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### **Research Article**

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# Optimal Convergence of the Newton Iterative Crank–Nicolson Finite Element Method for the Nonlinear Schrödinger Equation

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**Abstract:** An error estimate is presented for the Newton iterative Crank–Nicolson finite element method for the nonlinear Schrödinger equation, fully discretized by quadrature, without restriction on the grid ratio between temporal step size and spatial mesh size. It is shown that the Newton iterative solution converges double exponentially with respect to the number of iterations to the solution of the implicit Crank–Nicolson method uniformly for all time levels, with optimal convergence in both space and time.

Keywords: Nonlinear Schrödinger Equation, Crank–Nicolson, Newton Iteration, Quadrature, Convergence

MSC 2010: 65N12, 65N15, 35Q55

# **1** Introduction

We consider the initial-boundary value problem of the nonlinear Schrödinger (NLS) equation

$$\begin{cases} i\partial_t u + \Delta u + f(|u|^2)u = 0 & \text{ in } \Omega \times (0, T], \\ u = 0 & \text{ on } \partial\Omega \times (0, T], \\ u = u_0 & \text{ on } \Omega \times \{0\} \end{cases}$$
(1.1)

in a convex polygonal or polyhedral domain  $\Omega \subset \mathbb{R}^d$ ,  $d \in \{2, 3\}$ , with boundary  $\partial\Omega$ , where  $i = \sqrt{-1}$  is the imaginary unit and  $u: \Omega \times (0, T] \to \mathbb{C}$  is the complex-valued unknown solution, and  $f: \mathbb{R} \to \mathbb{R}$  is a real-valued function as the derivative of a potential function  $F: \mathbb{R} \to \mathbb{R}$ . The solution of the NLS equation (1.1) has conserved mass and energy, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega} |u|^2 \,\mathrm{d}x = 0 \quad \text{(mass conservation)}, \tag{1.2}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega} \frac{1}{2} [|\nabla u|^2 - F(|u|^2)] \,\mathrm{d}x = 0 \quad \text{(energy conservation)}. \tag{1.3}$$

In numerical computation, it is also desirable to preserve the mass and energy conservation properties (1.2)-(1.3), especially in simulating soliton waves or blow-up phenomena. The most popular numerical method which conserves both mass and energy is the modified Crank–Nicolson (CN) method, which was ini-

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tially introduced by Delfour, Fortin and Payre [9] in 1981 for the NLS equation with the specific nonlinearity

$$f(|u|^2) = \pm |u|^{p-1}$$
 and  $F(|u|^2) = \pm \frac{1}{p+1} |u|^{p+1}$  for  $p > 1$ .

The modified CN method was generalized by Sanz-Serna [22] in 1984 to the NLS equation with general nonlinearity. Based on the formulation of Sanz-Serna [22], the modified CN method with finite element method (FEM) in space approximates (1.1) as follows.

For a given  $u_h^{n-1}$  in a finite element subspace  $S_h \in H^1_0(\Omega)$ , find  $u_h^n \in S_h$  such that

$$\left(i\frac{u_h^n - u_h^{n-1}}{\tau}, v_h\right) - \left(\nabla \frac{u_h^n + u_h^{n-1}}{2}, \nabla v_h\right) + \left(\tilde{f}(|u_h^n|^2, |u_h^{n-1}|^2)\frac{u_h^n + u_h^{n-1}}{2}, v_h\right) = 0$$
(1.4)

holds for all test functions  $v_h \in S_h$ , where the nonlinear term  $\tilde{f}(\zeta, \eta)$  is defined by

$$\tilde{f}(\zeta,\eta) := \frac{F(\zeta) - F(\eta)}{\zeta - \eta} = \int_{0}^{1} f((1 - \theta)\zeta + \theta\eta) \,\mathrm{d}\theta \quad \text{for all } \zeta,\eta \in \mathbb{R}^{+}.$$
(1.5)

The solution of the implicit CN-FEM (1.4) conserves both mass and energy, i.e.,

$$\int_{\Omega} |u_h^n|^2 \, dx = \int_{\Omega} |u_h^{n-1}|^2 \, dx,$$
$$\int_{\Omega} \frac{1}{2} [|\nabla u_h^n|^2 - F(|u_h^n|^2)] \, dx = \int_{\Omega} \frac{1}{2} [|\nabla u_h^{n-1}|^2 - F(|u_h^{n-1}|^2)] \, dx.$$

The method has become popular and is widely used in the solution of the NLS equation combined with different spatial discretization methods; see [2, 5–7].

Under a grid-ratio condition  $\tau = o(h)$ , optimal-order convergence of the implicit CN-FEM was proved in [22], i.e.,

$$\|u_h^n - u(t_n)\|_{L^2} \le C(\tau^2 + h^{r+1}), \tag{1.6}$$

where *r* denotes the degree of finite elements in space. For the specific cubic NLS equation, Akrivis, Dougalis and Karakashian [3] proved optimal-order convergence of the implicit CN-FEM and the Newton iteration scheme under a weaker grid-ratio condition  $\tau = o(h^{\frac{d}{4}})$ . If the solution of the NLS equation is sufficiently smooth, then for any given number  $\ell$ , it was shown that the Newton iterative solution  $u_h^{n,\ell}$  obtained by  $\ell$  iterations at every time level has the following error bound:

$$\|u_h^{n,\ell} - u_h^n\|_{L^2} \le C_\ell(\tau^2 + h^{r+1}), \tag{1.7}$$

where  $u_h^n$  denotes the solution of the implicit CN-FEM. This proves optimal convergence of the Newton iterative solution  $u_h^{n,\ell}$  with respect to the time step size and spatial mesh size. However, the constant in estimate (1.7) depends implicitly on the number of Newton iterations, and we do not really know how the number of Newton iterations may affect the conservation of both mass and energy as well as the actual numerical accuracy of finite element solutions. It is mathematically and physically important whether the Newton iterative solutions meet the conservation of both mass and energy up to a desired double exponential accuracy, and indeed converge double exponentially with respect to the number of iterations uniformly for all time levels, without being affected by the time stepping methods as well as numerical integration. This question is still open, not only for the NLS equation but also for other important physical nonlinear evolutionary PDEs. This will be our main motivation and focus of the current work.

Karakashian and Makridakis [18, 19] proved high-order convergence of continuous and discontinuous space-time Galerkin FEMs for the cubic NLS equation under a weaker grid-ratio condition  $\tau^{k-1}|\ln h| \rightarrow 0$  in two dimensions, where  $k \ge 2$  is the degree of finite elements in time. For the defocusing cubic NLS equation (or the focusing cubic NLS equation with sufficiently small initial data), error estimates were established without grid-ratio condition in [14, 25] by using the energy conservation of the numerical scheme. For general nonlinearity (possibly focusing), Wang [24] proved the optimal convergence (1.6) for a linearized CN-FEM without grid-ratio conditions. Henning and Peterseim [17] established an error estimate for the implicit

CN-FEM without grid-ratio conditions. Both [17, 24] use an error splitting approach, in which the authors established a  $\tau$ -independent regularity estimate for the temporally semidiscrete solution and then compared the fully discrete solution with the temporally semidiscrete solution by using the established regularity. By this approach, they avoided grid-ratio conditions in using the inverse inequality.

To our knowledge, all the existing mass- and energy-conserving methods have at most second-order accuracy in time; see the discussion of this topic in [13]. It was shown in [12] that a nonlinearly implicit SAV-Gauss collocation method for the NLS equation, by using the recently developed SAV techniques in [23], can achieve arbitrarily high-order accuracy while preserving the conservation of mass and the SAV energy. The convergence of Newton iterative solutions in the SAV-Gauss collocation method with respect to the number of iterations uniformly for all time levels is still not available.

In this paper, we present more delicate analysis for the Newton iterative CN-FEM, fully discretized by a simple quadrature rule, with  $\ell$  Newton iterations at every time level. For linear FEMs we improve result (1.7) to the following double exponential convergence:

$$\|u_h^{n,\ell} - u_h^n\|_{H^1} \le [C(\tau^2 + h^2)]^{2^{\ell-1} - 1}$$
(1.8)

in  $H^1$  norm for any  $\ell \ge 2$ , with a constant *C* independent of  $\tau$ , *h*,  $\ell$  and *n* (but it may depend on *T*). As far as we know, this is the first rigorous justification of the double exponential convergence of the Newton iteration for the time-dependent NLS equation uniformly for all time levels. In fact, there are no similar results in the literature for any other nonlinearly implicit schemes for important physical nonlinear evolution PDEs. As we see, estimate (1.8) further implies that the Newton iterative solution almost preserves mass and energy conservation, with double exponential accuracy in  $\ell$ ; see Corollary 2.1.

For semilinear elliptic equations, the convergence and adaptivity procedure of the Newton iterative methods have already been discussed in the literature; for example, see [4, 10]. However, the convergence analysis of Newton iterative methods for the time-dependent NLS turns out to be much more involved due to the following features of the NLS equation.

- (1) The nonlinear function f may not be globally Lipschitz continuous (only locally Lipschitz continuous). As a result, the second-order derivative is f is bounded only if the argument inside f (i.e., the numerical solution) is bounded in  $L^{\infty}$  uniformly with respect to h and  $\tau$ . This requires us to work in a norm which is stronger than  $L^{\infty}$  in the analysis of the Newton iterative methods.
- (2) The NLS equation is a wave equation, and it does not have  $L^{\infty}$  estimates or smoothing property as parabolic equations. Therefore, we have to work in  $H^s$  norm with  $s > \frac{d}{2}$  in the *d*-dimensional space (as  $H^s \hookrightarrow L^{\infty}$  only for  $s > \frac{d}{2}$ ) in the analysis of Newton iterative methods.
- (3) In the time level  $t = t_m$ , the Newton iteration scheme for solving  $u_h^m$  contains  $i\frac{1}{\tau}u_h^{m-1}$  on the right-hand side of the equation, which depends on  $\frac{1}{\tau}$ . This is different from a single elliptic equation, which does not contain such a factor in the source term. Moreover, there are  $\frac{1}{\tau}$  different time levels, and therefore, the errors may accumulate in time in a naive convergence analysis by summing up the errors at all time levels. Since it is desirable to obtain the convergence analysis independent of  $\frac{1}{\tau}$ , we have to use an argument which fully makes use of the evolution structure of a wave equation, instead of analyzing every time level as an elliptic equation.

Another interesting contribution of this work is to establish the optimal error estimate (1.6) for the implicit CN-FEM when the piecewise linear FEM is used and the cubic nonlinear term is discretized by a simple quadrature rule. The optimal error estimate is achieved without any grid-ratio conditions and under the standard  $H^2$  spatial regularity of the solution. The main difference between our work and [17, 24] is that we established all the error estimates under the most realistic and practically acceptable situation, that is, for the incomplete Newton iteration in the nonlinear CN scheme, while Wang [24] considered a linearly implicit scheme (without iterations) and Henning and Peterseim [17] considered the fully implicit scheme (with exact solutions generated by infinite Newton iterations). As an intermediate step, we also present an optimal-order error estimate for a fully implicit CN-FEM with quadrature approximation in the nonlinear terms, while the results in [17] are for the fully implicit CN-FEM without quadrature.

The rest of this paper is organized as follows. In Section 2, we present our main results on the convergence of numerical solutions given by the implicit CN-FEM with quadrature and Newton iterative method. The proofs for the implicit CN-FEM and the Newton iterative method are presented in Sections 3 and 4, respectively. Throughout, we denote by *C* a generic positive constant which may be different at different occurrences, but is independent of h,  $\tau$ , n and k (to be introduced in the proof).

# 2 Main Results

### 2.1 Notation

For  $s \ge 0$  and  $1 \le p \le \infty$ , we denote by  $W^{s,p}(\Omega)$  the conventional complex-valued Sobolev space of functions on  $\Omega$ , with abbreviations  $H^s(\Omega) = W^{s,2}(\Omega)$  and  $L^p(\Omega) = W^{0,p}(\Omega)$ ; see [1]. The space  $H^1_0(\Omega)$  consists of functions in  $H^1(\Omega)$  vanishing on the boundary  $\partial\Omega$ . The space of continuous functions on  $\overline{\Omega}$  is denoted by  $C(\overline{\Omega})$ . The inner product on  $L^2(\Omega)$  is denoted by

$$(w, v) := \int_{\Omega} wv \, dx \quad \text{for all } w, v \in L^2(\Omega).$$

For simplicity of notation, we denote by  $\|\cdot\|_{L^p}$  and  $\|\cdot\|_{H^s}$  the norms of  $L^p(\Omega)$  and  $H^s(\Omega)$ , omitting the dependence on  $\Omega$  in the subscripts.

Let  $S_h 
ightharpoonup H_0^1(\Omega)$  and  $\hat{S}_h 
ightharpoonup H_0^1(\Omega)$  be the Lagrange finite element spaces of piecewise linear and quadratic polynomials, respectively, subject to a quasi-uniform triangulation of the domain  $\Omega$ , and let  $I_h$  and  $\hat{I}_h$  be the Lagrange interpolations from  $C(\overline{\Omega})$  onto  $S_h$  and  $\hat{S}_h$ , respectively.

We shall denote by  $\mathcal{K}$  the set of all triangles (in 2D) or tetrahedra (in 3D) in the triangulation, and by  $(\cdot, \cdot)_h$  a quadrature approximation of the inner product  $(\cdot, \cdot)$ , defined by

$$(w, v)_h := \int_{\Omega} \hat{I}_h(vw) \, \mathrm{d}x \quad \text{for all } w, v \in C(\overline{\Omega}).$$
(2.1)

We shall frequently use a discrete Laplacian  $\Delta_h : S_h \to S_h$  defined by

$$(\Delta_h w_h, v_h) = -(\nabla w_h, \nabla v_h)$$
 for all  $w_h, v_h \in S_h$ ,

and an induced fractional Sobolev norm  $\|\cdot\|_{H_h^s}$  for  $s \in [0, 2]$  on  $S_h$ ,

$$\|v_h\|_{H^s_h} := \|(-\Delta_h)^{\frac{s}{2}} v_h\|_{L^2}$$
 for all  $v_h \in S_h$ .

### 2.2 The Numerical Method

Let  $u_h^{0,\ell} = I_h u^0$ . For given  $u_h^{n-1,\ell} \in S_h$  and  $u_h^{n,m-1} \in S_h$  with  $1 \le m \le \ell$  (with  $u_h^{n,0} =: u_h^{n-1,\ell}$ ), we consider the following Newton iterative CN-FEM: find  $u_h^{n,m} \in S_h$  such that

$$\left( i \frac{u_h^{n,m} - u_h^{n-1,\ell}}{\tau}, v_h \right) - \left( \nabla \frac{u_h^{n,m} + u_h^{n-1,\ell}}{2}, \nabla v_h \right) + \left( \tilde{f}(|u_h^{n,m-1}|^2, |u_h^{n-1,\ell}|^2) \frac{u_h^{n,m-1} + u_h^{n-1,\ell}}{2}, v_h \right)_h + \left( \tilde{f}(|u_h^{n,m-1}|^2, |u_h^{n-1,\ell}|^2) \frac{u_h^{n,m} - u_h^{n,m-1}}{2}, v_h \right)_h + \left( \partial_1 \tilde{f}(|u_h^{n,m-1}|^2, |u_h^{n-1,\ell}|^2) \frac{u_h^{n,m-1} + u_h^{n-1,\ell}}{2} 2 \operatorname{Re}(\bar{u}_h^{n,m-1}(u_h^{n,m} - u_h^{n,m-1})), v_h \right)_h = 0 \quad \text{for all } v_h \in S_h.$$

$$(2.2)$$

In the method above,  $\partial_1 \tilde{f}(|u_h^{n,m-1}|^2, |u_h^{n-1,\ell}|^2)$  is an abbreviation of the expression

$$\partial_1 \tilde{f}(|u_h^{n,m-1}|^2,|u_h^{n-1,\ell}|^2) = \int_0^1 f'((1-\theta)|u_h^{n,m-1}|^2 + \theta|u_h^{n-1,\ell}|^2)(1-\theta)\,\mathrm{d}\theta,$$

which can be obtained by differentiating expression (1.5) with respect to  $|u_h^n|^2$ . The use of quadrature rule (2.1) in (2.2) is to simplify the implementation of the three nonlinear terms involving  $\tilde{f}$  and  $\partial_1 \tilde{f}$  without sacrificing the accuracy or the mass/energy conservation, as demonstrated by the subsequent analysis in this paper.

The linearly implicit method (2.2) can be viewed as the Newton iterative method for the following implicit CN-FEM with quadrature:

$$\left(i\frac{u_h^n - u_h^{n-1}}{\tau}, v_h\right) - \left(\nabla \frac{u_h^n + u_h^{n-1}}{2}, \nabla v_h\right) + \left(\tilde{f}(|u_h^n|^2, |u_h^{n-1}|^2)\frac{u_h^n + u_h^{n-1}}{2}, v_h\right)_h = 0 \quad \text{for all } v_h \in S_h,$$
(2.3)

which is the implicit CN-FEM (1.4) with its cubic nonlinear term approximated by quadrature rule (2.1).

### 2.3 Main Results

**Theorem 2.1.** Under the following regularity of the solution to the NLS equation (1.1),

$$u \in W^{2,1}(0, T; H^1_0(\Omega) \cap H^2(\Omega)),$$
 (2.4)

there exist positive constants  $\tau_0$  and  $h_0$  such that the following results hold for  $\tau \le \tau_0$  and  $h \le h_0$ .

(i) Implicit CN-FEM with quadrature: (2.3) has a unique solution satisfying

$$\|u_h^n - u(t_n)\|_{L^{\infty}} \le 1, \tag{2.5}$$

with conservation of mass and energy

$$\int_{\Omega} |u_h^n|^2 \, \mathrm{d}x = \int_{\Omega} |u_h^{n-1}|^2 \, \mathrm{d}x,$$
$$\int_{\Omega} \frac{1}{2} [|\nabla u_h^n|^2 - \hat{I}_h F(|u_h^n|^2)] \, \mathrm{d}x = \int_{\Omega} \frac{1}{2} [|\nabla u_h^{n-1}|^2 - \hat{I}_h F(|u_h^{n-1}|^2)] \, \mathrm{d}x,$$

and the error bound

$$\|u_h^n - u(t_n)\|_{L^2} \le C(\tau^2 + h^2).$$
(2.6)

Moreover, the solution  $u_h^n$  satisfies

$$\|u_h^n\|_{H^2_h} \le C. \tag{2.7}$$

(ii) Newton iterative CN-FEM with quadrature: (2.2) has a unique solution, with the following error bound for  $\ell \ge 1$  (double exponential convergence in  $\ell$ ) and  $s \in (\frac{d}{2}, 2)$ :

$$\|u_{h}^{n,\ell} - u_{h}^{n}\|_{L^{\infty}} + \|u_{h}^{n,\ell} - u_{h}^{n}\|_{H^{1}} + \|u_{h}^{n,\ell} - u_{h}^{n}\|_{H^{s}_{h}} \le C(C\tau)^{2^{\ell}-2}(\tau^{2-s} + h^{2-s})^{2^{\ell}},$$
(2.8)

where *C* is a constant independent of  $\tau$ , h,  $\ell$  and n (but may depend on *T* and s).

Remarks on Theorem 2.1. (1) Using the identity

$$(C\tau)^{2^{\ell}-2} = (C^2\tau^2)^{2^{\ell-1}-1} = C^2(C^4\tau^2)^{2^{\ell-2}-1}(\tau^2)^{2^{\ell-2}}$$

and the simple estimate

$$(\tau^{2-s}+h^{2-s})^{2^{\ell}} \le (C\tau^{8-4s}+Ch^{8-4s})^{2^{\ell-2}},$$

we readily get from (2.8) that

$$\begin{aligned} \|u_{h}^{n,\ell} - u_{h}^{n}\|_{L^{\infty}} + \|u_{h}^{n,\ell} - u_{h}^{n}\|_{H^{1}} + \|u_{h}^{n,\ell} - u_{h}^{n}\|_{H^{s}_{h}} &\leq C^{2}(C^{4}\tau^{2})^{2^{\ell-2}-1}(C\tau^{10-4s} + Ch^{10-4s})^{2^{\ell-2}} \\ &\leq [C(\tau^{2} + h^{2})]^{2^{\ell-1}-1} \end{aligned}$$
(2.9)

for  $s \le 2$ . Hence, the error of Newton iteration is double exponential in  $\ell$  with base  $\tau^2 + h^2$ , uniformly for all time levels (with a constant *C* independent of *n*).

Estimates (2.6) and (2.9) imply, through applying the triangle inequality,

$$\|u_h^{n,\ell} - u(t_n)\|_{L^2} \le C(\tau^2 + h^2) + CM_{\tau,h,\ell}(\tau^2 + h^2),$$

with  $M_{\tau,h,\ell} = [C(\tau^2 + h^2)]^{2^{\ell-1}-2}$ . This indicates that the optimal-order accuracy with respect to  $\tau$  and h will not be affected by the incomplete Newton iteration as long as we run at least two iterations ( $\ell \ge 2$ ) at every time level.

(2) Theorem 2.1 covers the cases  $\ell \ge 2$ . For the special case  $\ell = 1$ , an  $L^2$ -norm error estimate

$$\|u_h^{n,1} - u(t_n)\|_{L^2} \le C(\tau^2 + h^2)$$

can also be obtained for method (2.2), similarly to the error analysis for the linearly implicit FEM in [24]. Detailed discussions of  $\ell = 1$  are omitted here.

(3) The regularity condition in Theorem 2.1 is slightly weaker than the regularity conditions in [17, 24]. Similar to [17, 24], no grid-ratio condition is required for the error analysis. The error analysis presented here is for the fully discretized method with quadrature and Newton iteration, which is closer to the result obtained in practical computation (only the round-off errors are neglected).

Theorem 2.1 implies that the Newton iterative method approximates the solution of the implicit scheme with double exponential convergence. Hence, the mass and energy conservation can be conserved with an error bound of  $O([C(\tau^2 + h^2)]^{2^{\ell-1}-1})$  as in (2.9). This is stated in the following corollary.

**Corollary 2.1.** Under the assumptions of Theorem 2.1, the numerical solution given by (2.2) has an approximate conservation of mass and energy with double exponential accuracy, i.e.,

$$\int_{\Omega} |u_h^{n,\ell}|^2 \, dx = \int_{\Omega} |u_h^0|^2 \, dx + \mathcal{E}_1^n,$$
$$\int_{\Omega} \frac{1}{2} [|\nabla u_h^{n,\ell}|^2 - \hat{I}_h F(|u_h^{n,\ell}|^2)] \, dx = \int_{\Omega} \frac{1}{2} [|\nabla u_h^0|^2 - \hat{I}_h F(|u_h^0|^2)] \, dx + \mathcal{E}_2^n$$

with errors  $\mathcal{E}_1^n$  and  $\mathcal{E}_2^n$  satisfying  $|\mathcal{E}_1^n| + |\mathcal{E}_2^n| \le [C(\tau^2 + h^2)]^{2^{\ell-1}-1}$ , where the constant *C* is independent of  $\tau$ , *h*,  $\ell$  and *n* (but may depend on *s* and *T*).

# **3** Proof of Theorem 2.1 (i): Implicit Scheme with Quadrature

Let  $R_h$  and  $P_h$  be the Ritz and  $L^2$  projections onto the finite element space  $S_h$ , respectively,

$$(\nabla(w - R_h w), \nabla v_h) = 0 \quad \text{for all } w \in H^1_0(\Omega), \ v_h \in S_h,$$
$$(w - P_h w, v_h) = 0 \quad \text{for all } w \in L^2(\Omega), \ v_h \in S_h.$$

The Lagrange interpolation, the Ritz and  $L^2$  projections have the standard approximation properties (cf. [8]),

$$\begin{split} \|w - I_h w\|_{L^2} + h\|w - I_h w\|_{H^1} &\leq C \|w\|_{H^2} h^2, & \text{for all } w \in H^2(\Omega) \cap H^1_0(\Omega), & (3.1) \\ \|w - R_h w\|_{L^2} + h\|w - R_h w\|_{H^1} &\leq C \|w\|_{H^k} h^k, & 1 \leq k \leq 2, & \text{for all } w \in H^k(\Omega) \cap H^1_0(\Omega), & (3.2) \\ \|w - P_h w\|_{L^2} + h\|w - P_h w\|_{H^1} &\leq C \|w\|_{H^k} h^k, & 1 \leq k \leq 2, & \text{for all } w \in H^k(\Omega) \cap H^1_0(\Omega), & (3.2) \\ \|P_h w\|_{L^2} &\leq \|w\|_{L^2} & \text{for all } w \in L^2(\Omega). \end{split}$$

### 3.1 Consistency

We derive the consistency error of the CN-FEM (2.3) with quadrature in this section, for which we first present some important estimates.

**Lemma 3.1.** The approximate inner product defined in (2.1) has the following properties:

$$\begin{split} |(w, v_h)_h| &\leq \sum_{K \in \mathcal{K}} Ch^{\frac{d}{2}} \|w\|_{L^{\infty}(K)} \|v_h\|_{L^2(K)} \quad \text{for all } v_h \in S_h \text{ and all } w \in C(\overline{\Omega}), \\ |(gw_h, v_h)_h| &\leq C \|g\|_{L^{\infty}} \|w_h\|_{L^2} \|v_h\|_{L^2} \qquad \text{for all } w_h, v_h \in S_h \text{ and all } g \in C(\overline{\Omega}), \\ |(w, v_h)_h - (w, v_h)| &\leq Ch^2 \|w\|_{H^2} \|v_h\|_{L^2} \qquad \text{for all } w \in H^2(\Omega) \text{ and all } v_h \in S_h. \end{split}$$

*Proof.* Note that  $\hat{I}_h$  and  $I_h$  are the Lagrange interpolation operators using quadratic and linear finite elements, respectively. By using the basic stability property  $\|\hat{I}_h(wv_h)\|_{L^{\infty}(K)} \leq C \|wv_h\|_{L^{\infty}(K)}$  for every element  $K \in \mathcal{K}$ , we have

$$|(w, v_h)_h| = \left| \sum_{K \in \mathcal{K}} \int_K \hat{I}_h(wv_h) \, \mathrm{d}x \right| \le \sum_{K \in \mathcal{K}} Ch^d \|w\|_{L^{\infty}(K)} \|v_h\|_{L^{\infty}(K)} \le \sum_{K \in \mathcal{K}} Ch^{\frac{d}{2}} \|w\|_{L^{\infty}(K)} \|v_h\|_{L^{2}(K)},$$

where we have used the inverse inequality  $||v_h||_{L^2(K)} \leq Ch^{-\frac{d}{2}} ||v_h||_{L^{\infty}(K)}$ . Replacing *w* by  $gw_h$  in the inequality above, we obtain

$$\begin{aligned} |(gw_h, v_h)_h| &\leq \sum_{K \in \mathcal{K}} Ch^d ||g||_{L^{\infty}} ||w_h||_{L^{\infty}(K)} ||v_h||_{L^{\infty}(K)} \\ &\leq C ||g||_{L^{\infty}} \sum_{K \in \mathcal{K}} ||w_h||_{L^2(K)} ||v_h||_{L^2(K)} \quad \text{(inverse inequality)} \\ &\leq C ||g||_{L^{\infty}} ||w_h||_{L^2} ||v_h||_{L^2}. \end{aligned}$$

This proves the first two results of Lemma 3.1. The third result can be proved as follows:

$$\begin{split} |(w, v_h)_h - (w, v_h)| &= \left| \sum_{K \in \mathcal{K}} \int_K (\hat{I}_h(wv_h) - wv_h) \, dx \right| \\ &= \left| \sum_{K \in \mathcal{K}} \int_K \left( \hat{I}_h[(w - I_h w)v_h] - (w - I_h w)v_h \right) \, dx \right| \\ &\leq Ch^2 \sum_{K \in \mathcal{K}} \sum_{i,j=1}^d \|\partial_j \partial_i [(w - I_h w)v_h]\|_{L^2(K)} \\ &\leq Ch^2 \sum_{K \in \mathcal{K}} \sum_{i,j=1}^d \|\partial_j \partial_i (w - I_h w)\|_{L^2(K)} \|v_h\|_{L^2(K)} \\ &+ Ch^2 \sum_{K \in \mathcal{K}} \sum_{i,j=1}^d \|\partial_i (w - I_h w)\|_{L^2(K)} \|\partial_j v_h\|_{L^2(K)} \\ &\leq Ch^2 \sum_{K \in \mathcal{K}} \|w\|_{H^2(K)} \|v_h\|_{L^2(K)} + Ch^3 \sum_{K \in \mathcal{K}} \|w\|_{H^2(K)} \|v_h\|_{H^1(K)} \\ &\leq Ch^2 \|w\|_{H^2} \|v_h\|_{L^2}, \end{split}$$

where we have used the identity  $\partial_j \partial_i (I_h w) = 0$  in the second to last inequality, and the inverse inequality  $\|v_h\|_{H^1(K)} \leq Ch^{-1} \|v_h\|_{L^2(K)}$  in deriving the last inequality.

The following estimates of the interpolation errors will be frequently used in this paper.

**Lemma 3.2.** For every element  $K \in \mathcal{K}$ , there holds

$$\|v - I_h v\|_{L^{\infty}(K)} \le Ch^{2-\frac{d}{2}} \|v\|_{H^2(K)} \quad \text{for all } v \in H^2(K),$$
(3.3)

$$\|v - R_h v\|_{L^{\infty}} \le Ch^{2 - \frac{d}{2}} \|v\|_{H^2} \quad \text{for all } v \in H^2(\Omega).$$
(3.4)

*Proof.* The inequality in (3.3) is proved in [8, Corollary 4.4.7], which implies that

$$\|v - I_h v\|_{L^{\infty}} \le Ch^{2-\frac{\alpha}{2}} \|v\|_{H^2} \quad \text{for all } v \in H^2(\Omega).$$

Using the inverse inequality, we also have

$$\|R_h v - I_h v\|_{L^{\infty}} \le Ch^{-\frac{a}{2}} \|R_h v - I_h v\|_{L^2} \le Ch^{2-\frac{a}{2}} \|v\|_{H^2} \quad \text{for all } v \in H^2(\Omega).$$

Then, by using the triangle inequality, the two estimates above imply (3.4).

We are now ready to derive the consistency error of the CN-FEM (2.3) with quadrature. To do so, we let  $u(t_n)$  be the exact solution of the NLS equation (1.1) at  $t = t_n$ , and  $u_{h,*}^n = R_h u(t_n)$ . We first consider a quantity  $I_h^n$  that is defined by the left-hand side of (2.3) with  $u_h^n$  and  $u_h^{n-1}$  replaced by  $u_{h,*}^n$  and  $u_{h,*}^{n-1}$ , respectively. Then we derive an equation by taking the value of (1.1) at  $t = t_{n-\frac{1}{2}}$  and replace the time derivative  $\partial_t u(t_{n-\frac{1}{2}})$  by the first-order central difference. Now, taking the  $L^2$ -inner product of this equation with  $v_h \in S_h$ , adding the resulting equation to the quantity  $I_h^n$  and making some natural manipulations, we can readily derive the equation for  $u_{h,*}^n$  by using the definitions of projections  $R_h$  and  $P_h$ ,

$$\left(i\frac{u_{h,*}^{n}-u_{h,*}^{n-1}}{\tau},v_{h}\right)-\left(\nabla\frac{u_{h,*}^{n}+u_{h,*}^{n-1}}{2},\nabla v_{h}\right) + \left(\tilde{f}(|u_{h,*}^{n}|^{2},|u_{h,*}^{n-1}|^{2})\frac{u_{h,*}^{n}+u_{h,*}^{n-1}}{2},v_{h}\right)_{h} = (d_{*}^{n},v_{h}) \text{ for all } v_{h} \in S_{h},$$
(3.5)

where  $d_*^* \in S_h$  is the consistency error of the CN-FEM with quadrature, defined via a duality pairing

$$(d_*^n, v_h) = \left( i(R_h - P_h) \frac{u(t_n) - u(t_{n-1})}{\tau}, v_h \right) + \left( i \frac{u(t_n) - u(t_{n-1})}{\tau} - i \partial_t u(t_{n-\frac{1}{2}}), v_h \right) + \left( \Delta \frac{u(t_n) + u(t_{n-1})}{2} - \Delta u(t_{n-\frac{1}{2}}), v_h \right) + \left( \tilde{f}(|u_{h,*}^n|^2, |u_{h,*}^{n-1}|^2) \frac{u_{h,*}^n + u_{h,*}^{n-1}}{2} - \tilde{f}(|u(t_n)|^2, |u(t_{n-1})|^2) \frac{u(t_n) + u(t_{n-1})}{2}, v_h \right)_h + \left( \tilde{f}(|u(t_n)|^2, |u(t_{n-1})|^2) \frac{u(t_n) + u(t_{n-1})}{2} - \tilde{f}(|u(t_{n-\frac{1}{2}})|^2, |u(t_{n-\frac{1}{2}})|^2) u(t_{n-\frac{1}{2}}), v_h \right)_h + \left( \tilde{f}(|u(t_{n-\frac{1}{2}})|^2, |u(t_{n-\frac{1}{2}})|^2) u(t_{n-\frac{1}{2}}), v_h \right)_h - \left( \tilde{f}(|u(t_{n-\frac{1}{2}})|^2, |u(t_{n-\frac{1}{2}})|^2) u(t_{n-\frac{1}{2}}), v_h \right).$$
(3.6)

**Lemma 3.3.** If the solution of the NLS equation (1.1) has regularity (2.4), then the consistency error  $d_*^n$  defined in (3.6) satisfies the following estimate:

$$\tau \sum_{n=1}^{N} \|d_*^n\|_{L^2} \leq C(\tau^2 + h^2).$$

*Proof.* We write  $I_n = [t_{n-1}, t_n]$ . Using regularity (2.4), we know from equation (1.1) that

$$\mathrm{i}\partial_t u = -\Delta u - f(|u|^2)u \in W^{2,1}(0,T;L^2(\Omega)) \implies \partial_{ttt} u \in L^1(0,T;L^2(\Omega)).$$

Then the first three terms in (3.6) can be estimated by using Taylor's formula of integral form, which implies that (details are omitted)

$$\begin{split} \left| \left( \mathbf{i}(R_h - P_h) \frac{u(t_n) - u(t_{n-1})}{\tau}, v_h \right) \right| &\leq Ch^2 \| u \|_{W^{2,1}(0,T;H^2)} \| v_h \|_{L^2} \\ \left| \left( \mathbf{i} \frac{u(t_n) - u(t_{n-1})}{\tau} - \mathbf{i} \partial_t u(t_{n-\frac{1}{2}}), v_h \right) \right| &\leq C\tau \| \partial_{ttt} u \|_{L^1(I_n;L^2)} \| v_h \|_{L^2}, \\ \left| \left( \Delta \left( \frac{u(t_n) + u(t_{n-1})}{2} - u(t_{n-\frac{1}{2}}) \right), v_h \right) \right| &\leq C\tau \| \partial_{tt} u \|_{L^1(I_n;H^2)} \| v_h \|_{L^2}. \end{split}$$

To estimate the fourth and fifth terms in (3.6) (with quadrature), we first use the second result of Lemma 3.2 to get

 $\|u_{h,*}^n - u(t_n)\|_{L^{\infty}} \le Ch^{2-\frac{d}{2}}, \text{ and therefore } \|u_{h,*}^n\|_{L^{\infty}} \le C.$ 

Then, by using Lemmas 3.1 and 3.2 and the local Lipschitz continuity of  $\tilde{f}$ , we have

$$\begin{split} \left\| \left( \tilde{f}(|u_{h,*}^{n}|^{2},|u_{h,*}^{n-1}|^{2}) \frac{u_{h,*}^{n}+u_{h,*}^{n-1}}{2} - \tilde{f}(|u(t_{n})|^{2},|u(t_{n-1})|^{2}) \frac{u(t_{n})+u(t_{n-1})}{2},v_{h} \right)_{h} \right\| \\ & \leq \sum_{K \in \mathcal{K}} Ch^{\frac{d}{2}} \left\| \tilde{f}(|u_{h,*}^{n}|^{2},|u_{h,*}^{n-1}|^{2}) \frac{u_{h,*}^{n}+u_{h,*}^{n-1}}{2} - \tilde{f}(|u(t_{n})|^{2},|u(t_{n-1})|^{2}) \frac{u(t_{n})+u(t_{n-1})}{2} \right\|_{L^{\infty}(K)} \|v_{h}\|_{L^{2}(K)} \end{split}$$

$$\leq \sum_{K \in \mathcal{K}} Ch^{\frac{d}{2}} (\|u_{h,*}^{n} - u(t_{n})\|_{L^{\infty}(K)} + \|u_{h,*}^{n-1} - u(t_{n-1})\|_{L^{\infty}(K)})\|v_{h}\|_{L^{2}(K)}$$

$$\leq \sum_{K \in \mathcal{K}} Ch^{\frac{d}{2}} (\|u_{h,*}^{n} - I_{h}u(t_{n})\|_{L^{\infty}(K)} + \|u_{h,*}^{n-1} - I_{h}u(t_{n-1})\|_{L^{\infty}(K)})\|v_{h}\|_{L^{2}(K)}$$

$$+ \sum_{K \in \mathcal{K}} Ch^{\frac{d}{2}} (\|I_{h}u(t_{n}) - u(t_{n})\|_{L^{\infty}(K)} + \|I_{h}u(t_{n-1}) - u(t_{n-1})\|_{L^{\infty}(K)})\|v_{h}\|_{L^{2}(K)}$$

$$\leq \sum_{K \in \mathcal{K}} C(\|u_{h,*}^{n} - I_{h}u(t_{n})\|_{L^{2}(K)} + \|u_{h,*}^{n-1} - I_{h}u(t_{n-1})\|_{L^{2}(K)})\|v_{h}\|_{L^{2}(K)}$$

$$\leq C(\|u_{h,*}^{n} - I_{h}u(t_{n})\|_{L^{2}} + \|u_{h,*}^{n-1} - I_{h}u(t_{n-1})\|_{L^{2}})\|v_{h}\|_{L^{2}} + Ch^{2}\|u\|_{L^{\infty}(0,T;H^{2})}\|v_{h}\|_{L^{2}}$$

$$\leq Ch^{2}\|u\|_{L^{\infty}(0,T;H^{2})}\|v_{h}\|_{L^{2}}.$$

Similarly, we can derive

$$\left| \left( \tilde{f}(|u(t_n)|^2, |u(t_{n-1})|^2) \frac{u(t_n) + u(t_{n-1})}{2} - \tilde{f}(|u(t_{n-\frac{1}{2}})|^2, |u(t_{n-\frac{1}{2}})|^2) u(t_{n-\frac{1}{2}}), v_h \right)_h \right| \le C\tau \|\partial_{tt} u\|_{L^1(I_n; H^2)} \|v_h\|_{L^2},$$

where inequality holds because there are  $O(h^{-d})$  elements in the triangulation  $\mathcal{K}$ . By using the third result of Lemma 3.1, we have

$$\begin{split} \big| \big( \tilde{f} \big( |u(t_{n-\frac{1}{2}})|^2, |u(t_{n-\frac{1}{2}})|^2 \big) u(t_{n-\frac{1}{2}}), v_h \big)_h - \big( \tilde{f} \big( |u(t_{n-\frac{1}{2}})|^2, |u(t_{n-\frac{1}{2}})|^2 \big) u(t_{n-\frac{1}{2}}), v_h \big) \big| \\ &\leq Ch^2 \big\| f \big( |u(t_{n-\frac{1}{2}})|^2, |u(t_{n-\frac{1}{2}})|^2 \big) u(t_{n-\frac{1}{2}}) \big\|_{H^2} \|v_h\|_{L^2} \leq Ch^2 \|v_h\|_{L^2}. \end{split}$$

Substituting all the estimates above into the expression of  $d_*^n$  in (3.6), we obtain

$$|(d_*^n, v_h)| \le (C\tau \|u\|_{W^{2,1}(I_n; H^2)} + C\tau \|\partial_{ttt} u\|_{L^1(I_n; L^2)} + Ch^2) \|v_h\|_{L^2}.$$

By the duality pairing between  $L^2$  and itself, the inequality above implies that

$$\|d_*^n\|_{L^2} \leq (C\tau \|u\|_{W^{2,1}(I_n;H^2)} + C\tau \|\partial_{ttt}u\|_{L^1(I_n;L^2)} + Ch^2).$$

Hence,

$$\begin{split} \tau \sum_{n=1}^N \|d_*^n\|_{L^2} &\leq \sum_{n=1}^N (C\tau^2 \|u\|_{W^{2,1}(I_n;H^2)} + C\tau^2 \|\partial_{ttt} u\|_{L^1(I_n;L^2)} + C\tau h^2) \\ &\leq C\tau^2 (\|u\|_{W^{2,1}(0,T;H^2)} + \|\partial_{ttt} u\|_{L^1(0,T;L^2)}) + Ch^2. \end{split}$$

This proves the desired result of Lemma 3.3.

### 3.2 Existence, Uniqueness and Error Estimates

This subsection is divided into four parts. In the first part, we prove a discrete interpolation inequality that will be frequently used in the subsequent analysis. In the second part, we construct a nonlinear map whose fixed point is a solution to the implicit CN-FEM. The existence of a fixed point and the error estimates are presented in the third and fourth parts.

#### Part I: A Discrete Interpolation Inequality

The following lemma can be proved similarly to [20, Lemma 3.2].

Lemma 3.4 (Discrete Sobolev Interpolation Inequality). We have

$$\|v_h\|_{L^{\infty}} \leq C \|v_h\|_{L^2}^{1-\frac{d}{4}} \|\Delta_h v_h\|_{L^2}^{\frac{d}{4}} \text{ for all } v_h \in S_h.$$

#### Part II: Construction of a Nonlinear Map Whose Fixed Point Is a Solution

By considering the difference between (2.3) and (3.5), we obtain the following equation for the error  $e_h^n = u_h^n - u_{h,*}^n$  (recall  $u_{h,*}^n = R_h u(t_n)$ ):

$$\left( i \frac{e_h^n - e_h^{n-1}}{\tau}, v_h \right) - \left( \nabla \frac{e_h^n + e_h^{n-1}}{2}, \nabla v_h \right) + \left( \tilde{f}(|u_h^n|^2, |u_h^{n-1}|^2) \frac{u_h^n + u_h^{n-1}}{2} - \tilde{f}(|u_{h,*}^n|^2, |u_{h,*}^{n-1}|^2) \frac{u_{h,*}^n + u_{h,*}^{n-1}}{2}, v_h \right)_h = -(d_*^n, v_h) \quad \text{for all } v_h \in S_h.$$

$$(3.7)$$

It is easy to see that  $u_h^n$  is a solution of (2.3) if and only if  $e_h^n$  is a solution of (3.7) with  $u_h^n = u_{h,*}^n + e_h^n$ . To prove the existence of solutions to (3.7) (for sufficiently small  $\tau$  and h), we construct a map  $M: (S_h)^N \to (S_h)^N$  as follows: for any given  $w = (w_h^n)_{n=1}^N \in (S_h)^N$ , we set

$$\phi[w] = \min\left(\frac{1}{\max_{1 \le n \le N} \|w_h^n\|_{L^{\infty}}}, 1\right),\tag{3.8}$$

and define  $u_h^n := u_{h,*}^n + \phi[w] w_h^n$  for n = 1, ..., N. This definition guarantees that

$$||u_h^n - u_{h,*}^n||_{L^{\infty}} \le 1$$
 for  $n = 1, ..., N$ .

Then we view the two  $\tilde{f}$ -involved terms in (3.7) fixed and known from  $w_h^n$  and  $u_{h,*}^n$ , and define  $(e_h^n)_{n=1}^N \in (S_h)^N$  to be the solution of the *linear problem* (3.7). Since all norms on  $(S_h)^N$  are equivalent (for fixed  $\tau$  and h), it is straightforward to verify that this map M is continuous (and therefore compact in the finite-dimensional space). Next, we prove the existence of a fixed point for the map M by using the following Schaefer fixed point theorem [11, Chapter 9.2, Theorem 4].

**Theorem 3.1.** If  $M: (S_h)^N \to (S_h)^N$  is a continuous and compact mapping, and the set

$$B = \{ w \in (S_h)^N : \text{ there exists } \theta \in [0, 1] \text{ such that } w = \theta M w \}$$
(3.9)

is bounded in  $(S_h)^N$ , then the map M has at least one fixed point.

We can easily see from Theorem 3.1 that if *w* is a fixed point of *M*, then w = Mw. This corresponds to  $\theta = 1$  in the set *B*.

#### Part III: Boundedness of the Set B

If  $w = (w_h^n)_{n=1}^N \in B$ , then  $w = \theta M w$ . By denoting  $e = M w = (e_h^n)_{n=1}^N$ , we have  $w = \theta e$ , and therefore,  $e_h^n$  is the solution of (3.7) with  $u_h^n = u_{h,*}^n + \phi[\theta e_h^n]\theta e_h^n$ , and

$$\max_{1\leq n\leq N} \|u_h^n - u_{h,*}^n\|_{L^{\infty}} \leq \phi[\theta e] \max_{1\leq n\leq N} \|\theta e_h^n\|_{L^{\infty}} \leq 1,$$

where the last inequality is a result of (3.8). Hence,  $u = (u_{h}^n)_{n=1}^N$  is in an  $L^{\infty}$  neighborhood of  $u_* = (u_{h,*}^n)_{n=1}^N$  in  $(S_h)^N$ . Since  $u_{h,*}^n$  is the Ritz projection of  $u(t_n)$ , by using (3.4), we have

$$||u_{h,*}^n - u(t_n)||_{L^{\infty}} \le Ch^{2-\frac{u}{2}} ||u(t_n)||_{H^2}.$$

The two estimates above imply that (using the triangle inequality)

$$\max_{1 \le n \le N} \|u_h^n\|_{L^{\infty}} \le C.$$

The boundedness of *e* in  $(S_h)^N$  can be proved by substituting  $v_h = \frac{1}{2}(e_h^n + e_h^{n-1})$  into (3.7) and considering the imaginary part. Then we obtain, by using the local Lipschitz continuity of  $\tilde{f}$  and the boundedness of  $u_h^n$ 

shown above,

$$\frac{\|e_{h}^{n}\|_{L^{2}}^{2} - \|e_{h}^{n-1}\|_{L^{2}}^{2}}{2\tau} \leq C(\|u_{h}^{n} - u_{h,*}^{n}\|_{L^{2}} + \|u_{h}^{n-1} - u_{h,*}^{n-1}\|_{L^{2}})\|e_{h}^{n} + e_{h}^{n-1}\|_{L^{2}} + \frac{1}{2}|(d_{*}^{n}, e_{h}^{n} + e_{h}^{n-1})| \leq C(\|e_{h}^{n}\|_{L^{2}}^{2} + \|e_{h}^{n-1}\|_{L^{2}}^{2}) + \frac{1}{2}|(d_{*}^{n}, e_{h}^{n} + e_{h}^{n-1})|.$$

Summing up the inequality above for n = 1, ..., k, we have

$$\begin{split} \|e_{h}^{k}\|_{L^{2}}^{2} &\leq \|e_{h}^{0}\|_{L^{2}}^{2} + C\tau \sum_{n=1}^{k} (\|e_{h}^{n}\|_{L^{2}}^{2} + \|e_{h}^{n-1}\|_{L^{2}}^{2}) + \frac{1}{2}\tau \sum_{n=1}^{k} |(d_{*}^{n}, e_{h}^{n} + e_{h}^{n-1})| \\ &\leq \|e_{h}^{0}\|_{L^{2}}^{2} + C\tau \sum_{n=1}^{k} (\|e_{h}^{n}\|_{L^{2}}^{2} + \|e_{h}^{n-1}\|_{L^{2}}^{2}) + C\tau \sum_{n=1}^{k} \|d_{*}^{n}\|_{L^{2}} \max_{0 \leq n \leq k} \|e_{h}^{n}\|_{L^{2}} \\ &\leq \frac{3}{2} \|e_{h}^{0}\|_{L^{2}}^{2} + C\tau \sum_{n=1}^{k} (\|e_{h}^{n}\|_{L^{2}}^{2} + \|e_{h}^{n-1}\|_{L^{2}}^{2}) + C\left(\tau \sum_{n=1}^{k} \|d_{*}^{n}\|_{L^{2}}\right)^{2} + \frac{1}{2} \max_{1 \leq n \leq k} \|e_{h}^{n}\|_{L^{2}}^{2}. \end{split}$$

Since this inequality holds for all  $1 \le k \le N$ , it follows that

$$\max_{1 \le n \le k} \|e_h^k\|_{L^2}^2 \le \frac{3}{2} \|e_h^0\|_{L^2}^2 + C\tau \sum_{n=1}^k (\|e_h^n\|_{L^2}^2 + \|e_h^{n-1}\|_{L^2}^2) + C\left(\tau \sum_{n=1}^k \|d_*^n\|_{L^2}\right)^2 + \frac{1}{2} \max_{1 \le n \le k} \|e_h^n\|_{L^2}^2.$$

Note that the last term above can be absorbed by the left-hand side. Therefore, we have

$$\max_{1 \le n \le k} \|e_h^n\|_{L^2}^2 \le 3 \|e_h^0\|_{L^2}^2 + C\tau \sum_{n=1}^k (\|e_h^n\|_{L^2}^2 + \|e_h^{n-1}\|_{L^2}^2) + C\left(\tau \sum_{n=1}^k \|d_*^n\|_{L^2}\right)^2.$$

This proves, by using Gronwall's inequality for sufficiently small step size  $\tau$ , the following estimate:

$$\max_{1 \le n \le N} \|e_h^n\|_{L^2}^2 \le C \|e_h^0\|_{L^2}^2 + C \bigg(\tau \sum_{n=1}^N \|d_*^n\|_{L^2}\bigg)^2.$$
(3.10)

By using Lemma 3.3 and  $||e_h^0||_{L^2} \leq Ch^2$ , we obtain

$$\max_{1 \le n \le N} \|e_h^n\|_{L^2} \le C(\tau^2 + h^2).$$
(3.11)

If  $\tau \leq h$ , then the application of inverse inequality to (3.11) yields

$$\|e_h^n\|_{L^{\infty}} \leq Ch^{-\frac{d}{2}}(\tau^2 + h^2) \leq Ch^{2-\frac{d}{2}}.$$

If  $\tau \ge h$ , then (3.11) reduces to  $||e_h^n||_{L^2} \le C\tau^2$ . As a result, we have

$$\left\|\frac{e_h^n - e_h^{n-1}}{\tau}\right\|_{L^2} \le C\tau^{-1}(\|e_h^n\|_{L^2} + \|e_h^{n-1}\|_{L^2}) \le C\tau.$$

From (3.7), we derive that

$$\begin{split} \left\| \Delta_h \frac{e_h^n + e_h^{n-1}}{2} \right\|_{L^2} &\leq \left\| \frac{e_h^n - e_h^{n-1}}{\tau} \right\|_{L^2} + C(\|u_h^n - u_{h,*}^n\|_{L^2} + \|u_h^{n-1} - u_{h,*}^{n-1}\|_{L^2}) + C\|d_*^n\|_{L^2} \\ &\leq C\tau + C\tau^2 + C\|d_*^n\|_{L^2}. \end{split}$$

By using the triangle inequality, the above estimate implies that

$$\|\Delta_h e_h^n\|_{L^2} - \|\Delta_h e_h^{n-1}\|_{L^2} \le C\tau + C\tau^2 + C\|d_*^n\|_{L^2}.$$

Summing up this inequality for n = 1, ..., k, with  $1 \le k \le N$ , we obtain

$$\max_{1 \le k \le N} \|\Delta_h e_h^k\|_{L^2} \le C + C \sum_{n=1}^N \|d_*^n\|_{L^2} \le C + C\tau^{-1}(\tau^2 + h^2) \le C,$$
(3.12)

where we have used Lemma 3.3 in estimating  $\sum_{n=1}^{N} ||d_*^n||_{L^2}$  and used  $h \le C\tau$  in the last inequality. Using the discrete interpolation inequality in Lemma 3.4, together with (3.11)–(3.12), we have

$$\|e_h^n\|_{L^{\infty}} \le C \|e_h^n\|_{L^2}^{1-\frac{d}{4}} \|\Delta_h e_h^n\|_{L^2}^{\frac{d}{4}} \le C(\tau^2 + h^2)^{1-\frac{d}{4}} \le C\tau^{2-\frac{d}{2}} \quad \text{when } \tau \ge h.$$

By combining the two cases  $\tau \le h$  and  $\tau \ge h$  above, we obtain the following result:

$$\|e_h^n\|_{L^{\infty}} \leq C(\tau^{2-\frac{u}{2}} + h^{2-\frac{u}{2}}).$$

This proves that the set *B* defined in (3.9) is bounded in  $(S_h)^N$  in the  $L^{\infty}$  norm (and the bound is independent of  $\tau$  and *h*). According to Theorem 3.1, the map *M* has a fixed point, which is denoted below by  $e = (e_h^n)_{n=1}^N$ .

Moreover, when  $\tau$  and h are sufficiently small, the inequality above implies

$$\|\boldsymbol{e}_{h}^{n}\|_{L^{\infty}} \leq \frac{1}{2} \tag{3.13}$$

and therefore

$$\|u_{h}^{n}-u(t_{n})\|_{L^{\infty}} \leq \|e_{h}^{n}\|_{L^{\infty}} + \|u_{h,*}^{n}-u(t_{n})\|_{L^{\infty}} \leq \frac{1}{2} + Ch^{\frac{d}{2}}\|u(t_{n})\|_{H^{2}}.$$

For sufficiently small *h*, the inequality above implies

$$\|u_h^n - u(t_n)\|_{L^{\infty}} \le 1.$$
(3.14)

#### Part IV: Existence and Error Estimate

Inequality (3.13) implies  $\phi[\theta e] = 1$  according to the definition in (3.8). Therefore, the fixed point  $e = (e_h^n)_{n=1}^N$  of the map M (corresponding to  $\theta = 1$ ) is actually a solution of (3.7) with  $u_h^n = u_{h,*}^n + e_h^n$ . This proves equivalently the *existence* of a numerical solution to the implicit scheme (2.3), and the solution satisfies (2.5) in view of (3.14) as well as estimates (2.6)–(2.7) that follow from (3.11)–(3.12).

#### **Part V: Uniqueness**

If there are two solutions of the implicit scheme (2.3) satisfying (2.5), denoted by  $u_h^n$  and  $u_{h,*}^n$  (abusing the notation), it is direct to verify that the difference  $e_h = u_h^n - u_{h,*}^n$  satisfies (3.7) with  $d_*^n = 0$ . Then the same estimate as above yields (3.10), with  $e_h^0 = 0$  and  $d_*^n = 0$ . This proves the *uniqueness* of the solutions to (2.3).

The first part of Theorem 2.1 is now proved.

# 4 Proof of Theorem 2.1 (ii): Newton Iteration with Quadrature

### **4.1** Properties of $\Delta_h$ and $H_h^s$ Norm

We demonstrate in this subsection the double exponential convergence of the Newton iterative CN-FEM. To do so, we first derive some properties of the discrete Laplacian  $\Delta_h$  and the  $H_h^s$ -norm.

Let  $\lambda_j > 0$  and  $\phi_j$ , j = 1, ..., J, be the eigenvalues and  $L^2$ -normalized eigenfunctions of the operator  $-\Delta_h$ . The fractional power of  $-\Delta_h$  is defined as

$$(-\Delta_h)^{\frac{s}{2}}v_h := \sum_{j=1}^J \lambda_j^{\frac{s}{2}}(v_h, \phi_j)\phi_j \quad \text{for all } v_h \in S_h \text{ and all } s \in [0, 2].$$

The  $H_h^s$  norm on  $S_h$  is defined as

$$\|v_h\|_{H_h^s} := \|(-\Delta_h)^{\frac{s}{2}} v_h\|_{L^2} = \left(\sum_{j=1}^J \lambda_j^s |(v_h, \phi_j)|^2\right)^{\frac{1}{2}}.$$
(4.1)

The next lemma gives a basic interpolation inequality and inverse inequality using  $H_h^s$  norm. The proof of the lemma is presented in the appendix.

**Lemma 4.1** (Discrete interpolation and inverse inequalities). *The following inequalities hold*.

(i) Interpolation inequality:

$$\|v_h\|_{H^s_h} \le \|v_h\|_{L^2}^{1-\frac{3}{2}} \|v_h\|_{H^2_h}^{\frac{3}{2}}$$
 for all  $v_h \in S_h$  and all  $0 \le s \le 2$ .

(ii) Inverse inequality:

$$\|v_h\|_{H^{s_2}} \le Ch^{-(s_2-s_1)} \|v_h\|_{H^{s_1}}$$
 for all  $v_h \in S_h$  and all  $0 \le s_1 \le s_2 \le 2$ .

**Lemma 4.2.** The difference between  $(-\Delta_h)^{-\frac{s}{2}}$  and  $(-\Delta)^{-\frac{s}{2}}$  meets the estimate

$$\|(-\Delta_h)^{-\frac{s}{2}}\phi_h - (-\Delta)^{-\frac{s}{2}}\phi_h\|_{L^2} \le C\|\phi_h\|_{L^2}h^s \text{ for all } \phi_h \in S_h \text{ and all } s \in [0, 2].$$

*Proof.* Let  $w_h = (-\Delta_h)^{-1} \phi_h$  and  $w = (-\Delta)^{-1} \phi_h$ . Then  $w_h$  is the Ritz projection of w onto the finite element space. Hence, the following standard error estimates hold:

$$\|w_h - w\|_{L^2} \le C \|w\|_{H^2} h^2 \le C \|\phi_h\|_{L^2} h^2.$$

This can be written as

$$\|(-\Delta_h)^{-1}\phi_h - (-\Delta)^{-1}\phi_h\|_{L^2} \le C \|\phi_h\|_{L^2} h^2, \tag{4.2}$$

We consider the following analytic function of *z*:

$$G(z) = (-\Delta_h)^{-z} \phi_h - (-\Delta)^{-z} \phi_h$$
 for  $0 \le \operatorname{Re}(z) \le 1$ 

Since

$$\|(-\Delta_h)^{-i\eta}\phi_h\|_{L^2} \le \|\phi_h\|_{L^2}$$
 and  $\|(-\Delta)^{-i\eta}\phi_h\|_{L^2} \le \|\phi_h\|_{L^2}$  for all  $\eta \in \mathbb{R}$ 

it follows that G(z) is a bounded analytic function on the strip  $0 \le \text{Re}(z) \le 1$  and satisfying

$$\|G(z)\|_{L^{2}} \leq \begin{cases} C \|\phi_{h}\|_{L^{2}} & \text{when } \operatorname{Re}(z) = 0, \\ C \|\phi_{h}\|_{L^{2}} h^{2} & \text{when } \operatorname{Re}(z) = 1, \end{cases}$$

where the second inequality is due to (4.2). Hence, by Hadamard's three lines lemma (cf. [15, Lemma 1.3.5]), there holds

$$\|G(z)\|_{L^2} \le (C\|\phi_h\|_{L^2})^{1-\operatorname{Re}(z)} (C\|\phi_h\|_{L^2}h^2)^{\operatorname{Re}(z)} \le C\|\phi_h\|_{L^2}h^2 \operatorname{Re}(z) \quad \text{when } 0 < \operatorname{Re}(z) < 1.$$

Choosing  $z = \frac{s}{2}$  in the inequality above, we obtain the desired result.

It is known that  $D((-\Delta)^{\frac{s}{2}}) = H^s(\Omega) \cap H^1_0(\Omega)$  for  $s \in (\frac{1}{2}, 2]$  and  $D((-\Delta)^{\frac{s}{2}}) = H^s(\Omega)$  for  $s \in [0, \frac{1}{2})$ . The following result is a corollary of Lemma 4.2.

**Corollary 4.1** (Relation between  $(-\Delta_h)^{\frac{s}{2}}$  and  $(-\Delta)^{\frac{s}{2}}$ ).

$$\|(-\Delta)^{-\frac{s}{2}}\phi_{h}\|_{L^{2}} \leq C\|(-\Delta_{h})^{-\frac{s}{2}}\phi_{h}\|_{L^{2}} \quad for all \phi_{h} \in S_{h} and all s \in [0, 2], \\ \|(-\Delta_{h})^{\frac{s}{2}}P_{h}\phi\|_{L^{2}} \leq C\|\phi\|_{H^{s}} \qquad for all \phi \in D((-\Delta)^{\frac{s}{2}}) and all s \in [0, 2].$$

*Proof.* The first result of Corollary 4.1 is a consequence of Lemma 4.2, together with the triangle and inverse inequalities

$$\|\phi_h\|_{L^2}h^s = \|(-\Delta_h)^{\frac{s}{2}}(-\Delta_h)^{-\frac{s}{2}}\phi_h\|_{L^2}h^s \le C\|(-\Delta_h)^{-\frac{s}{2}}\phi_h\|_{L^2}.$$

Replacing  $\phi_h$  by  $(-\Delta_h)^{\frac{s}{2}}\phi_h$  in the first result of Corollary 4.1, we also obtain

$$\|(-\Delta)^{-\frac{3}{2}}(-\Delta_h)^{\frac{3}{2}}\phi_h\|_{L^2} \leq C\|\phi_h\|_{L^2} \quad \text{for all } \phi_h \in S_h \text{ and all } s \in [0, 2].$$

Hence, the operator  $(-\Delta)^{-\frac{s}{2}}(-\Delta_h)^{\frac{s}{2}}P_h$  is bounded on  $L^2(\Omega)$ . Its dual operator  $(-\Delta_h)^{\frac{s}{2}}P_h(-\Delta)^{-\frac{s}{2}}$  must also be bounded on  $L^2(\Omega)$ , i.e.,

$$\|(-\Delta_h)^{\frac{s}{2}}P_h(-\Delta)^{-\frac{s}{2}}\varphi\|_{L^2} \leq C\|\varphi\|_{L^2}.$$

Replacing  $\varphi$  by  $\varphi = (-\Delta)^{\frac{s}{2}} \phi$  for  $\phi \in D((-\Delta)^{\frac{s}{2}})$ , we obtain the second result of Corollary 4.1.

**Lemma 4.3.** For any fixed  $s \in (\frac{d}{2}, 2]$ , we have the discrete Sobolev embedding inequality

$$\|v_h\|_{L^{\infty}} \leq C \|v_h\|_{H^s_h} \quad \text{for all } v_h \in S_h.$$

*Proof.* Since  $(-\Delta)^{-\frac{s}{2}} \phi_h \in H^s(\Omega)$  for  $\phi_h \in S_h \subset L^2(\Omega)$ , the standard Sobolev embedding inequality implies that

$$\|(-\Delta)^{-\frac{s}{2}}\phi_{h}\|_{L^{\infty}} \le C\|(-\Delta)^{-\frac{s}{2}}\phi_{h}\|_{H^{s}} \le C\|\phi_{h}\|_{L^{2}} \quad \text{for } s \in (\frac{d}{2}, 2].$$
(4.3)

Hence we obtain by using the triangle and inverse inequalities, and the  $L^{\infty}$ -stability of the projection  $P_h$ , that

$$\begin{split} \|(-\Delta_{h})^{-\frac{s}{2}}\phi_{h}\|_{L^{\infty}} &\leq \|(-\Delta_{h})^{-\frac{s}{2}}\phi_{h} - P_{h}(-\Delta)^{-\frac{s}{2}}\phi_{h}\|_{L^{\infty}} + \|P_{h}(-\Delta)^{-\frac{s}{2}}\phi_{h}\|_{L^{\infty}} \\ &\leq Ch^{-\frac{d}{2}}\|(-\Delta_{h})^{-\frac{s}{2}}\phi_{h} - P_{h}(-\Delta)^{-\frac{s}{2}}\phi_{h}\|_{L^{2}} + C\|(-\Delta)^{-\frac{s}{2}}\phi_{h}\|_{L^{\infty}} \\ &\leq Ch^{-\frac{d}{2}}\|(-\Delta_{h})^{-\frac{s}{2}}\phi_{h} - (-\Delta)^{-\frac{s}{2}}\phi_{h}\|_{L^{2}} + C\|(-\Delta)^{-\frac{s}{2}}\phi_{h}\|_{L^{\infty}} \\ &\leq Ch^{s-\frac{d}{2}}\|\phi_{h}\|_{L^{2}} + C\|\phi_{h}\|_{L^{2}}, \end{split}$$

where the last inequality uses Lemma 4.2 and (4.3). For  $s \in (\frac{d}{2}, 2]$ , the inequality above implies

$$\|(-\Delta_h)^{-\frac{3}{2}}\phi_h\|_{L^{\infty}} \leq C \|\phi_h\|_{L^2}.$$

This implies the result of Lemma 4.3 if we write  $v_h = (-\Delta_h)^{-\frac{s}{2}} \phi_h$ .

**Lemma 4.4.** For  $s \in (\frac{d}{2}, 2]$ , any smooth function g(v) of v and any smooth function  $\phi(v_1, \ldots, v_m)$  of m arguments, the following estimates hold:

$\ vw\ _{H^s} \leq C \ v\ _{H^s} \ w\ _{H^s}$	for all $v, w \in H^{s}(\Omega)$ ,		
$\ g(v)\ _{H^s} \leq C_M$	for all $v \in H^{s}(\Omega)$ ,	$\ v\ _{H^s} \leq M,$	
$\ \phi(v_1,\ldots,v_m)\ _{H^s}\leq C_M$	for all $v_j \in H^s(\Omega)$ ,	$\ v_j\ _{H^s} \leq M,$	$j=1,\ldots,m$

where the constant  $C_M$  depends only on g and M.

*Proof.* For  $v, w \in H^s(\Omega)$  with  $s > \frac{d}{2}$ , we denote by  $\tilde{v}$  and  $\tilde{w}$  any extension of v and w to  $H^s(\mathbb{R}^d)$ , respectively. Then the following Kato–Ponce inequality is known on  $\mathbb{R}^d$  (cf. [16]):

$$\|\tilde{\nu}\tilde{w}\|_{H^s(\mathbb{R}^d)} \leq C \|\tilde{\nu}\|_{H^s(\mathbb{R}^d)} \|\tilde{w}\|_{H^s(\mathbb{R}^d)}.$$

Since  $\tilde{v}\tilde{w}$  is an extension of vw to  $H^s(\mathbb{R}^d)$  and  $\|vw\|_{H^s} \sim \inf_{\chi} \|\chi\|_{H^s(\mathbb{R}^d)}$ , where the infimum extends over all possible extensions of vw to  $H^s(\mathbb{R}^d)$ , it follows that  $\|vw\|_{H^s} \leq C \|\tilde{v}\|_{H^s(\mathbb{R}^d)} \|\tilde{w}\|_{H^s(\mathbb{R}^d)}$ . By taking infimum among all extensions  $\tilde{v}, \tilde{w} \in H^s(\mathbb{R}^d)$ , we obtain the first result of Lemma 4.4.

The second result can be shown similarly. Since  $\|v\|_{L^{\infty}} \leq C \|v\|_{H^s} \leq M$ , the function g can be regarded as Lipschitz continuous, with a Lipschitz constant depending on M. If  $\frac{d}{2} < s < 1$  (in the case d = 1), then the following result is a simple consequence of the equivalence between  $\|\cdot\|_{H^s}$  with the Sobolev–Slobodeckii norm (cf. [21, equation (3.18) on p. 73]):

$$\|g(v)\|_{H^s} \leq C_M \|v\|_{H^s}.$$

If  $s = 1 > \frac{d}{2}$  (in the case d = 1), then

$$\|g(v)\|_{H^1} \le C \|g(v)\|_{L^2} + C \|g'(v)\nabla v\|_{L^2} \le C_M + C_M \|\nabla v\|_{L^2} \le C_M$$

If  $\max(\frac{d}{2}, 1) < s < 2$ , then

$$\|g(v)\|_{H^{s}} \leq C \|g(v)\|_{H^{1}} + C \|g'(v)\nabla v\|_{H^{s-1}} \leq C_{M} + C \|g'(v)\nabla v\|_{H^{s-1}}.$$

According to the Kato–Ponce inequality (cf. [15, inequality (1)]), the following result holds for  $\frac{1}{2} = \frac{1}{p} + \frac{1}{q}$  and  $1 < p, q < \infty$ :

 $\|g'(v)\nabla v\|_{H^{s-1}} \leq C(\|g'(v)\|_{W^{s-1,p}}\|\nabla v\|_{L^q} + \|g'(v)\|_{L^\infty}\|\nabla v\|_{H^{s-1}}).$ 

For  $d \in \{2, 3\}$ , let  $1 < q < \infty$  be the number satisfying  $s - 1 = \frac{d}{2} - \frac{d}{q}$ . Then  $H^{s-1} \hookrightarrow L^q$ ,  $H^s \hookrightarrow W^{1,q}$  and  $p = \frac{d}{s-1}$ . Therefore, we have

$$\begin{split} \|g'(\nu)\nabla\nu\|_{H^{s-1}} &\leq C\big(\|g'(\nu)\|_{W^{s-1},\frac{d}{s-1}}\|\nabla\nu\|_{H^{s-1}} + \|g'(\nu)\|_{L^{\infty}}\|\nabla\nu\|_{H^{s-1}}\big) \\ &\leq C\big(\|g'(\nu)\|_{W^{s-1},\frac{d}{s-1}}\|\nu\|_{H^s} + C_M\|\nu\|_{H^s}\big) \leq C\big(\|g'(\nu)\|_{W^{1,q}}\|\nu\|_{H^s} + C_M\|\nu\|_{H^s}\big), \end{split}$$

where we have used the Sobolev embedding result  $W^{1,q} \hookrightarrow W^{s-1,\frac{d}{s-1}}$ , which holds whenever  $q \ge d$ . This is true because  $s - 1 = \frac{d}{2} - \frac{d}{a}$  and  $s > \frac{d}{2}$ . Since  $\|v\|_{H^s} \le M$  and  $H^s \hookrightarrow W^{1,q}$ , it follows that

$$\begin{aligned} \|g'(v)\nabla v\|_{H^{s-1}} &\leq C_M(\|g'(v)\|_{L^q} + \|g''(v)\nabla v\|_{L^q}) + C_M \\ &\leq C_M(C_M + C_M\|v\|_{W^{1,q}}) + C_M \leq C_M(C_M + C_M\|v\|_{H^s}) + C_M \leq C_M. \end{aligned}$$

This proves the second result of Lemma 4.4. The third result can be proved similarly.

We denote by  $C^2(\mathbb{C})$  the space of all functions on  $\mathbb{C}$  that are second-order differentiable with respect to the real and imaginary parts of their argument, and the partial derivatives up to second order are continuous on  $\mathbb{C}$  (therefore bounded on any compact subset of  $\mathbb{C}$ ).

**Lemma 4.5** (Action of  $(-\Delta_h)^{\frac{s}{2}}$  on a Nonlinear Function). Let  $P_h^*: C(\overline{\Omega}) \to S_h$  be defined by

$$(P_h^*w, v_h) = (w, v_h)_h$$
 for all  $w \in C(\Omega)$  and all  $v_h \in S_h$ .

Then, for any  $s \in (\frac{d}{2}, 2]$  and  $g \in C^2(\mathbb{C})$ , the following inequality holds:

$$\|P_{h}^{*}[g(v_{h})w_{h}]\|_{H_{h}^{s}} \leq C_{M}\|w_{h}\|_{H_{h}^{s}} \quad \text{for all } w_{h}, v_{h} \in S_{h}, \quad \|v_{h}\|_{H_{h}^{s}} \leq M,$$

where the constant  $C_M$  depends on g and M.

*Proof.* Let  $w = \Delta^{-1}\Delta_h w_h \in H^1_0(\Omega) \cap H^2(\Omega)$  and  $v = \Delta^{-1}\Delta_h v_h \in H^1_0(\Omega) \cap H^2(\Omega)$ . Then

$$\|(-\Delta)^{\frac{s}{2}}w\|_{L^{2}} = \|(-\Delta)^{-(1-\frac{s}{2})}(-\Delta_{h})^{1-\frac{s}{2}}(-\Delta_{h})^{\frac{s}{2}}w_{h}\|_{L^{2}},$$

and from the first result of Corollary 4.1, we know that

$$\|(-\Delta)^{-(1-\frac{s}{2})}(-\Delta_h)^{1-\frac{s}{2}}(-\Delta_h)^{\frac{s}{2}}w_h\|_{L^2} \le C\|(-\Delta_h)^{\frac{s}{2}}w_h\|_{L^2}.$$

The two estimates above imply that

$$\|w\|_{H^s} \le C \|w_h\|_{H^s_h}$$
 and  $\|v\|_{H^s} \le C \|v_h\|_{H^s_h}$  for  $s \in [0, 2]$ . (4.4)

Lemma 4.3 implies that, for  $s \in (\frac{d}{2}, 2]$ ,

$$\|w\|_{L^{\infty}} \leq C \|w\|_{H^{s}} \leq C \|w_{h}\|_{H^{s}_{h}}$$
 and similarly  $\|v\|_{L^{\infty}} \leq C \|v_{h}\|_{H^{s}_{h}} \leq CM$ .

Since  $\Delta_h w_h = \Delta w$ , it follows that  $w_h$  is the Ritz projection of w. As a result, (3.1) and (4.4) together imply that

$$||w_h - w||_{L^2} \le C ||w||_{H^2} h^2 \le C ||w_h||_{H^2_h} h^2$$
 and similarly  $||v_h - v||_{L^2} \le C ||v_h||_{H^2_h} h^2$ .

Hence, by using the definition of  $P_h^*$  and the first property of Lemma 3.1, and using the local Lipschitz continuity of *g* with Lemma 4.3, we have

$$\begin{split} |(P_{h}^{*}[g(v_{h})w_{h}] - P_{h}^{*}[g(v)w], \phi_{h})| \\ &= |(g(v_{h})w_{h} - g(v)w, \phi_{h})_{h}| \leq \sum_{K \in \mathcal{K}} Ch^{\frac{d}{2}} ||g(v_{h})w_{h} - g(v)w||_{L^{\infty}(K)} ||\phi_{h}||_{L^{2}(K)} \\ &\leq \sum_{K \in \mathcal{K}} C_{M}h^{\frac{d}{2}} (||v_{h} - v||_{L^{\infty}(K)} ||w||_{L^{\infty}(K)} + ||v_{h}||_{L^{\infty}(K)} ||w_{h} - w||_{L^{\infty}(K)}) ||\phi_{h}||_{L^{2}(K)} \\ &\leq \sum_{K \in \mathcal{K}} C_{M}h^{\frac{d}{2}} (||v_{h} - I_{h}v||_{L^{\infty}(K)} + ||I_{h}v - v||_{L^{\infty}(K)}) ||w||_{L^{\infty}} ||\phi_{h}||_{L^{2}(K)} \\ &+ \sum_{K \in \mathcal{K}} C_{M}h^{\frac{d}{2}} (||w_{h} - I_{h}w||_{L^{\infty}(K)} + ||I_{h}w - w||_{L^{\infty}(K)}) ||v_{h}||_{L^{\infty}} ||\phi_{h}||_{L^{2}(K)} \end{split}$$

$$\leq \sum_{K \in \mathcal{K}} (C_M \| v_h - I_h v \|_{L^2(K)} + C_M h^2 \| v \|_{H^2(K)}) \| w \|_{L^{\infty}} \| \phi_h \|_{L^2(K)} + \sum_{K \in \mathcal{K}} (C_M \| w_h - I_h w \|_{L^2(K)} + C_M h^2 \| w \|_{H^2(K)}) \| v_h \|_{L^{\infty}} \| \phi_h \|_{L^2(K)} \leq (C_M \| v_h - I_h v \|_{L^2} + C_M h^2 \| v \|_{H^2}) \| w \|_{L^{\infty}} \| \phi_h \|_{L^2} + (C_M \| w_h - I_h w \|_{L^2} + C_M h^2 \| w \|_{H^2}) \| v_h \|_{H^s_h} \| \phi_h \|_{L^2} \leq C_M (h^2 \| v_h \|_{H^2_h} \| w_h \|_{H^s_h} + h^2 \| v_h \|_{H^s_h} \| w_h \|_{H^2_h}) \| \phi_h \|_{L^2} \leq C_M h^s \| v_h \|_{H^s_h} \| w_h \|_{H^s_h} \| \phi_h \|_{L^2}$$
(inverse inequality in Lemma 4.1).

It follows from the above estimate that holds for all  $\phi_h \in S_h$  and the estimate  $\|v_h\|_{H^s_h} \leq M$  that

$$\|P_h^*[g(v_h)w_h] - P_h^*[g(v)w]\|_{L^2} \le C_M h^s \|w_h\|_{H^s_h}$$

Then, by using the inverse inequality in Lemma 4.1 and the inequality above, we have

$$\left\| (-\Delta_h)^{\frac{s}{2}} \left( P_h^*[g(v_h)w_h] - P_h^*[g(v)w] \right) \right\|_{L^2} \le Ch^{-s} \|P_h^*[g(v_h)w_h] - P_h^*[g(v)w]\|_{L^2} \le C_M \|w_h\|_{H^{s}_h}.$$

By using the notation  $P_h^*$ , the third result of Lemma 3.1 can be equivalently written as

$$\|P_h^*w - P_hw\|_{L^2} \le Ch^2 \|w\|_{H^2}.$$

As a result,

$$\begin{split} \|(-\Delta_{h})^{\frac{s}{2}}P_{h}^{*}[g(v)w] - (-\Delta_{h})^{\frac{s}{2}}P_{h}[g(v)w]\|_{L^{2}} &\leq Ch^{-s}\|P_{h}^{*}[g(v)w] - P_{h}[g(v)w]\|_{L^{2}} \leq Ch^{2-s}\|g(v)w\|_{H^{2}} \\ &\leq C_{M}h^{2-s}(\|w\|_{H^{2}} + \|v\|_{H^{s}}\|w\|_{H^{s}} + \|v\|_{H^{2}}\|w\|_{H^{s}}) \\ &\leq C_{M}h^{2-s}(\|w_{h}\|_{H^{2}_{h}} + \|v_{h}\|_{H^{2}_{h}}\|w_{h}\|_{H^{s}_{h}}) \\ &\leq C_{M}\|w_{h}\|_{H^{s}_{h}} + C_{M}\|v_{h}\|_{H^{s}_{h}}\|w_{h}\|_{H^{s}_{h}} \leq C_{M}\|w_{h}\|_{H^{s}_{h}}. \end{split}$$

Furthermore, by using the second result of Corollary 4.1, Lemma 4.4 and (4.4), for the  $L^2$  projection  $P_h$ , we have

$$\|(-\Delta_h)^{\frac{3}{2}}P_h[g(v)w]\|_{L^2} \le C \|g(v)w\|_{H^s} \le C \|g(v)\|_{H^s} \|w\|_{H^s} \le C_M \|w_h\|_{H^{\frac{1}{2}}}.$$

where the last inequality uses the second result of Lemma 4.4. Combining the three estimates above, we obtain the desired result in Lemma 4.5.  $\hfill \square$ 

**Corollary 4.2.** For any  $s \in (\frac{d}{2}, 2]$  and  $g \in C^2(\mathbb{C})$ , the following inequality holds:

$$\|P_h^*[g(v_h)w_hu_h]\|_{H_h^s} \le C_M \|w_h\|_{H_h^s} \|u_h\|_{H_h^s}$$

for all  $w_h$ ,  $u_h$ ,  $v_h \in S_h$  such that  $||v_h||_{H_h^s} \leq M$ , with  $C_M$  depending on g and M.

*Proof.* Note that the function  $w_h$  in Lemma 4.5 is replaced by a product  $w_h u_h$  in this lemma. We introduce two functions  $w = \Delta^{-1} \Delta_h w_h$  and  $u = \Delta^{-1} \Delta_h u_h$ . From (4.4), we know that  $||w||_{H^s} \leq C ||w_h||_{H^s_h}$  and  $||u||_{H^s} \leq C ||u_h||_{H^s_h}$ . By using the first result in Lemma 4.4 (the Kato–Ponce inequality), we have

$$\|wu\|_{H^s} \leq C \|w\|_{H^s} \|u\|_{H^s} \leq C \|w_h\|_{H^s_h} \|u_h\|_{H^s_h}$$

Then replacing *w* by *wu* in the proof of Lemma 4.5 immediately yields the desired result.

If  $g: \mathbb{C}^m \to \mathbb{C}$  is a function which is second-order continuously differentiable in the real and imaginary parts of each component, then we can regard g to be a function in  $C^2(\mathbb{R}^{2m}) \times C^2(\mathbb{R}^{2m})$ . In this case, a similar proof (using the third result of Lemma 4.4) would yield the following result.

**Corollary 4.3.** For any  $s \in (\frac{d}{2}, 2]$  and  $g \in C^2(\mathbb{C}^m)$ , the following inequalities hold:

$$\|P_{h}^{*}[g(v_{1,h},\ldots,v_{m,h})w_{h}]\|_{H_{h}^{s}} \leq C_{M}\|w_{h}\|_{H_{h}^{s}},$$
$$\|P_{h}^{*}[g(v_{1,h},\ldots,v_{m,h})w_{h}u_{h}]\|_{H_{h}^{s}} \leq C_{M}\|w_{h}\|_{H_{h}^{s}}\|u_{h}\|_{H_{h}^{s}}$$

for all  $w_h, v_{j,h} \in S_h$  such that  $\max_{1 \le j \le m} \|v_{j,h}\|_{H^s_h} \le M$ , with  $C_M$  depending on g and M.

### 4.2 Proof Theorem 2.1 (ii)

In this subsection, we prove the second part of Theorem 2.1, namely, estimate (2.8). For the sake of notation, we denote the error of the Newton iterative solution by  $e_h^{n,m} = u_h^n - u_h^{n,m}$ . By considering the nonlinear term in (2.3) as a function of  $(u_h^n, u_h^{n-1})$ , and the Taylor expansion of this

function at  $(u_h^{n,m-1}, u_h^{n-1,\ell})$ , we obtain

$$\left( i \frac{u_{h}^{n} - u_{h}^{n-1}}{\tau}, v_{h} \right) - \left( \nabla \frac{u_{h}^{n} + u_{h}^{n-1}}{2}, \nabla v_{h} \right)$$

$$+ \left( \tilde{f}(|u_{h}^{n,m-1}|^{2}, |u_{h}^{n-1,\ell}|^{2}) \frac{u_{h}^{n,m-1} + u_{h}^{n-1,\ell}}{2}, v_{h} \right)_{h}$$

$$+ \left( \tilde{f}(|u_{h}^{n,m-1}|^{2}, |u_{h}^{n-1,\ell}|^{2}) \frac{u_{h}^{n} - u_{h}^{n,m-1}}{2}, v_{h} \right)_{h}$$

$$+ \left( \partial_{1} \tilde{f}(|u_{h}^{n,m-1}|^{2}, |u_{h}^{n-1,\ell}|^{2}) \frac{u_{h}^{n,m-1} + u_{h}^{n-1,\ell}}{2} 2 \operatorname{Re}(\bar{u}_{h}^{n,m-1}(u_{h}^{n} - u_{h}^{n,m-1})), v_{h} \right)_{h}$$

$$+ \left( \tilde{f}(|u_{h}^{n,m-1}|^{2}, |u_{h}^{n-1,\ell}|^{2}) \frac{u_{h}^{n-1} - u_{h}^{n-1,\ell}}{2}, v_{h} \right)_{h}$$

$$+ \left( \partial_{2} \tilde{f}(|u_{h}^{n,m-1}|^{2}, |u_{h}^{n-1,\ell}|^{2}) \frac{u_{h}^{n,m-1} + u_{h}^{n-1,\ell}}{2} 2 \operatorname{Re}(\bar{u}_{h}^{n-1,\ell}(u_{h}^{n-1} - u_{h}^{n-1,\ell})), v_{h} \right)_{h}$$

$$= (\mathcal{E}_{h}^{n}, v_{h})_{h},$$

$$(4.5)$$

where  $\mathcal{E}_h^n$  are quadratic terms of the errors  $e_h^{n,m-1} = u_h^n - u_h^{n,m-1}$  and  $e_h^{n-1,\ell} = u_h^{n-1,\ell} - u_h^{n-1,\ell}$  in the abovementioned Taylor expansion.

Let  $s \in (\frac{d}{2}, 2) \cap [1, 2)$  be any fixed number. We consider mathematical induction on k and q (where  $1 \le k \le N$  and  $1 \le q \le \ell$  are some integers), by assuming that (mathematical induction on k and q),

$$\|e_h^{n,m-1}\|_{H_h^s} \le 1 + 2C_*, \quad \|e_h^{n-1,\ell}\|_{H_h^s} \le \tau^{2-s} + h^{2-s} \quad \text{for } 1 \le n \le k \text{ and } 1 \le m \le q,$$
(4.6)

where

$$C_* = \sup_{\tau \le \tau_0, h \le h_0} \sup_{s \in [0,2]} \max_{1 \le n \le N} \|u_h^n\|_{H_h^s}$$

is bounded as a result of (2.7). Under this induction assumption, the quadratic term in (4.5) satisfies the following estimate (in view of the second result in Corollary 4.3):

$$\|\mathcal{E}_{h}^{n}\|_{H_{h}^{s}} \le C(\|e_{h}^{n,m-1}\|_{H_{h}^{s}}^{2} + \|e_{h}^{n-1,\ell}\|_{H_{h}^{s}}^{2}) \quad \text{for } 1 \le n \le k \text{ and } 1 \le m \le q.$$

$$(4.7)$$

We shall prove that

$$\|e_h^{n,q}\|_{H^s_*} \le 1 + 2C_*,\tag{4.8}$$

$$\|e_h^{n,\ell}\|_{H^s_h} \le \tau^{2-s} + h^{2-s}.$$
(4.9)

Then, by mathematical induction on q, (4.8) implies that

$$\|e^{n,m}\|_{H^s_h} \le 1 + 2C_* \quad \text{for all } 0 \le m \le \ell.$$
 (4.10)

As a result, for  $\tau \le 1$  and all  $1 \le n \le k$ , there holds

$$\|e_{h}^{n+1,0}\|_{H_{h}^{s}} = \|u_{h}^{n,\ell} - u_{h}^{n+1}\|_{H_{h}^{s}} \le \|e_{h}^{n,\ell}\|_{H_{h}^{s}} + \|u_{h}^{n} - u_{h}^{n+1}\|_{H_{h}^{s}} \le \tau^{2-s} + h^{2-s} + 2 \max_{1 \le n \le N} \|u_{h}^{n}\|_{H_{h}^{s}} \le 1 + 2C_{*}.$$

$$(4.11)$$

Since (4.6) implies (4.10), it follows from (4.9) and (4.11) that

$$\|e_h^{n+1,m}\|_{H_h^s} \le 1 + 2C_* \quad \text{for all } 1 \le n \le k \text{ and } 0 \le m \le \ell.$$
(4.12)

By mathematical induction, from (4.9) and (4.12), we can conclude that (4.6) holds for k = N and q = l. It remains to prove (4.8)–(4.9) to complete the mathematical induction.

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The difference between (4.5) and (2.2) yields

$$\left(i\frac{e_{h}^{n,m}-e_{h}^{n-1,\ell}}{\tau},\nu_{h}\right) - \left(\nabla\frac{e_{h}^{n,m}+e_{h}^{n-1,\ell}}{2},\nabla\nu_{h}\right) = -(g_{h}^{n},\nu_{h})_{h} + (\mathcal{E}_{h}^{n},\nu_{h})_{h},\tag{4.13}$$

with

$$\begin{split} g_{h}^{n} &= \tilde{f}(|u_{h}^{n,m-1}|^{2},|u_{h}^{n-1,\ell}|^{2}) \frac{e_{h}^{n,m} + e_{h}^{n-1,\ell}}{2} \\ &+ \partial_{1}\tilde{f}(|u_{h}^{n,m-1}|^{2},|u_{h}^{n-1,\ell}|^{2}) \frac{u_{h}^{n,m-1} + u_{h}^{n-1,\ell}}{2} 2 \operatorname{Re}(\bar{u}_{h}^{n,m-1}e_{h}^{n,m}) \\ &+ \partial_{2}\tilde{f}(|u_{h}^{n,m-1}|^{2},|u_{h}^{n-1,\ell}|^{2}) \frac{u_{h}^{n,m-1} + u_{h}^{n-1,\ell}}{2} 2 \operatorname{Re}(\bar{u}_{h}^{n-1,\ell}e_{h}^{n-1,\ell}) \end{split}$$

By using the operator  $P_h^*$  introduced in Lemma 4.5, equation (4.13) can be rewritten as

$$i\frac{e_h^{n,m} - e_h^{n-1,\ell}}{\tau} + \Delta_h \frac{e_h^{n,m} + e_h^{n-1,\ell}}{2} = -P_h^* g_h^n + P_h^* \mathcal{E}_h^n.$$
(4.14)

Under induction assumption (4.6), we have  $||u^{n,m-1}||_{H_h^s} \le C$  and  $||u^{n-1,\ell}||_{H_h^s} \le C$  for  $1 \le n \le k$  and  $1 \le m \le q$ , and therefore, the following result holds (the first result of Corollary 4.3):

$$\|P_h^*g_h^n\|_{H_h^s} \le C(\|e_h^{n,m}\|_{H_h^s} + \|e_h^{n-1,\ell}\|_{H_h^s}) \quad \text{for } 1 \le n \le k \text{ and } 1 \le m \le q.$$
(4.15)

We rewrite (4.14) as

$$e_h^{n,m} = M_h e_h^{n-1,\ell} - \tau B_h P_h^* g_h^n + \tau B_h P_h^* \mathcal{E}_h^n,$$
(4.16)

with the operators

$$M_h = \left(\mathrm{i} + \frac{\tau}{2}\Delta_h\right)^{-1} \left(\mathrm{i} - \frac{\tau}{2}\Delta_h\right) \quad \text{and} \quad B_h = \left(\mathrm{i} + \frac{\tau}{2}\Delta_h\right)^{-1}.$$

Since the CN method has mass conservation and  $M_h$  commutes with  $(-\Delta_h)^{\frac{s}{2}}$ , it follows that  $M_h$  preserves the  $H_h^s$ -norm, i.e.,

$$\|M_h v_h\|_{H^s_h} = \|M_h(-\Delta_h)^{\frac{s}{2}} v_h\|_{L^2} = \|(-\Delta_h)^{\frac{s}{2}} v_h\|_{L^2} = \|v_h\|_{H^s_h} \quad \text{for all } v_h \in S_h.$$

Similarly,  $||B_h v_h||_{H_h^s} \le ||v_h||_{H_h^s}$  for all  $v_h \in S_h$ . Using these properties and taking the  $H_h^s$  norm in (4.16), we obtain, for  $1 \le n \le k$  and  $1 \le m \le q$ ,

$$\begin{split} \|e_{h}^{n,m}\|_{H_{h}^{s}} &\leq \|e_{h}^{n-1,\ell}\|_{H_{h}^{s}} + \tau \|P_{h}^{*}g_{h}^{n}\|_{H_{h}^{s}} + \tau \|P_{h}^{*}\mathcal{E}_{h}^{n}\|_{H_{h}^{s}} \\ &\leq (1+C\tau)\|e_{h}^{n-1,\ell}\|_{H_{h}^{s}} + C\tau \|e_{h}^{n,m}\|_{H_{h}^{s}} + C\tau (\|e_{h}^{n,m-1}\|_{H_{h}^{s}}^{2} + \|e_{h}^{n-1,\ell}\|_{H_{h}^{s}}^{2}). \end{split}$$

where we have used (4.7) and (4.15) in the last inequality. Using induction assumption (4.6), the inequality above further implies

$$\|e_h^{n,m}\|_{H^s_h} \le (1+C\tau) \|e_h^{n-1,\ell}\|_{H^s_h} + C\tau \|e_h^{n,m-1}\|_{H^s_h}^2 \quad \text{for } 1 \le n \le k \text{ and } 1 \le m \le q.$$

Then, denoting  $\Lambda^{n-1} = (1 + C\tau) \|e_h^{n-1,\ell}\|_{H_h^s}$  and iterating the above inequality for m = 1, ..., q, we obtain

$$\begin{split} \|e_{h}^{n,q}\|_{H_{h}^{s}} &\leq \Lambda^{n-1} + C\tau \|e_{h}^{n,q-1}\|_{H_{h}^{s}}^{2} \\ &\leq \Lambda^{n-1} + C\tau \, 2^{2}|\Lambda^{n-1}|^{2} + (C\tau)^{1+2} 2^{2} \|e_{h}^{n,q-2}\|_{H_{h}^{s}}^{2^{2}} \\ &\leq \Lambda^{n-1} + C\tau \, 2^{2}|\Lambda^{n-1}|^{2} + (C\tau)^{1+2} 2^{2+2^{2}}|\Lambda^{n-1}|^{2^{2}} + (C\tau)^{1+2+2^{2}} 2^{2+2^{2}} \|e_{h}^{n,q-3}\|_{H_{h}^{s}}^{2^{3}} \\ &\vdots \\ &\leq \Lambda^{n-1} + \sum_{m=2}^{q} (C\tau)^{\sum_{j=0}^{m-2} 2^{j}} 2^{\sum_{j=0}^{m-1} 2^{j}} |\Lambda^{n-1}|^{2^{m-1}} + (C\tau)^{\sum_{j=0}^{q-1} 2^{j}} 2^{\sum_{j=0}^{q-1} 2^{j}} \|e_{h}^{n,0}\|_{H_{h}^{s}}^{2^{q}} \\ &= \Lambda^{n-1} + \sum_{m=2}^{q} (C\tau)^{2^{m-1}-1} 2^{2^{m-1}} |\Lambda^{n-1}|^{2^{m-1}} + (C\tau)^{2^{q}-1} 2^{2^{q}-1} \|e_{h}^{n,0}\|_{H_{h}^{s}}^{2^{q}} \end{split}$$

$$\begin{split} &= \Lambda^{n-1} + \sum_{m=2}^{q} (2C\tau)^{2^{m-1}-1} |2\Lambda^{n-1}|^{2^{m-1}} + (2C\tau)^{2^{q}-1} \|e_{h}^{n,0}\|_{H_{h}^{s}}^{2^{q}} \\ &= \Lambda^{n-1} \Big( 1 + 2\sum_{m=2}^{q} (4C\tau\Lambda^{n-1})^{2^{m-1}-1} \Big) + (2C\tau)^{2^{q}-1} \|e_{h}^{n,0}\|_{H_{h}^{s}}^{2^{q}} \\ &\leq (1+C_{1}\tau)\Lambda^{n-1} + (2C\tau)^{2^{q}-1} \|e_{h}^{n,0}\|_{H_{h}^{s}}^{2^{q}} \\ &\leq (1+C_{2}\tau) \|e_{h}^{n-1,\ell}\|_{H_{h}^{s}} + (2C\tau)^{2^{q}-1} \|e_{h}^{n,0}\|_{H_{h}^{s}}^{2^{q}}, \end{split}$$

where we have substituted the expression  $\Lambda^{n-1} = (1 + C\tau) \|e_h^{n-1,\ell}\|_{H_h^s}$  into the last inequality. To further estimate, we use the triangle inequality

$$\|e_h^{n,0}\|_{H_h^s} = \|u_h^{n-1,\ell} - u_h^n\|_{H_h^s} \le \|u_h^{n-1,\ell} - u_h^{n-1}\|_{H_h^s} + \|u_h^{n-1} - u_h^n\|_{H_h^s}.$$

Then induction assumption (4.6) implies that  $\|u_h^{n-1,\ell} - u_h^{n-1}\|_{H_h^s} \le \tau$ , while the interpolation between (2.6) and (2.7) yields  $\|e_h^{n-1} - e_h^n\|_{H_h^s} \le C(\tau + h)^{2-s}$ . Therefore,

$$\|u_h^{n-1} - u_h^n\|_{H_h^s} \le \|u^{n-1} - u^n\|_{H_h^s} + \|e_h^{n-1} - e_h^n\|_{H_h^s} \le C\tau + C(\tau^{2-s} + h^{2-s}).$$

Substituting the two estimates above into (4.17), we have

$$\|e_h^{n,0}\|_{H^s_h} \le C(\tau^{2-s} + h^{2-s}). \tag{4.17}$$

Then, substituting (4.17) into the estimate of  $||e_h^{n,q}||_{H_h^s}$ , we obtain

$$\|e_h^{n,q}\|_{H_h^s} \le (1+C_2\tau)\|e_h^{n-1,\ell}\|_{H_h^s} + C_3\tau(C_3\tau)^{2^q-2}(\tau^{2-s}+h^{2-s})^{2^q}.$$
(4.18)

For sufficiently small  $\tau$  (independent of k and q), the above inequality and (4.6) imply  $||e_h^{n,q}||_{H_h^s} \le 1$ . This proves (4.8). Hence, choosing  $q = \ell$  in (4.18) yields

$$\|e_h^{n,\ell}\|_{H_h^s} \le (1+C_2\tau) \|e_h^{n-1,\ell}\|_{H_h^s} + C_3\tau(C_3\tau)^{2^\ell-2} (\tau^{2-s}+h^{2-s})^{2^\ell}.$$

Then, applying Gronwall's inequality, we obtain

$$\|e_h^{n,\ell}\|_{H^s_h} \le C(C_3\tau)^{2^\ell - 2}(\tau^{2-s} + h^{2-s})^{2^\ell}.$$
(4.19)

If  $\ell \ge 1$ , for sufficiently small  $\tau$  (independent of k and q), the inequality above implies  $||e_h^{n,\ell}||_{H_h^s} \le \tau^{2-s} + h^{2-s}$ . This proves (4.9) and therefore completes the mathematical induction on (4.6), as explained in (4.8)–(4.12). Hence, (4.6) holds for k = N and  $q = \ell$ , and correspondingly, (4.19) holds for all  $1 \le k \le N$ . This completes the proof of Theorem 2.1 (ii).

# 5 Numerical Tests

In this section, we present numerical results to illustrate the temporal and spatial convergence of the Newton iterative Crank–Nicolson method for the NLS equation.

To test the order of convergence, we consider the following initial-boundary value problem of the NLS equation with T = 1:

$$\begin{aligned} i\frac{\partial u}{\partial t} + \Delta u + |u|^2 u &= \frac{8}{125}(\sin(\pi x))^3(\sin(\pi y))^3 e^{-2\pi^2 it}, \quad (x, y) \in [0, 1] \times [0, 1], \quad t \in [0, T], \\ u &= 0, \quad (x, y) \in \partial\Omega, \quad t \in [0, T], \\ u|_{t=0} &= \frac{2}{5}\sin(\pi x)\sin(\pi y), \quad (x, y) \in [0, 1] \times [0, 1]. \end{aligned}$$

The exact solution of this problem is known to be

$$u(x, y, t) = \frac{2}{5}\sin(\pi x)\sin(\pi y)e^{-2\pi^2 i t}$$

h	$\ u(\cdot,T)-u_h^N\ _{L^2}$	order	
$\frac{1}{8}$	1.8054e-1		
$\frac{1}{16}$	4.6441e-2	1.96	
$\frac{1}{32}$	1.1726e-2	1.99	
$\frac{1}{64}$	2.9031e-3	2.00	<b>Table 1:</b> Spatial discretization errors of the numerical method, with $\tau = \frac{1}{1000}$ .
τ	$\ u(\cdot,T)-u_h^N\ _{L^2}$	order	
$\frac{1}{30}$	1.7987e-1		
$\frac{1}{60}$	4.8676e-2	1.89	
$\frac{1}{120}$	1.2149e-2	2.00	
$\frac{1}{240}$	3.0153e-3	2.01	<b>Table 2:</b> Temporal discretization errors of the numerical method, with $h = \frac{1}{4}$



**Figure 1:** Evolution of Newton iteration errors for m = 1, 2, 3, with  $h = \frac{1}{64}$  and  $\tau = 0.01$ .



**Figure 2:** Evolution of mass and energy for m = 1, 2, 3, with  $h = \frac{1}{64}$  and  $\tau = 0.01$ .

We solve the problem by the Newton iterative Crank-Nicolson method (2.2) with different spatial mesh sizes and temporal step sizes, and present the errors of the numerical solutions in Tables 1-2, where the Newton iterations stop when the tolerance error reaches  $10^{-10}$ . From the tables, we see second-order convergence in both space and time by neglecting the Newton iteration errors.

The evolution of the Newton iteration errors are presented in Figure 1 for m = 1, 2, 3 (number of iterations). This super-exponential convergence with respect to the number of iterations is consistent with the theoretical result proved in Theorem 2.1.

The evolution of mass and energy of the numerical solution is presented in Figure 2, which shows that the mass and energy are conserved with similar accuracy as the Newton iteration errors, and therefore can be neglected in comparison with the errors of the numerical solutions in Tables 1–2. These numerical results also agree with the theoretical analysis in Theorem 2.1.

# 6 Conclusion

We have proved that the Newton iteration for the nonlinearly implicit CN method for the NLS equation has double exponential convergence with respect to the number of iterations uniformly for all time levels, with limited regularity of the solution. We have also obtained an optimal-order error estimate for a practically implementable algorithm of implicit CN-FEM for the NLS equation, with incomplete Newton iterations and a simple quadrature for assembling the matrix from the cubic nonlinear term. The theoretical justification of such double exponential convergence of Newton iterations uniformly for all time levels is important for the justification of the effectiveness of the nonlinearly implicit structure-preserving algorithms for physical nonlinear evolution PDEs.

# **Appendix: Proof of Lemma 4.1**

(i) By using the definition in (4.1) and Hölder's inequality, we have

$$\begin{split} \|v_{h}\|_{H_{h}^{s}} &= \|(-\Delta_{h})^{\frac{s}{2}}v_{h}\|_{L^{2}} = \left(\sum_{j=1}^{J}|(v_{h},\phi_{j})|^{2-s}\lambda_{j}^{s}|(v_{h},\phi_{j})|^{s}\right)^{\frac{1}{2}} \\ &\leq \left(\sum_{j=1}^{J}|(v_{h},\phi_{j})|^{2}\right)^{\frac{2-s}{4}} \left(\sum_{j=1}^{J}\lambda_{j}^{2}|(v_{h},\phi_{j})|^{2}\right)^{\frac{s}{4}} = \|v_{h}\|_{L^{2}}^{\frac{2-s}{2}}\|\Delta_{h}v_{h}\|_{L^{2}}^{\frac{s}{2}} = \|v_{h}\|_{L^{2}}^{1-\frac{s}{2}}\|v_{h}\|_{L^{2}}^{\frac{s}{2}}. \end{split}$$

(ii) By the definition of the discrete Laplacian operator, we have

$$\begin{aligned} |(\Delta_h u_h, v)| &= |(\Delta_h u_h, P_h v)| = |(\nabla u_h, \nabla P_h v)| \le C \|\nabla u_h\|_{L^2} \|\nabla P_h v\|_{L^2} \\ &\le Ch^{-2} \|u_h\|_{L^2} \|P_h v\|_{L^2} \le Ch^{-2} \|u_h\|_{L^2} \|v\|_{L^2} \quad \text{for all } v \in L^2(\Omega), \end{aligned}$$

where the second to last inequality is the standard inverse inequality for finite element functions. Since the inequality above holds for all  $v \in L^2(\Omega)$ , it follows that  $\|\Delta_h u_h\|_{L^2} \leq Ch^{-2} \|u_h\|_{L^2}$ . By using this estimate and the interpolation inequality proved in Lemma 4.1 (i), we have

$$\|(-\Delta_h)^{\frac{s}{2}}v_h\|_{L^2} = \|v_h\|_{H^s_h} \le \|v_h\|_{L^2}^{\frac{2-s}{2}} \|v_h\|_{H^s_h}^{\frac{s}{2}} = \|v_h\|_{L^2}^{\frac{2-s}{2}} \|\Delta_h v_h\|_{L^2}^{\frac{s}{2}} \le Ch^{-s} \|v_h\|_{L^2}$$

Since  $(-\Delta_h)^{\frac{s_2}{2}} v_h = (-\Delta_h)^{\frac{s_2-s_1}{2}} (-\Delta_h)^{\frac{s_1}{2}} v_h$ , the inequality above implies that

$$\|(-\Delta_h)^{\frac{s_2}{2}}v_h\|_{L^2} \le Ch^{-(s_2-s_1)}\|(-\Delta_h)^{\frac{s_1}{2}}v_h\|_{L^2}$$

This proves the second result of Lemma 4.1.

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