau \in (0, \hat{\tau}]$, where σ is defined as (25).

One can note that

$$|J_h(v)| \leq \|v\|_X, \tag{82}$$

for $v \in X_h$. Moreover, it is noteworthy that, as a consequence of (37) and (H5) (which will be verified below), there is a constant $\hat{h} > 0$ such that

$$J_h(0, u_\rho^0) > 1 \tag{83}$$

for any $h \in (0, \hat{h}]$.

Now we can state the following proof.

Proof of Theorem III. We first check (I)–(VI) in Section 4:

- (I) is satisfied if u_0 is smooth and satisfies the compatibility conditions with the boundary condition (see Proposition A.2);
- (II) is satisfied with $T_\infty \leq T_J < 1/(4\pi)$ by (31);
- (III) is satisfied by the definition of Δt_n;
- (IV) is given as the finite difference solution u_ρ^n;

- (V) is guaranteed by Theorem II;
- (VI) is satisfied with $C_J = 1$;
- (VII) is assumed;
- (VIII) is satisfied with $C'_J = 1$ (see (82)).

We consider functions $G(s) = s^{2p}$ and $H(s) = s^q$ for $p \geq 1$ and $q > 0$. Actually, $G(s)$ is a function of class (G) and $H(s)$ is a function of class (H) associated with G.

To apply Propositions 4.1 and 4.2, we verify (H1)–(H5):

- (H2) is satisfied as will be stated in Proposition 5.1 presented below;
- (H3) is satisfied, because, by (VI),
$$\Delta t_n \leq \frac{\tau}{\|u_\rho^n\|_{L^\infty(I)}^q} \leq \frac{\tau}{J_h(t_n, u_\rho^n)^q} = \frac{\tau}{H(J_h(t_n, u_\rho^n))};$$
- (H4) is satisfied (see (83));
- (H5) is a readily obtainable consequence of (V), (81), and $\beta(h) \to \pi/2$ as $h \to 0$;
- (H1) is satisfied (see (83)).

Finally, we verify (H6) using Proposition 4.2 in the following way. Assuming that $T(h,\tau) \leq M$ for some $0 < M \leq T_\infty$, then we prove $\|u_\rho^n\|_X \to \infty$ as $n \to \infty$ by showing a contradiction. Assume $\|u_\rho^n\|_X < \infty$ for $n \geq 0$. Then, by the definition of Δt_n, we must have $a_n \to 0$. Therefore, $T(h,\tau) = 1/(4\pi)$. However, in view of Proposition 4.2,
$$T_\infty \geq \limsup_{h,\tau\to 0} T(h,\tau) = \frac{1}{4\pi} > T_J \geq T_\infty,$$
which is a contradiction. Therefore, we have proved (H6).

We can therefore apply Proposition 4.3 and complete the proof of Theorem III. □

The following proposition must be stated.

Proposition 5.1. *Letting* $1/2 \leq \theta \leq 1$ *and assuming that* (37) *is satisfied, then,* $J_h(t_n, u_h^n)$ *is a positive and strictly increasing sequence in* $n \geq 0$ *(Consequently,* $J_h(t_n, u_h^n) \geq 0$ *for* $n \geq 0$*), and there exist positive constants* h_1 *and* τ_1 *such that*
$$\frac{J_h(t_{n+1}, u_h^{n+1}) - J_h(t_n, u_h^n)}{\Delta t_n} \geq \frac{1}{16} J_h(t_n, u_h^n)^{2p}, \tag{84}$$
for $n \geq 0$, $h \in (0, h_1]$ *and* $\tau \in (0, \tau_1]$.

Proof. Because $t_n \leq 1/(4\pi)$, we have
$$\mathrm{Re}(e^{i\pi^2 t_n}) = \cos(\pi^2 t_n) \geq \cos(\pi/4) = \frac{1}{\sqrt{2}}.$$

Therefore, in view of (81)

$$\operatorname{Re}\eta^n \geq \cos(\pi^2 t_n) - C_1\tau^2 > \frac{1}{2} \tag{85}$$

for $n \geq 0$ and $\tau \in (0, \hat{\tau}]$.

We write $J_n = J_h(t_n, u_\rho^n)$, $u_j^{n+\theta} = \theta u_j^{n+1} + (1-\theta)u_j^n$ and $\eta^{n+\theta} = (1-\theta)\eta^{n+1} + \theta\eta^n$ for abbreviation. Using (32), we can calculate it as

$$\begin{aligned}
\frac{J_{n+1} - J_n}{\Delta t_n} &= \frac{1}{2\beta(h)} \operatorname{Im} \sum_{j=1}^{N} \left[(D_{\Delta t_n}\eta^n) u_j^{n+\theta} + \eta^{n+\theta}(D_{\Delta t_n} u_j^n) \right] \sin(\pi x_j) h \\
&= \frac{1}{2\beta(h)} \operatorname{Re} \sum_{j=1}^{N} \pi^2 \eta^{n+\theta} u_j^{n+\theta} \sin(\pi x_j) h \\
&\quad + \frac{1}{2\beta(h)} \operatorname{Re} \sum_{j=1}^{N} \eta^{n+\theta} (\delta_h^2 u_j^{n+\theta}) \sin(\pi x_j) h \\
&\quad + \frac{1}{2\beta(h)} \operatorname{Re} \sum_{j=1}^{N} \eta^{n+\theta} \left[\theta |u_j^{n+1}|^{2p} + (1-\theta)|u_j^n|^{2p} \right] \sin(\pi x_j) h
\end{aligned}$$

for $n \geq 0$. An elementary identity is applied:

$$\sum_{j=1}^{N} \delta_h^2 u_j^n \sin(\pi x_j) h = -\pi^2 [1 - \kappa(h)] \sum_{j=1}^{N} \sin(\pi x_j) u_j^n h,$$

where

$$\kappa(h) = 1 - \frac{4}{\pi^2 h^2} \sin^2 \left(\frac{\pi h}{2} \right),$$

and obtain the following using (81),

$$\begin{aligned}
\frac{J_{n+1} - J_n}{\Delta t_n} &= \frac{\pi^2}{2\beta(h)} \operatorname{Re} \sum_{j=1}^{N} \eta^{n+\theta} u_j^{n+\theta} \sin(\pi x_j) h \\
&\quad - \frac{\pi^2 [1 - \kappa(h)]}{2\beta(h)} \operatorname{Re} \sum_{j=1}^{N} \eta^{n+\theta} u_j^{n+\theta} \sin(\pi x_j) h \\
&\quad + \frac{1}{2\beta(h)} \sum_{j=1}^{N} \operatorname{Re} \eta^{n+\theta} \left[\theta |u_j^{n+1}|^{2p} + (1-\theta)|u_j^n|^{2p} \right] \sin(\pi x_j) h \\
&= \frac{\pi^2 \kappa(h)}{2\beta(h)} \operatorname{Re} \sum_{j=1}^{N} \eta^{n+\theta} u_j^{n+\theta} \sin(\pi x_j) h \\
&\quad + \frac{1}{2\beta(h)} \sum_{j=1}^{N} \operatorname{Re} \eta^{n+\theta} \left[\theta |u_j^{n+1}|^{2p} + (1-\theta)|u_j^n|^{2p} \right] \sin(\pi x_j) h \\
&\geq -\frac{\pi^2 \kappa(h)}{\beta(h)} \sum_{j=1}^{N} \left[\theta |u_j^{n+1}| + (1-\theta)|u_j^n| \right] \sin(\pi x_j) h \\
&\quad + \frac{1}{4\beta(h)} \sum_{j=1}^{N} \left[\theta |u_j^{n+1}|^{2p} + (1-\theta)|u_j^n|^{2p} \right] \sin(\pi x_j) h
\end{aligned}$$

Next we prove (84) by induction in n. To do so, it is noteworthy that there exists a positive constant h_2 such that $0 < \pi^2\kappa(h) \leq 1/16$ holds for $h \in (0, h_2]$. In what follows, we presume that $h \in (0, h_3]$, where $h_3 = \min\{h_1, h_2\}$. Moreover, we use

$$J_n \leq \frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^n| \sin(\pi x_j) h, \tag{86a}$$

$$\frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^n|^{2p} \sin(\pi x_j) h \geq \left(\frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^n| \sin(\pi x_j) h \right)^{2p} \geq J_n^{2p} \tag{86b}$$

for $n \geq 0$. The first inequality (86b) is a consequence of Jensen's inequality.

First, we show that (84) holds for $n = 0$. It is noteworthy that

$$\frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^0| \sin(\pi x_j) h \geq J_0 > 1. \tag{87}$$

If assuming

$$\frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^1| \sin(\pi x_j) h \geq 1,$$

we can estimate it using (86),

$$\begin{aligned}
\frac{J_1 - J_0}{\Delta t_0} \geq{}& \frac{1}{4\beta(h)} \sum_{j=1}^{N} \left[(1-\theta)|u_j^1|^{2p} + \theta |u_j^0|^{2p} \right] \sin(\pi x_j) h \\
&- \frac{1}{16\beta(h)} \sum_{j=1}^{N} \left[(1-\theta)|u_j^1| + \theta |u_j^0| \right] \sin(\pi x_j) h \\
\geq{}& \frac{1}{4} \left[(1-\theta) J_1^{2p} + \theta J_0^{2p} \right] - \frac{1}{16} \left[(1-\theta) J_1^{2p} + \theta J_0^{2p} \right] \\
\geq{}& \frac{3}{16} \left[(1-\theta) J_1^{2p} + \theta J_0^{2p} \right] \geq \frac{3\theta}{16} J_0^{2p} \geq \frac{1}{16} J_0^{2p}.
\end{aligned}$$

However, if

$$\frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^1| \sin(\pi x_j) h < 1,$$

then by using

$$\frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^1| \sin(\pi x_j) h < 1 \leq \frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^0| \sin(\pi x_j) h,$$

we have

$$\begin{aligned}
\frac{J_1 - J_0}{\Delta t_0} &\geq \frac{1}{4\beta(h)} \sum_{j=1}^{N} \left[(1-\theta)|u_j^1|^{2p} + \theta |u_j^0|^{2p}\right] \sin(\pi x_j) h \\
&\qquad - \frac{1}{16\beta(h)} \sum_{j=1}^{N} \left[(1-\theta)|u_j^0| + \theta |u_j^0|\right] \sin(\pi x_j) h \\
&\geq \frac{1}{4\beta(h)} \sum_{j=1}^{N} \left[(1-\theta)|u_j^1|^{2p} + \theta |u_j^0|^{2p}\right] \sin(\pi x_j) h \\
&\qquad - \frac{1}{16\beta(h)} \sum_{j=1}^{N} |u_j^0| \sin(\pi x_j) h \\
&\geq \frac{1}{4}\left[(1-\theta) J_1^{2p} + \theta J_0^{2p}\right] - \frac{1}{16} J_0^{2p} \geq \frac{1}{16} J_0^{2p}.
\end{aligned}$$

Consequently, the case for which $n = 0$ is verified.

Next, we assume that $0 < n_0 \in \mathbb{Z}$ exists such that (84) holds for $0 \leq n \leq n_0 - 1$. Then we obtain a rough estimate

$$J_n \geq 1$$

for $0 \leq n \leq n_0$. By considering two cases

$$\frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^{n_0+1}| \sin(\pi x_j) h \geq 1$$

and

$$\frac{1}{\beta(h)} \sum_{j=1}^{N} |u_j^{n_0+1}| \sin(\pi x_j) h < 1,$$

we can prove that (84) is satisfied for $n = n_0 + 1$ as we have shown for $n_0 = 0$.

This completes the proof of Proposition 5.1. □

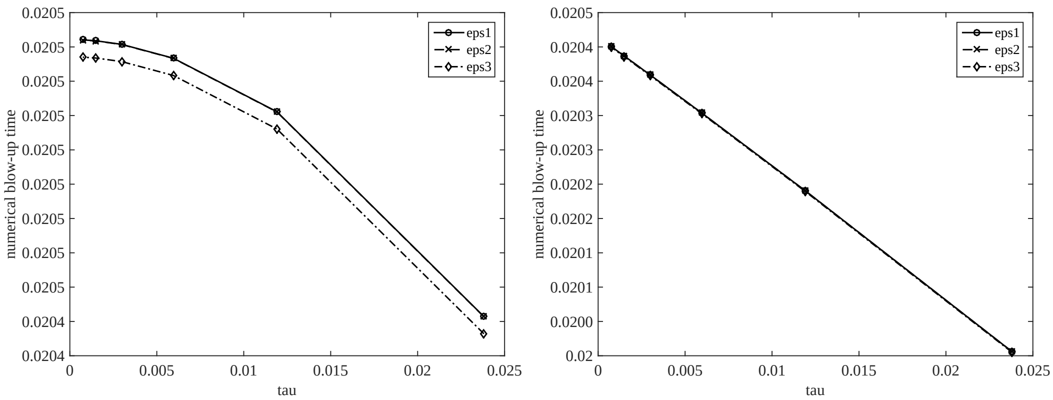
6. Numerical examples

This section presents some numerical examples to confirm Theorem III. The numerical blow-up time $T(h, \tau)$ is an infinite series defined as (36). Therefore, in actual computations, we take a sufficiently large n and regard t_n as a reasonable approximation of $T(h, \tau)$. We assume $1/2 \leq \theta \leq 1$, $\tau = h$ and $q = p$ (see Remark C.3). Furthermore, set $T(\tau) = T(h, \tau)$. For the time being, the initial function is set as $u_0(x) = 50i \sin(\pi x)$. We then introduce the *truncated numerical blow-up time* $T_\varepsilon(\tau)$ by setting

$$T_\varepsilon(\tau) = \min\left\{t_n \mid \|\boldsymbol{u}^n\|_\infty > \varepsilon^{-1}\right\}, \tag{88}$$

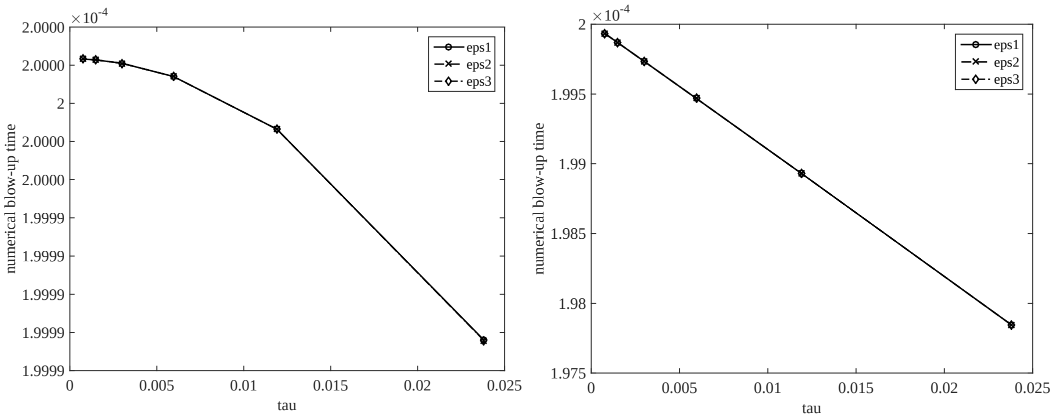
where $\varepsilon > 0$ is the stopping criterion given below.

For a given $\varepsilon_1 > 0$, we set $\varepsilon_2 = 100\varepsilon_1$, $\varepsilon_3 = 100\varepsilon_2$ and $T_j(\tau) = T_{\varepsilon_j}(\tau)$ for $j = 1, 2, 3$. We present $T_1(\tau)$, $T_2(\tau)$, and $T_3(\tau)$ for several values of τ in Fig. 3–5. If τ is sufficiently small, then $T_1(\tau)$ and $T_2(\tau)$ are almost equal. Therefore, we can



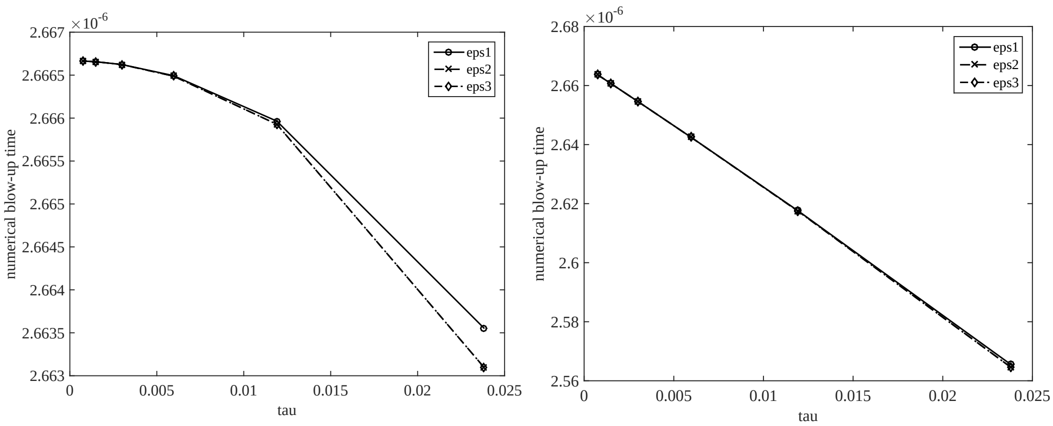
(a) $\theta = 1/2$ (b) $\theta = 1$

Figure 3: Truncated blow-up times $T_1(\tau)$ (`eps1`), $T_2(\tau)$ (`eps3`) and $T_3(\tau)$ (`eps2`) for solutions of (32) with $p = 1$ and $\varepsilon_1 = 10^{-10}$.



(a) $\theta = 1/2$ (b) $\theta = 1$

Figure 4: Truncated blow-up times $T_1(\tau)$ (`eps1`), $T_2(\tau)$ (`eps3`) and $T_3(\tau)$ (`eps2`) for solutions of (32) with $p = 3/2$ and $\varepsilon_1 = 10^{-10}$.



(a) $\theta = 1/2$ (b) $\theta = 1$

Figure 5: Truncated blow-up times $T_1(\tau)$ (`eps1`), $T_2(\tau)$ (`eps3`) and $T_3(\tau)$ (`eps2`) for solutions of (32) with $p = 2$ and $\varepsilon_1 = 10^{-10}$.

consider $T_\varepsilon(\tau)$ as an appropriate approximation of the exact blow-up time. Table 1 is the final result of the numerical blow-up time.

Moreover, we infer from Fig. 3–5 that there is the relation

$$T(\tau) = -C\tau^\alpha + T_\infty \tag{89}$$

where $C > 0$ and $\alpha \geq 1$ are constants. To verify this using numerical experiments, letting $k(\tau) = |T(2\tau, \varepsilon) - T(\tau, \varepsilon)|$, we observe

$$\alpha(\tau) = \frac{\log k(\tau) - \log k(2\tau)}{-\log 2}. \tag{90}$$

In fact, if $\alpha = \alpha(\tau)$ is independent of τ, then we have $k(\tau) = C'\tau^\alpha$ with $C' = C(2^\alpha - 1)$. The result is reported in Table 2. From this, we infer that, as $\tau \to 0$,

$$|T(\tau, h) - T_\infty| = O(\tau^\sigma)$$

holds, where σ is defined as (25). The proof of this conjecture is left as a subject for future study.

τ	$p=1$	$p=3/2$	$p=2$
0.00595238	0.0204633423	0.0002000014	0.0000026665
0.00297619	0.0204641504	0.0002000021	0.0000026666
0.00148810	0.0204643586	0.0002000023	0.0000026667
0.00074405	0.0204644119	0.0002000023	0.0000026667

Table 1: Numerical blow-up times $T_1(\tau)$ for $\theta = 1/2$ and $\varepsilon_1 = 10^{-10}$.

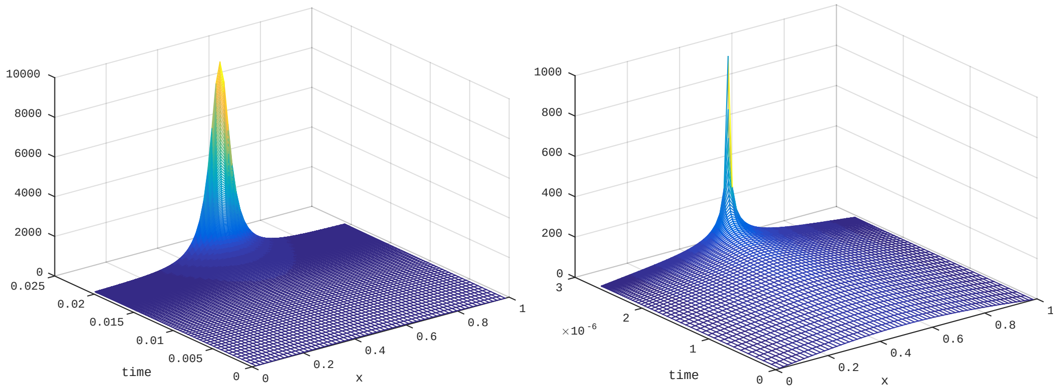
	$p=1$		$p=3/2$		$p=2$	
τ	$\theta=1/2$	$\theta=1$	$\theta=1/2$	$\theta=1$	$\theta=1/2$	$\theta=1$
0.00595238	2.18	1.07	2.00	1.01	1.94	1.05
0.00297619	2.03	1.03	1.99	1.01	1.95	1.03
0.00148810	2.02	1.01	1.99	1.00	1.96	1.01
0.00074405	2.03	1.01	1.99	1.00	1.97	1.01

Table 2: Numerical convergence rates $\alpha(\tau)$ of $T(\tau)$.

Finally, examples of shapes of numerical solutions $\boldsymbol{u}^n$ of (32) are given. We take two initial functions $u_0(x) = 50i\sin(\pi x)$ and $u_0(x) = 100\sin(2\pi x) + 50i\sin(\pi x)$. In Fig. 6 and 7, the absolute value $|\boldsymbol{u}^n|$ of $\boldsymbol{u}^n$ is shown.

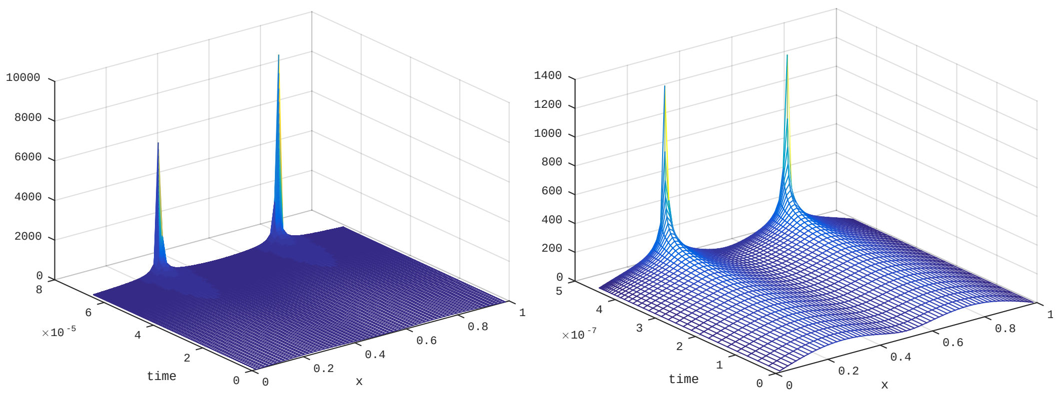
A. Well-posedness of (13)

The following results are not new for specialists of nonlinear Schrödinger equations. For example, Proposition A.1 is fundamentally described in [5, theorem 3.5.1]. However, results for more regular solutions are not given explicitly in [5]. If considering



(a) $p = 1$ (b) $p = 2$

Figure 6: Shapes of numerical solutions $|\boldsymbol{u}^n|$ of (32): $u_0(x) = 50i\sin(\pi x)$, $N = 63$, $\tau = h$ and $\theta = 1/2$.



(a) $p = 3/2$ (b) $p = 2$

Figure 7: Shapes of numerical solutions $|\boldsymbol{u}^n|$ of (32): $u_0(x) = 100\sin(2\pi x) + 50i\sin(\pi x)$, $N = 63$, $\tau = h$ and $\theta = 1/2$.

the Cauchy problem, we can use the smoothing property of the Schrödinger semigroup and obtain a regular (global-in-time) solution in a certain sense (see [11]). However, in the case of a bounded domain, any smoothing properties are not available. Therefore, we assume sufficiently smooth data f, g and u_0 to obtain a smooth solution.

Let $I = (0, L)$ for $L > 0$. Any function spaces considered in this appendix are still complex-valued. We introduce the following linear operators A and H of $L^2(I) \to L^2(I)$ by

$$\mathcal{D}(A) = H^2(I) \cap H_0^1(I), \quad Av = -\frac{d^2}{dx^2}v \quad (v \in \mathcal{D}(A)),$$
$$\mathcal{D}(H) = \mathcal{D}(A), \qquad Hv = iAv \quad (v \in \mathcal{D}(H)).$$

The following results are well known (see [16]). Operator A is a positive and self-adjoint operator in $L^2(I)$ and $-A$ generates the analytic semigroup (of class C_0) e^{-tA} in $L^2(I)$. The operator $-H$ generates a C_0 semigroup $S(t) = e^{-itH}$ in $L^2(I)$ and $\|S(t)\|_{L^2(I)} = 1$ for all $t > 0$.

When $I = \mathbb{R}$, one can prove

$$\|S(t)\|_{H^1(I)} = 1 \qquad (t > 0)$$

by the Fourier transform. However, it is not readily apparent that this equality remains valid if I is a bounded interval. Instead, we apply fractional powers $A^{\frac{1}{2}}$ of A. We know that

$$\mathcal{D}(A^{\frac{1}{2}}) = H_0^1(I).$$

Therefore, as a norm of $H_0^1(I)$, we can choose

$$|||v||| = \|A^{\frac{1}{2}}v\|_{L^2(I)} = \|\partial_x v\|_{L^2(I)} \qquad (v \in H_0^1(I)).$$

By Poincaré's inequality, we have

$$C^{-1}\|v\|_{H^1(I)} \le |||v||| \le C\|v\|_{H^1(I)} \qquad (v \in H_0^1(I)).$$

Then, we deduce the following results.

- $|||S(t)||| = 1$ for all $t > 0$.
- There exists a constant $C_I > 0$ such that $\|v\|_{L^\infty(I)} \le C_I|||v|||$ for $v \in H_0^1(I)$.

We make the following condition on the nonlinearity f of $H_0^1(I) \to L^2(I)$.

Condition (f1). There exists a continuous, non-decreasing and positive function $\omega(\eta)$ of $\eta > 0$ such that

$$\|A^{\frac{1}{2}}f(u) - A^{\frac{1}{2}}f(v)\|_{L^2(I)} \le \omega(M)\|A^{\frac{1}{2}}u - A^{\frac{1}{2}}v\|_{L^2(I)}$$

for any $u, v \in \mathcal{D}(A^{\frac{1}{2}})$ with $\|A^{\frac{1}{2}}u\|_{L^2(I)}, \|A^{\frac{1}{2}}v\|_{L^2(I)} \le M$ and $M > 0$. This inequality is written equivalently as

$$\|\partial_x f(u) - \partial_x f(v)\|_{L^2(I)} \le \omega(M)\|\partial_x u - \partial_x v\|_{L^2(I)}$$

for any $u, v \in H_0^1(I)$ with $\|u\|_{H^1(I)}, \|v\|_{H^1(I)} \le M$.

Proposition A.1. *Assume that Condition (f1) is satisfied and that* $g \in C^0([0,T]; H_0^1(I))$*. Then, for any* $u_0 \in H_0^1(I)$*, there exists* $T > 0$ *and a unique*

$$u \in C^0([0,T]; H_0^1(I)) \cap C^1((0,T); [H_0^1(I)]')$$

that satisfies

$$\int_I i(\partial_t u)v \, dx + \int_I (\partial_x u)(\partial_x v) \, dx = \int_I f(u)v \, dx + \int_I gv \, dx$$
$$(\forall v \in H_0^1(I), \quad a.e.\ t \in (0,T))$$

with $u(0,x) = u_0(x)$ *for* $x \in I$*. Moreover, if we define the maximal existence time* T_∞ *as* $T_\infty = \sup T$*, then* $T_\infty < \infty$ *implies* $\lim_{t \to T_\infty} |||u(t)||| = \infty$*.*

We then make the following condition for $f : H_0^1(I) \to L^2(I)$ and $2 \leq m \in \mathbb{Z}$.

Condition (fm). For $k = 1, \ldots, m$ and $u \in \mathcal{D}(A^{m/2})$, we have $f(u) \in \mathcal{D}(A^{k/2})$. Moreover, there exists a continuous, non-decreasing and positive function $\omega_k(\eta)$ of $\eta > 0$ such that

$$\|A^{k/2}[f(u) - f(v)]\|_{L^2(I)} \leq \omega_k(M) \|A^{k/2}(u - v)\|_{L^2(I)}$$

for any $u, v \in \mathcal{D}(A^{k/2})$ with $\|A^{k/2}u\|_{L^2(I)}, \|A^{k/2}v\|_{L^2(I)} \leq M$.

Proposition A.2. *Let* $2 \leq m \in \mathbb{Z}$*. Assume that Condition (fm) is satisfied and that* $g \in C^{[m/2]}([0,\infty); H_0^1(I))$*. Then, for any* $u_0 \in \mathcal{D}(A^{m/2})$*, there exists* $T > 0$ *and a unique*

$$u \in \bigcap_{k=0}^{[m/2]} C^k([0,T]; \mathcal{D}(A^{m/2-k}))$$

that satisfies

$$i\partial_t u + \partial_x^2 u = f(u) + g(t,x) \quad (0 < t < T,\ x \in I)$$

with $u(0,t) = u_0(x)$ *for* $x \in I$*.*

Those propositions A.1 and A.2 are proved fundamentally using the same method used by Segal [18] (see also [5, proof of Theorem 3.3.1]).

Remark A.3. For $m \geq 1$, $u_0 \in \mathcal{D}(A^{m/2})$ implies that $u_0 = \partial_x u_0 = \cdots = \partial_x^m u_0 = 0$ at $x = 0, L$.

B. Proof of Proposition 2.3

Let $f : \mathbb{C} \to \mathbb{C}$. Suppose that $\phi(x,y) = \operatorname{Re} f(z)$ and $\psi(x,y) = \operatorname{Im} f(z)$, $z = x + iy$, are both C^1 functions of $\mathbb{R}_x \times \mathbb{R}_y \to \mathbb{R}$ and that $f(0) = 0$ holds. First, we introduce a useful expression. We write

$$Df(z) = (\phi_x(x,y), \phi_y(x,y))^{\mathrm{T}} + i(\psi_x(x,y), \psi_y(x,y))^{\mathrm{T}} \qquad (z = x + iy).$$

In addition, for $w = \xi + i\eta$, define $Df(z) \cdot w$ as

$$Df(z) \cdot w = \phi_x(x,y)\xi + \phi_y(x,y)\eta + i[\psi_x(x,y)\xi + \psi_y(x,y)\eta].$$

Then, if setting

$$|Df(z)| = \sqrt{\phi_x(x,y)^2 + \phi_y(x,y)^2 + \psi_x(x,y)^2 + \psi_y(x,y)^2},$$

we have

$$|Df(z)\cdot w| \le |Df(z)|\cdot|w| \qquad (z,\ w\in\mathbb{C}).$$

Furthermore, for $R>0$, setting

$$\alpha(R) = \max_{|z|\le\sqrt{L}R} |Df(z)|,$$

we can estimate as

$$|Df(z) - Df(w)| \le 2\alpha(R) \qquad (|z|,|w|\le\sqrt{L}R). \tag{91}$$

Let $\boldsymbol{u} = (u_1,\dots,u_N)^{\mathrm{T}}, \boldsymbol{v} = (v_1,\dots,v_N)^{\mathrm{T}} \in \mathbb{C}^N$ and $u_0 = u_{N+1} = v_0 = v_{N+1} = 0$. Then,

$$\begin{aligned} q_j &\equiv f(u_j) - f(v_j) - [f(u_{j-1}) - f(v_{j-1})] \\ &= \int_0^1 Df(p_j(s))\cdot[(u_j - v_j) - (u_{j-1} - v_{j-1})]\, ds \\ &\quad + \int_0^1 [Df(p_j(s)) - Df(p_{j-1}(s))]\cdot(u_{j-1} - v_{j-1})\, ds \end{aligned}$$

for $1\le j\le N$, where $p_j(s) = sv_j + (1-s)u_j$.

At this stage, we let $R = |||\boldsymbol{u}|||_h \wedge |||\boldsymbol{v}|||_h$. Then, in view of Proposition 2.1 (i), we have $|p_j(s)|, |p_{j-1}(s)| \le \sqrt{L}R$, which we can estimate as

$$|q_j|^2 \le 2\alpha(R)^2[(u_j - v_j) - (u_{j-1} - v_{j-1})]^2 + 4\alpha(R)^2 L|||\boldsymbol{u}-\boldsymbol{v}|||_h^2.$$

Therefore,

$$\begin{aligned} |||\boldsymbol{f}(\boldsymbol{u}) - \boldsymbol{f}(\boldsymbol{v})|||_h^2 &= \sum_{j=1}^{N+1} \frac{|q_j|^2}{h^2} h \\ &\le 2\alpha(R)^2 \sum_{j=1}^{N+1} \frac{|(u_j - v_j) - (u_{j-1} - v_{j-1})|^2}{h^2} h + 4\alpha(R)^2 L^2 |||\boldsymbol{u}-\boldsymbol{v}|||_h^2 \\ &= (2+4L^2)\alpha(R)^2 |||\boldsymbol{u}-\boldsymbol{v}|||_h^2, \end{aligned}$$

which implies (21b) with $C_{2f}(R) = \sqrt{2+4L^2}\alpha(R) = c_0(R)$.

Finally, (21a) follows by setting $\boldsymbol{v} = \boldsymbol{0}$.

C. Modified Newton method

To solve our finite difference scheme (14), at each time step t_n, we must solve a nonlinear equation of the form

$$\mathcal{F}\boldsymbol{u} = H\boldsymbol{u} - K\boldsymbol{v} + i\Delta t\left[(1-\theta)\boldsymbol{f}(\boldsymbol{v}) + \theta\boldsymbol{f}(\boldsymbol{u}) + \boldsymbol{g}^{n+\theta}\right] = \boldsymbol{0}, \tag{92}$$

where $\boldsymbol{u} = \boldsymbol{u}^{n+1}$, $\boldsymbol{v} = \boldsymbol{u}^n$, $\Delta t = \Delta t_n$, $H = H_n$, and $K = K_n$.

If decomposing the equation (92) into the real and imaginary parts, then we can apply any iterative methods for solving the system of equations of real functions. The standard Newton method is a powerful method. Another method is proposed in [2, §5]. However, if the nonlinearity $f(z)$ is differentiable in the complex sense, we can use the complex Newton method (for the system of equations of complex functions). Consequently, MATLAB and Scilab are available to compute (92) using *complex variables*. However, $f(z) = \alpha z|z|^m$ and $f(z) = \alpha|z|^m$, $\alpha \in \mathbb{C}$, $m \geq 2$, are not differentiable in the complex sense so that the complex Newton method is not available. Instead, we offer a new iterative method that is a version of modified Newton methods to solve (92) using complex variables.

That is, we consider the following iteration: For an initial guess $\boldsymbol{u}_0 \in \mathbb{C}^N$, we generate $\{\boldsymbol{u}_k\}_{k\geq 1}$ by

$$\begin{aligned} \boldsymbol{u}_{k+1} &= \mathcal{N}\boldsymbol{u}_k \\ &\equiv \boldsymbol{u}_k - H^{-1}\mathcal{F}\boldsymbol{u}_k \\ &= -i\Delta t\theta H^{-1}\boldsymbol{f}(\boldsymbol{u}_k) + H^{-1}\left[K\boldsymbol{v} - i\Delta t(1-\theta)\boldsymbol{f}(\boldsymbol{v}) - i\Delta t\boldsymbol{g}^{n+\theta}\right]. \end{aligned} \tag{93}$$

This iterative method actually converges with a sufficiently small Δt, as stated in Proposition C.1. Set $B_R = \{z \in \mathbb{C} \mid |z| \leq R\}$ and take $\tilde{g} > 0$ satisfying $|||\boldsymbol{g}^n|||_h \leq \tilde{g}$ for $0 \leq t_n \leq T$.

Proposition C.1. *Assume that Condition (f) is satisfied. Let $\boldsymbol{v} \in \mathbb{C}^N$ and $R = |||\boldsymbol{v}|||_h$. Then, if*

$$\Delta t \leq \min\left\{\frac{R}{3\theta C_{1f}(2R)}, \frac{R}{3(1-\theta)C_{1f}(R)}, \frac{R}{3\tilde{g}}, \frac{1}{2\theta C_{2f}(2R)}\right\}, \tag{94}$$

then $\mathcal{N}$ is a contraction mapping from B_{2R} to B_{2R}. Consequently, there exists a unique fixed point $\boldsymbol{u} \in B_{2R}$.

The proof is a direct consequence of Condition (f).

Example C.2. We ignore the contribution of $\tilde{g}$ to set Δt appropriately because $\tilde{g}$ is not so large relative to R. Consider $f(z) = \alpha u|u|^m$, $\alpha \in \mathbb{C}$ and $m \geq 2$. Then, (94) is written equivalently as

$$\Delta t \leq \min\left\{\frac{1}{3\theta c_1 2^{m+1}}, \frac{1}{3(1-\theta)c_1}\right\}\frac{1}{R^m}, \tag{95}$$

where c_1 is the constant defined in Example 2.4. Therefore, in this case, to apply the iterative method (93), we must take

$$\Delta t_k = \tau \min\left\{1, \frac{1}{|||\boldsymbol{u}^n|||_h^m}\right\}, \quad 0 < \tau \leq \tau', \tag{96}$$

where

$$\tau' = \gamma \min\left\{\frac{1}{3\theta c_1 2^{m+1}}, \frac{1}{3(1-\theta)c_1}\right\} \tag{97}$$

and γ is a constant taken from $0 < \gamma < 1$. For the case $f(z) = \alpha|z|^m$, c_1 should be replaced by c_2 in Example 2.4.

Remark C.3. In view of (96), we must choose $q = 2p$ in (34) to solve (32). However, we have verified from numerical experimentation that a modified Newton method always converges by setting $q = p$.

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ADDRESS:
Graduate School of Mathematical Sciences, The University of Tokyo
3–8–1 Komaba Meguro-ku, Tokyo 153, JAPAN
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