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OPTIMAL ERROR BOUNDS ON THE EXPONENTIAL WAVE INTEGRATOR FOR THE NONLINEAR SCHRÖDINGER EQUATION WITH LOW REGULARITY POTENTIAL AND NONLINEARITY*

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Abstract. We establish optimal error bounds for the exponential wave integrator (EWI) applied to the nonlinear Schrödinger equation (NLSE) with L^∞-potential and/or locally Lipschitz nonlinearity under the assumption of H^2-solution of the NLSE. For the semidiscretization in time by the first-order Gautschi-type EWI, we prove an optimal L^2-error bound at $O(\tau)$ with $\tau > 0$ being the time step size, together with a uniform H^2-bound of the numerical solution. For the full-discretization scheme obtained by using the Fourier spectral method in space, we prove an optimal L^2-error bound at $O(\tau + h^2)$ without any coupling condition between τ and h, where $h > 0$ is the mesh size. In addition, for $W^{1,4}$-potential and a little stronger regularity of the nonlinearity, under the assumption of H^3-solution, we obtain an optimal H^1-error bound. Furthermore, when the potential is of low regularity but the nonlinearity is sufficiently smooth, we propose an extended Fourier pseudospectral method which has the same error bound as the Fourier spectral method, while its computational cost is similar to the standard Fourier pseudospectral method. Our new error bounds greatly improve the existing results for the NLSE with low regularity potential and/or nonlinearity. Extensive numerical results are reported to confirm our error estimates and to demonstrate that they are sharp.

Key words. nonlinear Schrödinger equation, exponential wave integrator, low regularity potential, low regularity nonlinearity, optimal error bound, extended Fourier pseudospectral method

MSC codes. 35Q55, 65M15, 65M70, 81Q05

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1. Introduction.

In this paper, we consider the following nonlinear Schrödinger equation (NLSE):

$$(1.1)\quad \begin{cases} i\partial_t\psi(\mathbf{x},t) = -\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + f(|\psi(\mathbf{x},t)|^2)\psi(\mathbf{x},t), & \mathbf{x}\in\Omega,\ t>0,\\ \psi(\mathbf{x},0) = \psi_0(\mathbf{x}), \quad \mathbf{x}\in\overline{\Omega}, \end{cases}$$

where t is time, $\mathbf{x} = (x_1, \cdots, x_d)^T \in \mathbb{R}^d$ $(d = 1, 2, 3)$ is the spatial coordinate, $\psi = \psi(\mathbf{x}, t)$ is a complex-valued wave function, and $\Omega = \Pi_{i=1}^d (a_i, b_i) \subset \mathbb{R}^d$ is a bounded domain equipped with periodic boundary condition. Here, $V = V(\mathbf{x}) : \Omega \to \mathbb{R}$ is a real-valued potential, and $f = f(\rho) : [0,\infty) \to \mathbb{R}$, with $\rho = |\psi|^2$ being the density, describes the nonlinear interaction. We assume that $V \in L^\infty(\Omega)$ and $f(|z|^2)z : \mathbb{C} \to \mathbb{C}$ is locally Lipschitz continuous, and thus both V and f may be of low regularity.

When $V(\mathbf{x}) = |\mathbf{x}|^2/2$ and $f(\rho) = \rho$, the NLSE (1.1) collapses to the NLSE with harmonic potential and cubic nonlinearity (or smooth potential and nonlinearity) or the Gross–Pitaevskii equation, which has been widely adopted for modeling and simulation in quantum mechanics, nonlinear optics, and Bose–Einstein condensation (BEC) [8, 28, 51]. For the smooth NLSE with sufficiently smooth initial data ψ_0, many accurate and efficient numerical methods have been proposed and analyzed in the past two decades, including the finite difference method [1, 9, 8, 6], the exponential

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wave integrator (EWI) [10, 33, 25], the time-splitting method [16, 20, 39, 27, 8, 6, 11], the finite element method [2, 49, 52, 53, 32], etc. Recently, many works have been done to analyze and design numerical methods for the cubic NLSE with low regularity initial data ψ_0 and with/without potential (see [27, 40, 42, 37, 41, 47, 44, 43, 5, 4] and references therein for other dispersive PDEs).

Arising from different physics applications, both V and f in (1.1) may be of low regularity. Typical examples of the low regularity L^∞-potential include, in many physical contexts, the square-well potential or step potential, both of which are discontinuous; in the study of BEC in different trapping shape, the power law potential $V(\mathbf{x}) = |\mathbf{x}|^\gamma$ ($\gamma > 0$) [46, 19]; and in the analysis of the Josephson effect and Anderson localization, some disorder potential [54, 48]. Low regularity nonlinearities, such as $f(\rho) = \rho^\sigma$ ($\sigma > 0$) or $f(\rho) = \rho \ln \rho$, are considered in, e.g., the Schrödinger–Poisson–Xα model [17, 21]; the Lee–Huang–Yang correction [38], which is adopted to model and simulate quantum droplets [35, 22, 7, 45]; and the mean-field model for the Bose–Fermi mixture [31, 23].

Most numerical methods for the cubic NLSE with smooth potential can be extended straightforwardly to solve the NLSE (1.1) with L^∞-potential and/or locally Lipschitz nonlinearity (different from the singular nonlinearity in [12, 13, 14, 15]). However, the performance of these methods is quite different from the smooth case, and the error analysis of them is a very subtle and challenging question. For (1.1) with power-type nonlinearity $f(\rho) = \rho^\sigma$ and sufficiently smooth potential, the Lie–Trotter time-splitting method is analyzed in [18, 26, 34] with reduced convergence order in L^2-norm when $\sigma < 1/2$ and in H^1-norm when $\sigma < 1$. The analysis of (1.1) with smooth nonlinearity and L^∞-potential seems more challenging, and the only known convergence result is the one obtained in [32] for the Crank–Nicolson Galerkin scheme, where first-order convergence in time and less-than-second-order convergence in space in L^2-norm are shown under strong assumptions on the exact solution (among others, $\partial_t \psi \in H^2$) and a coupling condition between the time step size τ and the mesh size h. Some low regularity integrators or resonance-based Fourier integrators are also proposed to reduce the regularity requirements on both V and ψ, while the regularity assumption on V is still stronger than H^1 [55, 4, 3], which still excludes the popular well potential and step potential widely adopted in the physics literature. The main difficulty comes from the low regularity of solution of the NLSE with L^∞-potential and locally Lipschitz nonlinearity, where only H^2 well-posedness is guaranteed [36, 24], and the low regularity of the potential and the nonlinearity, which causes order reduction in local truncation errors and prevents us from obtaining stability estimates in high-order Sobolev spaces H^α ($\alpha > d/2$) (see [18, 55, 32] for more detailed discussion). Besides, for the NLSE (1.1) with purely L^∞-potential, how to estimate the spatial discretization is also a challenging problem, and it turns out that it is very subtle and challenging to estimate the classical methods, including the finite difference method, the pseudospectral method, and the finite element method [32].

The main aim of this paper is to establish optimal error bounds for a first-order Gautschi-type EWI, also known as the exponential Euler scheme in the literature [33], applied to the NLSE with L^∞-potential and/or locally Lipschitz nonlinearity. Our main results are as follows:

(i) For the semidiscretization in time (EWI (2.2)), we prove an optimal L^2-error bound at $O(\tau)$, with $\tau > 0$ being the time step size, and a uniform H^2-bound of the numerical solution, under the assumption of H^2-solution of the NLSE (see (3.2) in Theorem 3.1).

(ii) For the full discretization of the EWI by using the Fourier spectral method for spatial derivatives (EWI-FS (2.11)), we prove an optimal L^2-error bound at $O(\tau + h^2)$ without any coupling condition between τ and the mesh size h (see (4.1) in Theorem 4.1).

(iii) For $W^{1,4}$-potential and a little more regular nonlinearity, under the assumption of H^3-solution, we obtain optimal H^1-error bounds for EWI and EWI-FS schemes. (see (3.3) in Theorem 3.1 and (4.2) in Theorem 4.1).

(iv) When the potential is of low regularity but the nonlinearity is sufficiently smooth, we propose an extended Fourier pseudospectral method for spatial discretization of the EWI, leading to the EWI-extended Fourier pseudospectral (EWI-EFP) scheme (2.13). For the EWI-EFP, we establish optimal error bounds in L^2- and H^1-norms under the same assumption on the potential and exact solution as the EWI-FS (see Corollary 4.4). However, the computational cost of EWI-EFP is similar to the standard Fourier pseudospectral discretization of the EWI.

Our error bounds greatly improve the previous results for the NLSE with low regularity potential and/or nonlinearity. In general, compared with the error estimates of classical EWIs [4] and time-splitting methods [18] in the literature, to obtain optimal error bounds, we reduce the differentiability requirement on the potential by two orders and on the nonlinearity by one order. Moreover, when $V \in L^\infty$ and f is smooth as considered in [32], compared with their results for the Crank–Nicolson Galerkin scheme, we improve the convergence order in L^2-norm to the optimal first order in time and the optimal second order in space, remove the coupling condition requirement between τ and h in [32], relax the regularity assumption on the exact solution such that it is theoretically guaranteed, and reduce the computational cost in practical implementation.

Here, we briefly explain why we can obtain the improved error bounds. In general, time-splitting methods and EWIs require weaker regularity on the exact solution to obtain the same order of convergence compared with finite difference methods. In practical computation, time-splitting methods tend to outperform EWIs when the solution is smooth, which requires that the potential and nonlinearity as well as the initial data are all smooth. The main reason is that time-splitting methods are usually a structure-preserving scheme; i.e., they preserve mass conservation, time symmetry, time-transverse invariance, and dispersion relation at the discretized level [6, 8]. On the contrary, when the NLSE (1.1) involves low regularity potential and/or nonlinearity, leading to a solution with low regularity, we find that the first-order Gautschi-type EWI offers two major advantages in obtaining optimal error bounds: (i) In obtaining local truncation errors, time-splitting methods need to apply the Laplacian Δ to the equation, while the EWI only needs to apply ∂_t to the equation, and thus the EWI needs a weaker regularity requirement on both potential and nonlinearity, and (ii) a smoothing operator is adopted in the EWI scheme to control the dispersion of high frequencies, and thus it helps to keep the numerical solution in H^2 at each time step, which makes it possible to obtain the stability estimates in high-order Sobolev spaces, while it is a challenging and subtle task to establish H^2-bounds of the numerical solution obtained from time-splitting methods.

The rest of the paper is organized as follows. In section 2, we present a semidiscretization in time by the first-order Gautschi-type EWI and then a full discretization by the Fourier spectral/extended pseudospectral method in space. Sections 3 and 4 are devoted to the error estimates of the semidiscretization scheme and the full-discretization scheme, respectively. Numerical results are reported in section 5 to confirm the error estimates. Finally, some conclusions are drawn in section 6. Throughout the paper, we adopt the standard Sobolev spaces as well as their corresponding norms and denote by C a generic positive constant independent of the mesh size h and time step size τ and by $C(\alpha)$ a generic positive constant depending only on the parameter α. The notation $A \lesssim B$ is used to represent that there exists a generic constant $C > 0$ such that $|A| \leq CB$.

2. The EWI Fourier spectral method. In this section, we introduce an EWI and its spatial discretization to solve the NLSE with low regularity potential and nonlinearity. For simplicity of the presentation and to avoid heavy notations, we only carry out the analysis in one dimension and take $\Omega = (a, b)$. The only dimension-sensitive estimates are Sobolev embeddings and the inverse inequality to control L^∞-norm by L^2-norm. In our analysis, we only use the embeddings which hold for one, two, and three dimensions, and for the inverse inequality, we clearly show how it depends on the space dimension. Thus, generalizations to two and three dimensions are straightforward, and the main results remain unchanged.

We define periodic Sobolev spaces as (see, e.g., [3, 29] for definition in phase space)

$$H^m_{\text{per}}(\Omega) := \{\phi \in H^m(\Omega) : \phi^{(k)}(a) = \phi^{(k)}(b),\ k = 0, \cdots, m-1\}, \quad m \geq 1.$$

2.1. Semidiscretization in time by an EWI. Choose a time step size $\tau > 0$, and denote time steps as $t_n = n\tau$ for $n = 0, 1, \cdots$. By Duhamel's formula, the exact solution of the NLSE (1.1) is given as

$$\begin{aligned} \psi(t_{n+1}) &= \psi(t_n + \tau) = e^{i\tau\Delta}\psi(t_n) \\ &\quad - i\int_0^\tau e^{i(\tau - s)\Delta}\left[V\psi(t_n + s) + f(|\psi(t_n + s)|^2)\psi(t_n + s)\right] \mathrm{d}s, \quad n \geq 0, \end{aligned} \tag{2.1}$$

where we abbreviate $\psi(x, t)$ as $\psi(t)$ for simplicity of notations when there is no confusion. Let $\psi^{[n]} := \psi^{[n]}(x)$ be the approximation of $\psi(x, t_n)$ for $n \geq 0$. Applying the approximation $\psi(t_n + s) \approx \psi(t_n)$ for the integrand in (2.1) and integrating out $e^{i(\tau - s)\Delta}$ exactly, we get a semidiscretization in time by the first-order Gautschi-type EWI as

$$\begin{aligned} &\psi^{[n+1]} = \Phi^\tau(\psi^{[n]}) := e^{i\tau\Delta}\psi^{[n]} - i\tau\varphi_1(i\tau\Delta)\left(V\psi^{[n]} + f(|\psi^{[n]}|^2)\psi^{[n]}\right), \quad n \geq 0, \\ &\psi^{[0]} = \psi_0, \end{aligned} \tag{2.2}$$

where φ_1 is an entire function defined as

$$\varphi_1(z) = \frac{e^z - 1}{z}, \qquad z \in \mathbb{C}.$$

The operator $\varphi_1(i\tau\Delta)$ is defined through its action in the Fourier space as

$$\begin{aligned} (\varphi_1(i\tau\Delta)v)(x) &= \sum_{l \in \mathbb{Z}} \varphi_1(-i\tau\mu_l^2)\widehat{v}_l e^{i\mu_l(x-a)} \\ &= \widehat{v}_0 + \sum_{l \in \mathbb{Z}\setminus\{0\}} \frac{1 - e^{-i\tau\mu_l^2}}{i\tau\mu_l^2}\widehat{v}_l e^{i\mu_l(x-a)}, \quad x \in \Omega, \end{aligned} \tag{2.3}$$

where $\mu_l = \frac{2\pi l}{b-a}$ for $l \in \mathbb{Z}$ and $\widehat{v}_l$ ($l \in \mathbb{Z}$) are the Fourier coefficients of the function $v \in L^2(\Omega)$ defined as

$$\widehat{v}_l = \frac{1}{b-a}\int_a^b v(x)e^{-i\mu_l(x-a)}\mathrm{d}x, \quad l \in \mathbb{Z}. \tag{2.4}$$

From (2.3), noting that $|1-e^{-i\theta}|\le 2$ for $\theta\in\mathbb{R}$, we see that

$$\left|(\widehat{\varphi_1(i\tau\Delta)}v)_l\right| \le \begin{cases} \frac{2}{\tau}\frac{|\widehat{v}_l|}{\mu_l^2}, & l\in\mathbb{Z}\setminus\{0\},\\ |\widehat{v}_0|, & l=0, \end{cases} \tag{2.5}$$

which implies that $\varphi_1(i\tau\Delta)v\in H^2_{\rm per}(\Omega)$ for all $v\in L^2(\Omega)$. Hence, Φ^τ is indeed a flow in $H^2_{\rm per}(\Omega)$ for any $V\in L^\infty(\Omega)$, making it possible to obtain uniform H^2-bound of the semidiscrete solution with some new analysis techniques we will introduce later.

In fact, the introduction of the smoothing function $\varphi_1(i\tau\Delta)$ in (2.2) is one of the major advantages of the EWI (2.2) over the time-splitting methods in terms of controlling the dispersion of high frequencies or resonance. With this smoothing function, one can show that the numerical solution is in H^2 at every time step. For comparison, based on the results in [18] for time-splitting methods applied to the NLSE with semismooth nonlinearity, the numerical solution of the semidiscretization is not in H^2 in general! The situation is even worse if there is purely L^∞-potential.

2.2. Full discretization by the Fourier spectral method. We further discretize the semidiscretization (2.2) in space by the Fourier spectral method to obtain a full-discretization scheme. Choose a mesh size $h=(b-a)/N$ with N being a positive integer, and denote grid points as

$$x_j=a+jh,\quad j=0,1,\cdots,N.$$

Define the index sets

$$\mathcal{T}_N=\left\{-\frac{N}{2},\cdots,\frac{N}{2}-1\right\},\quad \mathcal{T}_N^0=\{0,1,\cdots,N\},$$

and denote

$$X_N=\mathrm{span}\left\{e^{i\mu_l(x-a)}: l\in\mathcal{T}_N\right\}, \tag{2.6}$$

$$Y_N=\left\{v=(v_0,v_1,\cdots,v_N)^T\in\mathbb{C}^{N+1}: v_0=v_N\right\}. \tag{2.7}$$

Let $P_N: L^2(\Omega)\to X_N$ be the standard L^2-projection onto X_N and $I_N: Y_N\to X_N$ be the standard Fourier interpolation operator as

$$(P_N u)(x)=\sum_{l\in\mathcal{T}_N}\widehat{u}_l e^{i\mu_l(x-a)}, \tag{2.8}$$

$$(I_N v)(x)=\sum_{l\in\mathcal{T}_N}\widetilde{v}_l e^{i\mu_l(x-a)},\quad x\in\overline{\Omega}=[a,b], \tag{2.9}$$

where $u\in L^2(\Omega)$, $v\in Y_N$, $\widehat{u}_l$ $(l\in\mathbb{Z})$ are the Fourier coefficients of u defined in (2.4) and $\widetilde{v}_l$ $(l\in\mathcal{T}_N)$ are the discrete Fourier transform coefficients defined as

$$\widetilde{v}_l=\frac{1}{N}\sum_{j=0}^{N-1}v_j e^{-i\mu_l(x_j-a)},\quad l\in\mathcal{T}_N. \tag{2.10}$$

Let $\psi^n:=\psi^n(x)$ be the approximation of $\psi(x,t_n)$ for $n\ge 0$. Then an EWI-FS for the NLSE (1.1) is given as

$$\begin{aligned} &\psi^{n+1}=\Phi_h^\tau(\psi^n):=e^{i\tau\Delta}\psi^n-i\tau\varphi_1(i\tau\Delta)P_N\left(V\psi^n+f(|\psi^n|^2)\psi^n\right),\quad n\ge 0,\\ &\psi^0=P_N\psi_0. \end{aligned} \tag{2.11}$$

Note that $\psi^n \in X_N$ for $n \geq 0$, and we have

$$(2.12)\qquad \begin{aligned} &\widehat{(\psi^{n+1})}_l = e^{-i\tau\mu_l^2}\widehat{(\psi^n)}_l - i\tau\varphi_1(-i\tau\mu_l^2)\left(\widehat{(V\psi^n)}_l + \widehat{G(\psi^n)}_l\right), \quad n \geq 0,\\ &\widehat{(\psi^0)}_l = \widehat{(\psi_0)}_l, \quad l \in \mathcal{T}_N, \end{aligned}$$

where $G(\psi^n)(x) = G(\psi^n(x)) := f(|\psi^n(x)|^2)\psi^n(x)$ for $x \in \Omega$. We remark here that the EWI-FS is usually implemented by the Fourier pseudospectral method (see, e.g., [10, 29]) in practical computations. Of course, due to the low regularity of the potential and/or nonlinearity, it is very hard to establish error bounds for the full discretization by the Fourier pseudospectral method.

2.3. Full discretization by an extended Fourier pseudospectral method. In practice, the Fourier spectral method cannot be efficiently implemented. Here, we propose an extended Fourier pseudospectral method when the potential is of low regularity but the nonlinearity is sufficiently smooth; i.e., we adopt the Fourier spectral method to discretize the linear potential and use the Fourier pseudospectral method to discretize the nonlinearity. This full discretization has two advantages: (i) We can establish its optimal error bounds, and (ii) the computational cost of this discretization is similar to the standard Fourier pseudospectral method.

Let $\psi_j^{\langle n\rangle}$ be the numerical approximation of $\psi(x_j, t_n)$ for $j \in \mathcal{T}_N^0$ and $n \geq 0$, and denote $\psi^{\langle n\rangle} := (\psi_0^{\langle n\rangle}, \psi_1^{\langle n\rangle}, \cdots, \psi_N^{\langle n\rangle})^T \in Y_N$. Then an EWI-EFP method for the NLSE (1.1) reads

$$(2.13)\qquad \begin{aligned} \psi_j^{\langle n+1\rangle} &= \sum_{l\in\mathcal{T}_N} e^{-i\tau\mu_l^2}\widetilde{(\psi^{\langle n\rangle})}_l e^{i\mu_l(x_j-a)}\\ &\quad - i\tau\sum_{l\in\mathcal{T}_N}\varphi_1(-i\tau\mu_l^2)\left(\left(\widehat{VI_N\psi^{\langle n\rangle}}\right)_l + \widetilde{G(\psi^{\langle n\rangle})}_l\right)e^{i\mu_l(x_j-a)}, \quad n \geq 0,\\ \psi_j^{\langle 0\rangle} &= \psi_0(x_j), \quad j \in \mathcal{T}_N^0, \end{aligned}$$

where $G(\psi^{\langle n\rangle})_j = f(|\psi_j^{\langle n\rangle}|^2)\psi_j^{\langle n\rangle}$ for $j \in \mathcal{T}_N^0$. To compute the Fourier projection coefficients $\left(\widehat{VI_N\psi^{\langle n\rangle}}\right)_l$, we use an extended fast Fourier transform (FFT) as shown below. Note that $I_N\psi^{\langle n\rangle} \in X_N$ for all $n \geq 0$, and thus we have

$$(2.14)\qquad P_N(VI_N\psi^{\langle n\rangle}) = P_N\left(P_{2N}(V)I_N\psi^{\langle n\rangle}\right), \quad n \geq 0.$$

Moreover, since $P_{2N}(V)I_N\psi^{\langle n\rangle} \in X_{4N}$ and I_{4N} is an identity on X_{4N}, we have

$$P_{2N}(V)I_N\psi^{\langle n\rangle} = I_{4N}\left(P_{2N}(V)I_N\psi^{\langle n\rangle}\right), \quad n \geq 0,$$

which, plugged into (2.14), yields

$$(2.15)\qquad P_N\left(VI_N\psi^{\langle n\rangle}\right) = P_N I_{4N}\left(P_{2N}(V)I_N\psi^{\langle n\rangle}\right), \quad n \geq 0,$$

where $P_{2N}(V)$ can be precomputed numerically or analytically, and thus the right-hand side of (2.15) can be computed exactly and efficiently using the extended FFT, using FFT for $P_{2N}(V)I_N\psi^{\langle n\rangle}$ with length $4N$ instead of N. As a result, the memory cost is $O(4N)$, and the computational cost per time step is $O(4N\log(4N))$. Note that $\psi^{\langle n\rangle}$ $(n \geq 0)$ obtained from (2.13) satisfies

$$(2.16)\qquad \begin{aligned} &I_N\psi^{\langle n+1\rangle} = e^{i\tau\Delta}I_N\psi^{\langle n\rangle} - i\tau\varphi_1(i\tau\Delta)\left(P_N\left(VI_N\psi^{\langle n\rangle}\right) + I_N G(\psi^{\langle n\rangle})\right),\\ &I_N\psi^{\langle 0\rangle} = I_N\psi_0, \qquad n \geq 0. \end{aligned}$$

3. Optimal error bounds for the semidiscretization (2.2). In this section, we establish optimal error bounds in L^2-norm and H^1-norm for the semidiscretization (2.2) of the NLSE (1.1).

3.1. Main results. For the optimal L^2-norm error bound, we assume that the nonlinearity is locally Lipschitz continuous; i.e., there exists a fixed function $C_{\mathrm{Lip}}(\cdot):\mathbb{R}^+\to\mathbb{R}^+$ such that

$$\text{(A)}\quad |f(|z_1|^2)z_1 - f(|z_2|^2)z_2| \le C_{\mathrm{Lip}}(M_0)|z_1-z_2|,\quad z_j\in\mathbb{C},\ |z_j|\le M_0,\quad j=1,2.$$

Assumption (A) is satisfied by $f\in C^1((0,\infty))$ satisfying

$$|f(\rho)|+|\rho f'(\rho)|\le L(M_0),\quad 0<\rho\le M_0,$$

with $C_{\mathrm{Lip}}(M_0)\sim L(M_0)$ for $M_0>0$. In particular, (A) allows

(i) $f(\rho)=\lambda_1\rho^{\sigma_1}+\lambda_2\rho^{\sigma_2}$ for any $0<\sigma_1<\sigma_2$ and $\lambda_1,\lambda_2\in\mathbb{R}$ with $C_{\mathrm{Lip}}(M_0)\sim|\lambda_1|M_0^{\sigma_1}+|\lambda_2|M_0^{\sigma_2}$;

(ii) $f(\rho)=\lambda\rho^{\sigma}\ln\rho$ for any $\sigma>0$ and $\lambda\in\mathbb{R}$ with $C_{\mathrm{Lip}}(M_0)\sim 1+M_0^{\sigma}+M_0^{\sigma}|\ln M_0|$.

For the optimal H^1-norm error bound, we assume that

$$\text{(B)}\quad \|f(|v|^2)v-f(|w|^2)w\|_{H^1}\le C(\|v\|_{H^3},\|w\|_{H^2})\|v-w\|_{H^1},\ v\in H^3(\Omega), w\in H^2(\Omega).$$

Assumption (B) is satisfied by

(i) $f(\rho)=\lambda_1\rho^{\sigma_1}+\lambda_2\rho^{\sigma_2}$ for $\sigma_2>\sigma_1\ge 1/2$ and $\lambda_1,\lambda_2\in\mathbb{R}$ with $C(\cdot,\cdot)$ depending on $\|v\|_{H^3}$ and $\|w\|_{H^2}$;

(ii) $f(\rho)=\lambda\rho^{\sigma}\ln\rho$ for any $\sigma>1/2$ and $\lambda\in\mathbb{R}$ with $C(\cdot,\cdot)$ depending on $\|v\|_{H^3}$ and $\|w\|_{H^2}$.

We remark here that (B) implies (A) by taking $v(x)\equiv z_1$ and $w(x)\equiv z_2$ in (B). Nonlinearity satisfying (B) occurs in physical applications, including the Lee–Huang–Yang correction [38, 35, 22, 7, 45] and the Bose–Fermi mixture [31, 23] in one, two, and three dimensions and the Schrodinger–Poisson–Xα model [17, 21] in two dimensions. Assumption (A) covers, in addition to all those mentioned before, the case of the Schrodinger–Poisson–Xα model in three dimensions.

Let $T_{\max}$ be the maximal existing time of the solution of the NLSE (1.1), and take $0<T<T_{\max}$ be a fixed time. Define

$$M:=\max\left\{\|\psi\|_{L^\infty([0,T];H^2)},\|\psi\|_{L^\infty([0,T];L^\infty)},\|\partial_t\psi\|_{L^\infty([0,T];L^2)},\|V\|_{L^\infty}\right\}. \tag{3.1}$$

Let $\psi^{[n]}$ be the numerical approximation obtained by the EWI (2.2). Then we have the following.

THEOREM 3.1. *Under the assumptions that $V\in L^\infty(\Omega)$, f satisfies Assumption* (A)*, and the exact solution $\psi\in C([0,T];H^2_{\mathrm{per}}(\Omega))\cap C^1([0,T];L^2(\Omega))$, there exists $\tau_0>0$ depending on M and T and sufficiently small such that for any $0<\tau<\tau_0$, we have $\psi^{[n]}\in H^2_{\mathrm{per}}(\Omega)$ for $0\le n\le T/\tau$ and*

$$\begin{aligned}&\|\psi(\cdot,t_n)-\psi^{[n]}\|_{L^2}\lesssim\tau,\quad \|\psi^{[n]}\|_{H^2}\le C(M),\\ &\|\psi(\cdot,t_n)-\psi^{[n]}\|_{H^1}\lesssim\sqrt{\tau},\qquad 0\le n\le T/\tau.\end{aligned} \tag{3.2}$$

Moreover, if $V\in W^{1,4}(\Omega)\cap H^1_{\mathrm{per}}(\Omega)$, f satisfies (B)*, and $\psi\in C([0,T];H^3_{\mathrm{per}}(\Omega))\cap C^1([0,T];H^1(\Omega))$, then we have, for $0<\tau<\tau_0$,*

$$\|\psi(\cdot,t_n)-\psi^{[n]}\|_{H^1}\lesssim\tau,\qquad 0\le n\le T/\tau. \tag{3.3}$$

Remark 3.2. According to the known regularity results (see, e.g., Corollary 4.8.6 of [24]), under the assumptions that $V \in L^\infty(\Omega)$ and (A), it can be expected that $\psi \in C([0,T]; H^2_{\text{per}}(\Omega)) \cap C^1([0,T]; L^2(\Omega))$ for some $0 < T < T_{\max}$ if $\psi_0 \in H^2_{\text{per}}(\Omega)$.

Remark 3.3. Recall that, for the time-splitting methods analyzed in [18] with $f(\rho) = \rho^\sigma$, the optimal L^2-norm error bound in time is obtained for $V \in H^2(\Omega)$ and $\sigma \geq 1/2$ and that the optimal H^1-norm error bound in time is obtained for $V \in H^3(\Omega)$ and $\sigma \geq 1$. Hence, our results greatly relax the regularity requirements on both potential and nonlinearity.

In the following, we shall prove Theorem 3.1. We start with the proof of (3.2), and the proof of (3.3) can be obtained by the standard Lady Windermere's fan argument with the established uniform H^2-bound of the semidiscretization solution in (3.2).

In the rest of this section, we assume that $V \in L^\infty(\Omega)$, f satisfies Assumption (A) and $\psi \in C([0,T]; H^2_{\text{per}}(\Omega)) \cap C^1([0,T]; L^2(\Omega))$.

3.2. Local truncation error. We define an operator $B : L^\infty(\Omega) \to L^\infty(\Omega)$ as

$$B(v) = Vv + f(|v|^2)v, \quad v \in L^\infty(\Omega), \tag{3.4}$$

and define a constant $C_L(\cdot) := \|V\|_{L^\infty} + C_{\text{Lip}}(\cdot)$ with $C_{\text{Lip}}(\cdot)$ given by Assumption (A). For the operator B, we have the following.

LEMMA 3.4. *Let $v, w \in L^\infty(\Omega)$ satisfying $\|v\|_{L^\infty} \leq M_0$ and $\|w\|_{L^\infty} \leq M_0$. Then*

$$\|B(v) - B(w)\|_{L^2} \leq C_L(M_0)\|v - w\|_{L^2}. \tag{3.5}$$

Proof. Recalling (3.4) and (A), we have

$$\begin{aligned}\|B(v) - B(w)\|_{L^2} &= \|V(v-w) + f(|v|^2)v - f(|w|^2)w\|_{L^2}\\ &\leq \|V\|_{L^\infty}\|v-w\|_{L^2} + C_{\text{Lip}}(M_0)\|v-w\|_{L^2}\\ &= C_L(M_0)\|v-w\|_{L^2},\end{aligned}$$

which completes the proof. ∎

LEMMA 3.5. *For $0 \leq n \leq T/\tau - 1$, define*

$$g_n(t) := B(\psi(t_n + t)) - B(\psi(t_n)), \qquad 0 \leq t \leq \tau. \tag{3.6}$$

Then $g_n \in C([0,\tau]; L^2(\Omega)) \cap W^{1,\infty}([0,\tau]; L^2(\Omega))$ satisfies

$$\|g_n\|_{L^\infty([0,\tau];L^2)} \leq C_L(M)M\tau, \tag{3.7}$$

$$\|\partial_t g_n\|_{L^\infty([0,\tau];L^2)} \leq C_L(M)M. \tag{3.8}$$

Proof. Using Lemma 3.4, we have, for $0 \leq s < t \leq \tau$,

$$\begin{aligned}\|g_n(t) - g_n(s)\|_{L^2} &= \|B(\psi(t_n+t)) - B(\psi(t_n+s))\|_{L^2}\\ &\leq C_L(M)\|\psi(t_n+t) - \psi(t_n+s)\|_{L^2}\\ &\leq C_L(M)\int_s^t \|\partial_t\psi(t_n+\sigma)\|_{L^2}\mathrm{d}\sigma.\end{aligned} \tag{3.9}$$

From (3.9), recalling (A), one has $g_n \in C([0,\tau]; L^2(\Omega))$, and, by using Lemma 3.4 again, one has

$$\begin{aligned}\|g_n(t)\|_{L^2} &= \|B(\psi(t_n+t)) - B(\psi(t_n))\|_{L^2} \leq C_L(M)\|\psi(t_n+t) - \psi(t_n)\|_{L^2}\\ &\leq \tau C_L(M)\|\partial_t\psi\|_{L^\infty([t_n,t_n+\tau];L^2)} \leq C_L(M)M\tau,\end{aligned}$$

which proves (3.7). Noting (3.9), from the standard theory of Sobolev spaces (see, e.g., Proposition 1.3.12 of [24]), we have $g_n \in W^{1,\infty}([0,T];L^2(\Omega))$, and by letting $\varphi(\sigma) = C_L(M)\|\partial_t\psi(t_n+\sigma)\|_{L^2}$ for $0 \le \sigma \le \tau$,

$$\|\partial_t g_n\|_{L^\infty([0,\tau];L^2)} \le \|\varphi\|_{L^\infty([0,\tau])} \le C_L(M)M,$$

which concludes the proof. ◻

Similar to Lemma 4.8.5 in [24], we have the following.

LEMMA 3.6. *Assume that* $\tau > 0$ *and* $g \in C([0,\tau];L^2(\Omega)) \cap W^{1,1}([0,\tau];L^2(\Omega))$. *If*

$$w(t) = -i\int_0^t e^{i(t-s)\Delta} g(s)\mathrm{d}s, \quad t \in [0,\tau], \tag{3.10}$$

then we have

$$\|\Delta w\|_{L^\infty([0,\tau];L^2)} \le \|g\|_{L^\infty([0,\tau];L^2)} + \|g(0)\|_{L^2} + \|\partial_t g\|_{L^1([0,\tau];L^2)}. \tag{3.11}$$

Proof. Taking the time derivative on both sides of (3.10) and noting that $g \in W^{1,1}([0,\tau];L^2(\Omega))$, we have, for $0 \le t \le \tau$,

$$\begin{aligned}\partial_t w(t) = -i\frac{d}{dt}\int_0^t e^{is\Delta} g(t-s)\mathrm{d}s &= -ie^{it\Delta}g(0) - i\int_0^t e^{is\Delta}\partial_t g(t-s)\mathrm{d}s \\ &= -ie^{it\Delta}g(0) - i\int_0^t e^{i(t-s)\Delta}\partial_t g(s)\mathrm{d}s. \end{aligned}\tag{3.12}$$

From (3.12), using the isometry property of $e^{it\Delta}$, we have

$$\|\partial_t w(t)\|_{L^2} \le \|g(0)\|_{L^2} + \|\partial_t g\|_{L^1([0,\tau];L^2)}, \quad 0 \le t \le \tau. \tag{3.13}$$

Note that w defined in (3.10) satisfies the equation

$$i\partial_t w = -\Delta w + g, \quad 0 \le t \le \tau,$$

which implies, by using (3.13), that

$$\|\Delta w(t)\|_{L^2} \le \|\partial_t w(t)\|_{L^2} + \|g(t)\|_{L^2} \le \|g(0)\|_{L^2} + \|\partial_t g\|_{L^1([0,\tau];L^2)} + \|g(t)\|_{L^2}, \tag{3.14}$$

and the conclusion follows from taking the supremum of t on both sides. ◻

Now we can obtain the following local truncation error estimates.

PROPOSITION 3.7 (local truncation error). *For* $0 \le n \le T/\tau - 1$, *we have*

$$\|\psi(t_{n+1}) - \Phi^\tau(\psi(t_n))\|_{H^\alpha} \le C(M)\tau^{2-\alpha/2}, \quad 0 \le \alpha \le 2, \tag{3.15}$$

where $C(M) \sim C_L(M)M$.

Proof. Recalling (2.1) and (3.4), we have

$$\psi(t_{n+1}) = e^{i\tau\Delta}\psi(t_n) - i\int_0^\tau e^{i(\tau-s)\Delta}B(\psi(t_n+s))\mathrm{d}s, \quad 0 \le n \le T/\tau - 1. \tag{3.16}$$

By the construction of the EWI (2.2) and (3.4), we have

$$\Phi^\tau(\psi(t_n)) = e^{i\tau\Delta}\psi(t_n) - i\int_0^\tau e^{i(\tau-s)\Delta}B(\psi(t_n))\mathrm{d}s, \quad 0 \le n \le T/\tau - 1. \tag{3.17}$$

Subtracting (3.17) from (3.16) and recalling (3.6), we have

$$
\begin{aligned}
\psi(t_{n+1}) - \Phi^\tau(\psi(t_n)) &= -i\int_0^\tau e^{i(\tau-s)\Delta}(B(\psi(t_n+s)) - B(\psi(t_n)))\mathrm{d}s \\
&= -i\int_0^\tau e^{i(\tau-s)\Delta} g_n(s)\mathrm{d}s, \quad 0\le n\le T/\tau - 1. \qquad (3.18)
\end{aligned}
$$

From (3.18), using (3.7), one gets

$$
\|\psi(t_{n+1}) - \Phi^\tau(\psi(t_n))\|_{L^2} \le \int_0^\tau \|g_n(s)\|_{L^2}\mathrm{d}s \le C_L(M)M\tau^2, \qquad (3.19)
$$

which proves (3.15) for $\alpha = 0$. Then we shall establish (3.15) with $\alpha = 2$, and (3.15) with $0 < \alpha < 2$ will follow from the Gagliardo–Nirenberg interpolation inequalities. Applying Lemma 3.6 to (3.18), using (3.8), and noting that $g_n(0) = 0$, we have

$$
\begin{aligned}
&\|\Delta(\psi(t_{n+1}) - \Phi^\tau(\psi(t_n)))\|_{L^2} \\
&\quad \le \|g_n\|_{L^\infty([0,\tau];L^2)} + \|g_n(0)\|_{L^2} + \|\partial_t g_n\|_{L^1([0,\tau];L^2)} \\
&\quad \le C_L(M)M\tau + \tau\|\partial_t g_n\|_{L^\infty([0,\tau];L^2)} \le 2C_L(M)M\tau, \qquad (3.20)
\end{aligned}
$$

which, combined with (3.19), implies that

$$
\|\psi(t_{n+1}) - \Phi^\tau(\psi(t_n))\|_{H^2} \le C(M)\tau, \quad 0\le n\le T/\tau - 1, \qquad (3.21)
$$

where $C(M) \sim C_L(M)M$. The conclusion follows from (3.19) and (3.21) and the Gagliardo–Nirenberg interpolation inequalities. ∎

Remark 3.8. In (3.19), the optimal local truncation error in L^2-norm is obtained with the boundedness of $\|\partial_t B(\psi(t))\|_{L^2}$ (recalling Lemma 3.5) instead of $\|\Delta B(\psi(t))\|_{L^2}$ in the time-splitting methods [18].

3.3. L^∞-conditional stability estimate of (2.2). We shall establish the L^∞-conditional stability estimate of the numerical flow (2.2). The key is the following lemma, which can be understood as the smoothing effect of the operator $\varphi_1(i\tau\Delta)$, which is another major advantage of the EWI (2.2).

LEMMA 3.9. *Let $v, w \in L^2(\Omega)$ and $0 < \tau < 1$. Then we have*

$$
\|\varphi_1(i\tau\Delta)v - \varphi_1(i\tau\Delta)w\|_{H^\alpha} \le C(\alpha)\tau^{-\alpha/2}\|v - w\|_{L^2}, \quad 0\le\alpha\le 2,
$$

where $C(\alpha) = 2^{\frac{\alpha}{2}}(1+\mu_1^{-2})^{\frac{\alpha}{2}}$.

Proof. It suffices to show that for any $v \in L^2(\Omega)$,

$$
\|\varphi_1(i\tau\Delta)v\|_{H^\alpha} \le C(\alpha)\tau^{-\alpha/2}\|v\|_{L^2}, \quad 0\le\alpha\le 2. \qquad (3.22)
$$

Note that

$$
|e^{i\theta} - 1| \le 2^\gamma\theta^{1-\gamma}, \quad \theta\in\mathbb{R}, \quad 0\le\gamma\le 1. \qquad (3.23)
$$

By Parseval's identity, using (3.23) with $\gamma = \alpha/2$ and recalling (2.3), we have

$$\begin{aligned}\frac{1}{b-a}\|\varphi_1(i\tau\Delta)v\|_{H^\alpha}^2 &= \sum_{l\in\mathbb{Z}}(1+\mu_l^2)^\alpha|\varphi_1(-i\tau\mu_l^2)|^2|\widehat{v}_l|^2\\ &= |\widehat{v}_0|^2 + \sum_{l\in\mathbb{Z}\setminus\{0\}}(1+\mu_l^2)^\alpha\left|\frac{e^{i\tau\mu_l^2}-1}{\tau\mu_l^2}\right|^2|\widehat{v}_l|^2\\ &\le |\widehat{v}_0|^2 + 2^\alpha\sum_{l\in\mathbb{Z}\setminus\{0\}}(1+\mu_l^2)^\alpha\left(\tau\mu_l^2\right)^{-\alpha}|\widehat{v}_l|^2\\ &= |\widehat{v}_0|^2 + 2^\alpha\tau^{-\alpha}\sum_{l\in\mathbb{Z}\setminus\{0\}}\left(\frac{1+\mu_l^2}{\mu_l^2}\right)^\alpha|\widehat{v}_l|^2\\ &\le |\widehat{v}_0|^2 + C(\alpha)^2\tau^{-\alpha}\sum_{l\in\mathbb{Z}\setminus\{0\}}|\widehat{v}_l|^2\\ &\le C(\alpha)^2\tau^{-\alpha}\sum_{l\in\mathbb{Z}}|\widehat{v}_l|^2 = C(\alpha)^2\tau^{-\alpha}\frac{1}{b-a}\|v\|_{L^2}^2,\end{aligned}$$

which proves (3.22) and concludes the proof. ∎

With Lemma 3.9, we are able to obtain the stability estimate of the numerical flow (2.2) up to H^2 without additional regularity on the potential and nonlinearity.

PROPOSITION 3.10 (stability estimate). *Let $v, w \in H^2_{\mathrm{per}}(\Omega)$ such that $\|v\|_{L^\infty} \le M_0$ and $\|w\|_{L^\infty} \le M_0$, and let $0 < \tau < 1$. Then we have, for $0 \le \alpha \le 2$,*

$$\|\Phi^\tau(v) - \Phi^\tau(w)\|_{H^\alpha} \le \|v-w\|_{H^\alpha} + C(M_0)\tau^{1-\alpha/2}\|v-w\|_{L^2}.$$

Proof. Recalling (2.2) and 3.4, we have

$$\Phi^\tau(u) = e^{i\tau\Delta}u - i\tau\varphi_1(i\tau\Delta)B(u), \qquad u \in H^2_{\mathrm{per}}(\Omega). \tag{3.24}$$

Taking $u = v$ and $u = w$ in (3.24), subtracting one from the other, and using the isometry property of $e^{it\Delta}$ and Lemmas 3.9 and 3.4, we have

$$\begin{aligned}\|\Phi^\tau(v) - \Phi^\tau(w)\|_{H^\alpha} &\le \|e^{i\tau\Delta}v - e^{i\tau\Delta}w\|_{H^\alpha} + \tau\|\varphi_1(i\tau\Delta)(B(v)-B(w))\|_{H^\alpha}\\ &\le \|v-w\|_{H^\alpha} + C(\alpha)\tau^{1-\alpha/2}\|B(v)-B(w)\|_{L^2}\\ &\le \|v-w\|_{H^\alpha} + C(\alpha)\tau^{1-\alpha/2}C_L(M_0)\|v-w\|_{L^2}.\end{aligned}$$

The conclusion follows from letting $C(M_0) = C(\alpha)C_L(M_0)$ with $\alpha = 2$. ∎

3.4. Proof of the optimal L^2-error bound (3.2). With the local truncation error estimate in Proposition 3.7 and the L^∞-conditional stability estimate in Proposition 3.10, we can prove (3.2) by mathematical induction.

Proof of (3.2) *in Theorem* 3.1. Define the error function $e^{[n]} := \psi(t_n) - \psi^{[n]}$ for $0 \le n \le T/\tau$. For $0 \le n \le T/\tau - 1$ and $0 \le \alpha \le 2$, we have

$$\begin{aligned}\|e^{[n+1]}\|_{H^\alpha} &= \|\psi(t_{n+1}) - \psi^{[n+1]}\|_{H^\alpha} = \|\psi(t_{n+1}) - \Phi^\tau(\psi^{[n]})\|_{H^\alpha}\\ &\le \|\psi(t_{n+1}) - \Phi^\tau(\psi(t_n))\|_{H^\alpha} + \|\Phi^\tau(\psi(t_n)) - \Phi^\tau(\psi^{[n]})\|_{H^\alpha}.\end{aligned} \tag{3.25}$$

In the following, we first establish the error bounds in L^2-norm and $H^{\frac{7}{4}}$-norm together by the mathematical induction, which, in particular, yields the uniform L^∞-bound of $\psi^{[n]}$. With the uniform L^∞-bound, we can obtain the uniform H^2-bound of $\psi^{[n]}$. The error bound in H^1-norm will follow from the error bound in L^2-norm and the uniform H^2-bound by using the standard interpolation inequalities.

Let $C_0 := \max\{C(1+M), M, 1\} \geq 1$ with M given in (3.1) and $C(\cdot)$ defined in Proposition 3.10, and let $C_1 := C(M)$ with $C(\cdot)$ defined in Proposition 3.7. Let $0 < \tau_0 < 1$ be chosen such that

$$2C_0 T e^{C_0 T} C_1 \tau_0^{\frac{1}{8}} \leq 1/c, \tag{3.26}$$

where c is the constant given by the Sobolev embedding $H^{\frac{7}{4}} \hookrightarrow L^\infty$. We are going to prove that when $0 < \tau < \tau_0$, we have, for $0 \leq n \leq T/\tau$,

$$\|e^{[n]}\|_{L^2} \leq e^{C_0 T} C_1 \tau, \quad \|e^{[n]}\|_{H^{\frac{7}{4}}} \leq 2C_0 T e^{C_0 T} C_1 \tau^{\frac{1}{8}}. \tag{3.27}$$

We shall prove (3.27) by mathematical induction. When $n = 0$, $e^{[n]} = \psi^{[0]} - \psi_0 = 0$, and (3.27) holds trivially. We assume that (3.27) holds for $0 \leq n \leq m \leq T/\tau - 1$. Under this assumption, we have, by Sobolev embedding, $\tau < \tau_0$, and (3.26),

$$\|\psi^{[n]}\|_{L^\infty} \leq \|\psi(t_n)\|_{L^\infty} + \|e^{[n]}\|_{L^\infty} \leq M + c\|e^{[n]}\|_{H^{\frac{7}{4}}} \leq M + 1, \quad 0 \leq n \leq m. \tag{3.28}$$

Taking $\alpha = 0$ and $\alpha = 7/4$ in (3.25), we have, for $0 \leq n \leq T/\tau - 1$,

$$\|e^{[n+1]}\|_{L^2} \leq \|\psi(t_{n+1}) - \Phi^\tau(\psi(t_n))\|_{L^2} + \|\Phi^\tau(\psi(t_n)) - \Phi^\tau(\psi^{[n]})\|_{L^2}, \tag{3.29}$$

$$\|e^{[n+1]}\|_{H^{\frac{7}{4}}} \leq \|\psi(t_{n+1}) - \Phi^\tau(\psi(t_n))\|_{H^{\frac{7}{4}}} + \|\Phi^\tau(\psi(t_n)) - \Phi^\tau(\psi^{[n]})\|_{H^{\frac{7}{4}}}. \tag{3.30}$$

Using Propositions 3.7 and 3.10 with $\alpha = 0$ and $\alpha = 7/4$ for (3.29) and (3.30), respectively, and noting (3.28), we have, for $0 \leq n \leq m$,

$$\|e^{[n+1]}\|_{L^2} \leq (1 + C_0\tau)\|e^{[n]}\|_{L^2} + C_1\tau^2, \tag{3.31}$$

$$\|e^{[n+1]}\|_{H^{\frac{7}{4}}} \leq \|e^{[n]}\|_{H^{\frac{7}{4}}} + C_0\tau^{\frac{1}{8}}\|e^{[n]}\|_{L^2} + C_1\tau^{1+\frac{1}{8}}. \tag{3.32}$$

From (3.31), using the standard discrete Gronwall's inequality, we have

$$\|e^{[m+1]}\|_{L^2} \leq e^{C_0 T} C_1 \tau. \tag{3.33}$$

From (3.32), using the assumption that (3.27) holds for $0 \leq n \leq m$, we have

$$\|e^{[n+1]}\|_{H^{\frac{7}{4}}} \leq \|e^{[n]}\|_{H^{\frac{7}{4}}} + C_0\tau^{\frac{1}{8}} e^{C_0 T} C_1 \tau + C_1 \tau^{1+\frac{1}{8}}, \quad 0 \leq n \leq m. \tag{3.34}$$

Summing over n from 0 to m in (3.34), noting that $e^{[0]} = 0$ and $C_0 \geq 1$, we obtain

$$\begin{aligned} \|e^{[m+1]}\|_{H^{\frac{7}{4}}} &\leq C_0 \tau^{\frac{1}{8}} e^{C_0 T} C_1 m\tau + C_1 m \tau^{1+\frac{1}{8}} \\ &\leq C_0 T e^{C_0 T} C_1 \tau^{\frac{1}{8}} + C_1 T \tau^{\frac{1}{8}} \\ &\leq 2C_0 T e^{C_0 T} C_1 \tau^{\frac{1}{8}}. \end{aligned} \tag{3.35}$$

Combining (3.33) and (3.35), we prove (3.27) for $n = m+1$ and thus for all $0 \leq n \leq T/\tau$ by mathematical induction.

Then we prove the uniform H^2 bound of $\psi^{[n]}$. We first note that (3.28) now holds for any $0 \leq n \leq T/\tau$. Taking $\alpha = 2$ in (3.25), using Propositions 3.10 and 3.7 with $\alpha = 2$ and (3.27), we have, for $0 \leq n \leq T/\tau - 1$,

$$\begin{aligned} \|e^{[n+1]}\|_{H^2} &\leq \|\Psi^\tau(\psi(t_n)) - \Phi^\tau(\psi(t_n))\|_{H^2} + \|\Phi^\tau(\psi(t_n)) - \Phi^\tau(\psi^{[n]})\|_{H^2} \\ &\leq \|e^{[n]}\|_{H^2} + C_0\|e^{[n]}\|_{L^2} + C_1\tau \\ &\leq \|e^{[n]}\|_{H^2} + C_0 e^{C_0 T} C_1 \tau + C_1 \tau. \end{aligned} \tag{3.36}$$

Summing (3.36) from 0 to $n-1$, we obtain

$$\|e^{[n]}\|_{H^2} \le C_0 e^{C_0 T} C_1 n\tau + C_1 n\tau \le 2C_0 e^{C_0 T} C_1 T, \quad 0 \le n \le T/\tau. \tag{3.37}$$

Finally, combining (3.27) and (3.37) and using the interpolation inequality for the H^1-error bound, we prove (3.2). ∎

3.5. Proof of the optimal H^1-error bound (3.3). To prove (3.3), we assume that $V \in W^{1,4}(\Omega) \cap H^1_{\rm per}(\Omega)$, f satisfies Assumption (B), $\psi \in C([0,T]; H^3_{\rm per}(\Omega)) \cap C^1([0,T]; H^1(\Omega))$, and $0 < \tau < \tau_0$ with τ_0 given in (3.26). Under the assumptions above, $B : H^2_{\rm per}(\Omega) \to H^1_{\rm per}(\Omega)$ satisfies

$$\|B(v) - B(w)\|_{H^1} \le C(\|v\|_{H^3}, \|w\|_{H^2}, \|V\|_{W^{1,4}(\Omega)})\|v - w\|_{H^1}, \quad v, w \in H^2_{\rm per}(\Omega). \tag{3.38}$$

Proof of (3.3) *in Theorem* 3.1. From (3.18), using (3.38) and the isometry property of $e^{it\Delta}$ and noting that $\psi \in C^1([0,T]; H^1(\Omega))$, we have, for $0 \le n \le T/\tau - 1$,

$$\|\psi(t_{n+1}) - \Phi^\tau(\psi(t_n))\|_{H^1} \le \int_0^\tau \|B(\psi(t_n + s)) - B(\psi(t_n))\|_{H^1} {\rm d}s \lesssim \tau^2. \tag{3.39}$$

Noting that $|\varphi_1(i\theta)| \le 1$ for $\theta \in \mathbb{R}$, we have

$$\|\varphi_1(i\tau\Delta)v\|_{H^1} \le \|v\|_{H^1}, \quad v \in H^1_{\rm per}(\Omega), \tag{3.40}$$

which implies, by recalling (3.24) and using (3.38) again, that

$$\begin{aligned} \|\Phi^\tau(\psi(t_n)) - \Phi^\tau(\psi^{[n]})\|_{H^1} &\le \|\psi(t_n) - \psi^{[n]}\|_{H^1} + \tau\|B(\psi(t_n)) - B(\psi^{[n]})\|_{H^1} \\ &\le (1 + C\tau)\|\psi(t_n) - \psi^{[n]}\|_{H^1}, \quad 0 \le n \le T/\tau - 1, \end{aligned} \tag{3.41}$$

where C depends on $\|V\|_{W^{1,4}}$, $\|\psi(t_n)\|_{H^3}$, and $\|\psi^{[n]}\|_{H^2}$, which are uniformly bounded. Then (3.3) follows from (3.39) and (3.41) by the standard Lady Windermere's fan argument. ∎

4. Optimal error bounds for the full discretization (2.11). In this section, we establish optimal error bounds in L^2- and H^1-norms for the full-discretization scheme EWI-FS (2.11) and generalize them to the EWI-EFP scheme (2.13).

4.1. Main results. For ψ^n $(0 \le n \le T/\tau)$ obtained by the EWI-FS scheme (2.11), we have the following.

THEOREM 4.1. *Assuming that $V \in L^\infty(\Omega)$, f satisfies Assumption* (A)*, and the exact solution $\psi \in C([0,T]; H^2_{\rm per}(\Omega)) \cap C^1([0,T]; L^2(\Omega))$, there exists $\tau_0 > 0$ and $h_0 > 0$ depending on M and T and sufficiently small such that for any $0 < \tau < \tau_0$ and $0 < h < h_0$, we have*

$$\begin{aligned} &\|\psi(\cdot, t_n) - \psi^n\|_{L^2} \lesssim \tau + h^2, \quad \|\psi^n\|_{H^2} \le C(M), \\ &\|\psi(\cdot, t_n) - \psi^n\|_{H^1} \lesssim \sqrt{\tau} + h, \qquad 0 \le n \le T/\tau. \end{aligned} \tag{4.1}$$

Moreover, if $V \in W^{1,4}(\Omega) \cap H^1_{\rm per}(\Omega)$, f satisfies (B)*, and $\psi \in C([0,T]; H^3_{\rm per}(\Omega)) \cap C^1([0,T]; H^1(\Omega))$, then we have, for $0 < \tau < \tau_0$ and $0 < h < h_0$,*

$$\|\psi(\cdot, t_n) - \psi^n\|_{L^2} \lesssim \tau + h^3, \quad \|\psi(\cdot, t_n) - \psi^n\|_{H^1} \lesssim \tau + h^2, \qquad 0 \le n \le T/\tau. \tag{4.2}$$

Remark 4.2. Thanks to the strong H^2-control of the semidiscretization solution in (3.2), there is no coupling condition between τ and h for all $1 \leq d \leq 3$ in Theorem 4.1.

In the following, we shall prove Theorem 4.1. We use different methods to prove (4.1) and (4.2). For the L^2-norm error bound (4.1), we compare the full-discretization solution ψ^n with the semidiscretization solution $\psi^{[n]}$ to avoid the coupling condition between τ and h when using the inverse inequalities. Then, for the H^1-norm error bound (4.2), we can directly compare the full-discretization solution with the exact solution since we already have control of the full-discretization solution in H^2-norm.

In the rest of this section, we assume that $V \in L^\infty(\Omega)$, f satisfies Assumption (A), and $\psi \in C([0,T]; H^2_{\text{per}}(\Omega)) \cap C^1([0,T]; L^2(\Omega))$.

4.2. Proof of the optimal L^2-error bound (4.1). We start with the error estimates between the semidiscretization solution $\psi^{[n]}$ and the full-discretization solution ψ^n.

PROPOSITION 4.3. *Let $0 < \tau < \tau_0$ with τ_0 given in Theorem* 3.1. *Then there exists h_0 depending on M and T and small enough such that for $0 < h < h_0$, we have*

$$\|P_N \psi^{[n]} - \psi^n\|_{L^2} \leq C(M,T)h^2, \quad 0 \leq n \leq T/\tau.$$

Proof. Define the error function $e^n := P_N \psi^{[n]} - \psi^n$ for $0 \leq n \leq T/\tau$. Then $e^0 = P_N \psi^{[0]} - \psi^0 = 0$. Applying P_N on both sides of (2.2), noting that P_N commutes with $e^{i\tau\Delta}$ and $\varphi_1(i\tau\Delta)$, and recalling (3.4), we have

$$P_N \psi^{[n+1]} = e^{i\tau\Delta} P_N \psi^{[n]} - i\tau\varphi_1(i\tau\Delta) P_N B(\psi^{[n]}), \quad 0 \leq n \leq T/\tau - 1. \tag{4.3}$$

Recalling (2.11) and (3.4), we have

$$\psi^{n+1} = e^{i\tau\Delta} \psi^n - i\tau\varphi_1(i\tau\Delta) P_N B(\psi^n), \quad 0 \leq n \leq T/\tau - 1. \tag{4.4}$$

Subtracting (4.4) from (4.3), we have, for $0 \leq n \leq T/\tau - 1$,

$$e^{n+1} = e^{i\tau\Delta} e^n - i\tau\varphi_1(i\tau\Delta) P_N (B(\psi^{[n]}) - B(\psi^n)). \tag{4.5}$$

From (4.5), using the isometry property of $e^{it\Delta}$, the L^2-projection property of P_N, and Lemma 3.9 with $\alpha = 0$, we have, for $0 \leq n \leq T/\tau - 1$,

$$\begin{aligned} \|e^{n+1}\|_{L^2} &\leq \|e^n\|_{L^2} + \tau \|\varphi_1(i\tau\Delta) P_N ((B(\psi^{[n]}) - B(\psi^n))\|_{L^2} \\ &\leq \|e^n\|_{L^2} + \tau \|(B(\psi^{[n]}) - B(\psi^n)\|_{L^2} \\ &\leq \|e^n\|_{L^2} + \tau \|(B(\psi^{[n]}) - B(P_N\psi^{[n]})\|_{L^2} + \tau \|(B(P_N\psi^{[n]}) - B(\psi^n)\|_{L^2}. \end{aligned} \tag{4.6}$$

By (3.2), using Sobolev embedding and the boundedness of P_N, we have

$$\|P_N \psi^{[n]}\|_{L^\infty} \leq \tilde{c} \|P_N \psi^{[n]}\|_{H^2} \leq \tilde{c} \|\psi^{[n]}\|_{H^2} \leq \tilde{c} C(M) =: M_0, \quad 0 \leq n \leq T/\tau, \tag{4.7}$$

where $\tilde{c}$ is given by the Sobolev embedding $H^2 \hookrightarrow L^\infty$. Similarly, $\|\psi^{[n]}\|_{L^\infty} \leq M_0$. From (4.6), noting (4.7) and using Lemma 3.4, the uniform H^2-bound in (3.2), and the standard projection error estimate $\|\phi - P_N \phi\|_{L^2} \lesssim h^2 |\phi|_{H^2}$ $\forall \phi \in H^2_{\text{per}}(\Omega)$, we have, for $0 \leq n \leq T/\tau - 1$,

$$\|e^{n+1}\|_{L^2} \leq \|e^n\|_{L^2} + C_L(\max\{M_0, \|\psi^n\|_{L^\infty}\})\tau \|e^n\|_{L^2} + \tilde{C}_1 \tau h^2, \tag{4.8}$$

where $\tilde{C}_1$ depends exclusively on M. The conclusion then follows from the discrete Gronwall's inequality and the standard induction argument by using the inverse inequality [50]

$$\|\phi\|_{L^\infty} \le C_{\text{inv}} h^{-\frac{d}{2}} \|\phi\|_{L^2}, \quad \phi \in X_N, \tag{4.9}$$

where d is the dimension of the space, i.e., $d=1$ in the current case. For the convenience of the reader, we present this process in the following.

Let $\tilde{C}_0 := C_L(1+M_0)+1$ with $C_L(\cdot)$ given in Lemma 3.4, and recall $\tilde{C}_1$ given by (4.8). Let $0<h_0<1$ be chosen such that

$$C_{\text{inv}} e^{\tilde{C}_0 T} \tilde{C}_1 h_0^{2-d/2} \le 1. \tag{4.10}$$

We shall show that, when $0<h<h_0$, for $0 \le n \le T/\tau$,

$$\|e^n\|_{L^2} \le e^{\tilde{C}_0 T} \tilde{C}_1 h^2, \quad \|\psi^n\|_{L^\infty} \le 1+M_0. \tag{4.11}$$

Recall that $e^0=0$, and by (4.7), $\|\psi^0\|_{L^\infty} = \|P_N \psi_0\|_{L^\infty} = \|P_N \psi^{[0]}\|_{L^\infty} \le M_0$. Then (4.11) holds for $n=0$. Assume that (4.11) holds for $0 \le n \le m \le T/\tau - 1$, which implies, from (4.8), that

$$\|e^{n+1}\|_{L^2} \le (1+\tilde{C}_0\tau)\|e^n\|_{L^2} + \tilde{C}_1 \tau h^2, \quad 0 \le n \le m, \tag{4.12}$$

which further implies, by using the discrete Gronwall's inequality, that

$$\|e^{m+1}\|_{L^2} \le e^{\tilde{C}_0 T} \tilde{C}_1 h^2. \tag{4.13}$$

From (4.13), using (4.9) and recalling (4.7) and (4.10), we have, by the triangle inequality,

$$\begin{aligned} \|\psi^{m+1}\|_{L^\infty} &\le \|e^{m+1}\|_{L^\infty} + \|P_N \psi^{[m+1]}\|_{L^\infty} \le C_{\text{inv}} h^{2-d/2} \|e^{m+1}\|_{L^2} + M_0 \\ &\le C_{\text{inv}} e^{\tilde{C}_0 T} \tilde{C}_1 h^{2-d/2} + M_0 \le 1 + M_0. \end{aligned} \tag{4.14}$$

Combing (4.13) and (4.10) proves (4.11) for $n=m+1$ and thus for all $0 \le n \le T/\tau$ by mathematical induction, which completes the proof. ∎

Proof of (4.1) *in Theorem* 4.1. By the triangle inequality, for $0 \le \alpha \le 2$,

$$\|\psi(t_n) - \psi^n\|_{H^\alpha} \le \|\psi(t_n) - \psi^{[n]}\|_{H^\alpha} + \|\psi^{[n]} - P_N \psi^{[n]}\|_{H^\alpha} + \|P_N \psi^{[n]} - \psi^n\|_{H^\alpha}. \tag{4.15}$$

From (3.2), using the interpolation inequalities, we have

$$\|\psi(t_n) - \psi^{[n]}\|_{H^\alpha} \lesssim \tau^{1-\alpha/2}, \quad 0 \le \alpha \le 2. \tag{4.16}$$

From (4.15), using (4.16) and the standard Fourier projection error estimates

$$\|\phi - P_N \phi\|_{H^\alpha} \lesssim h^{2-\alpha} |\phi|_{H^2}, \quad 0 \le \alpha \le 2, \quad \phi \in H^2_{\text{per}}(\Omega), \tag{4.17}$$

and noting (3.2), we have

$$\|\psi(t_n) - \psi^n\|_{H^\alpha} \lesssim \tau^{1-\alpha/2} + h^{2-\alpha} + \|P_N \psi^{[n]} - \psi^n\|_{H^\alpha}. \tag{4.18}$$

From (4.18), using the inverse estimate $\|\phi\|_{H^\alpha} \lesssim h^{-\alpha} \|\phi\|_{L^2}$ $\forall \phi \in X_N$ [30, 50] and Proposition 4.3, we have

$$\|\psi^n - \psi(t_n)\|_{H^\alpha} \lesssim \tau^{1-\alpha/2} + h^{2-\alpha} + h^{-\alpha} h^2 \lesssim \tau^{1-\alpha/2} + h^{2-\alpha}, \quad 0 \le \alpha \le 2, \tag{4.19}$$

which proves (4.1) by taking $\alpha = 0, 1, 2$. ∎

4.3. Proof of the optimal H^1-error bound (4.2). To prove (4.2), we assume that $V \in W^{1,4}(\Omega) \cap H^1_{\text{per}}(\Omega)$, f satisfies Assumption (B), $\psi \in C([0,T]; H^3_{\text{per}}(\Omega)) \cap C^1([0,T]; H^1(\Omega))$, and $0 < \tau < \tau_0$, $0 < h < h_0$. Since we already have the uniform control of ψ^n in H^2-norm, (4.2) can be proved similarly to (3.3), and we just sketch the outline here.

Proof of (4.2) *in Theorem* 4.1. Recalling (2.11) and (3.16), we have

$$\begin{aligned} &P_N\psi(t_{n+1}) - \Phi_h^\tau(P_N\psi(t_n)) \\ &\quad = -i\int_0^\tau e^{i(\tau-s)\Delta} P_N\left(B(\psi(t_n+s)) - B(P_N\psi(t_n))\right) \mathrm{d}s, \quad 0 \le n \le \frac{T}{\tau} - 1, \end{aligned} \tag{4.20}$$

which implies, by the property of $e^{it\Delta}$ and P_N for $X = L^2$ or H^1, that

$$\begin{aligned} &\|P_N\psi(t_{n+1}) - \Phi_h^\tau(P_N\psi(t_n))\|_X \\ &\quad \le \int_0^\tau \left(\|B(\psi(t_n+s)) - B(\psi(t_n))\|_X + \|B(\psi(t_n)) - B(P_N\psi(t_n))\|_X\right) \mathrm{d}s. \end{aligned} \tag{4.21}$$

From (4.21), using Lemma 3.4 and (3.38), we have, for $0 \le n \le T/\tau - 1$,

$$\begin{aligned} &\|P_N\psi(t_{n+1}) - \Phi_h^\tau(P_N\psi(t_n))\|_{L^2} \lesssim \tau^2 + \tau h^3, \\ &\|P_N\psi(t_{n+1}) - \Phi_h^\tau(P_N\psi(t_n))\|_{H^1} \lesssim \tau^2 + \tau h^2. \end{aligned} \tag{4.22}$$

Besides, recalling (2.11), using Lemmas 3.9 and 3.4, (3.22), and (3.38), we have

$$\begin{aligned} &\|\Phi_h^\tau(P_N\psi(t_n)) - \Phi_h^\tau(\psi^n)\|_{L^2} \le (1 + C_1\tau)\|P_N\psi(t_n) - \psi^n\|_{L^2}, \\ &\|\Phi_h^\tau(P_N\psi(t_n)) - \Phi_h^\tau(\psi^n)\|_{H^1} \le (1 + C_2\tau)\|P_N\psi(t_n) - \psi^n\|_{H^1}, \end{aligned} \tag{4.23}$$

where C_1 depends on $\|P_N\psi(t_n)\|_{L^\infty}$ and $\|\psi^n\|_{L^\infty}$ and C_2 depends on $\|P_N\psi(t_n)\|_{H^3}$ and $\|\psi^n\|_{H^2}$ for $0 \le n \le T/\tau - 1$. Thus, both C_1 and C_2 are under control. Then the proof can be completed by the Lady Windermere's fan argument and the standard projection error estimates of P_N. ◻

4.4. Extension to the EWI-EFP (2.13). For $I_N\psi^{\langle n\rangle}(0 \le n \le T/\tau)$ obtained from the EWI-EFP scheme (2.13), it satisfies the same error bounds as $\psi^n(0 \le n \le T/\tau)$ in Theorem 4.1 under the same assumptions on potential and the exact solution but with a little more regular nonlineairty. To be precise, we introduce another assumption on the nonlinearity as

(C) $$f(|v|^2)v \in H^\alpha_{\text{per}}(\Omega) \quad \forall v \in H^\alpha_{\text{per}}(\Omega).$$

For the optimal L^2-norm error bound, we assume that f satisfies Assumptions (A) and (C) with $\alpha = 2$. Two typical examples of f include (i) $f(\rho) = \lambda_1\rho^{\sigma_1} + \lambda_2\rho^{\sigma_2}$ with $\sigma_2 > \sigma_1 \ge 1/2$ and $\lambda_1, \lambda_2 \in \mathbb{R}$ and (ii) $f(\rho) = \lambda\rho^\sigma \ln\rho$ with $\sigma > 1/2$ and $\lambda \in \mathbb{R}$.

For the optimal H^1-norm error bound, we assume, in addition to Assumption (B), that f satisfies (C) with $\alpha = 3$ and the discrete counterpart of Assumption (B),

(B') $$\|I_N(f(|v|^2)v - f(|w|^2)w)\|_{H^1} \le C(\|v\|_{H^3}, \|w\|_{H^2})\|v - w\|_{H^1}, \quad v, w \in X_N,$$

with two typical examples of f: (i) $f(\rho) = \lambda_1\rho^{\sigma_1} + \lambda_2\rho^{\sigma_2}$ with $\sigma_2 > \sigma_1 \ge 1$ and $\lambda_1, \lambda_2 \in \mathbb{R}$ and (ii) $f(\rho) = \lambda\rho^\sigma \ln\rho$ with $\sigma > 1$ and $\lambda \in \mathbb{R}$ (see, e.g., [18] for the proof).

Then we have the following error bounds for the EWI-EFP scheme (2.13).

COROLLARY 4.4. *Assume that* $V \in L^\infty(\Omega)$, f *satisfies Assumptions* (A) *and* (C) *with* $\alpha = 2$, *and the exact solution* $\psi \in C([0,T]; H^2_{\rm per}(\Omega)) \cap C^1([0,T]; L^2(\Omega))$. *There exists* $\tau_0 > 0$ *and* $h_0 > 0$ *depending on* M *and* T *and sufficiently small such that for any* $0 < \tau < \tau_0$ *and* $0 < h < h_0$, *we have*

$$\begin{aligned}&\|\psi(\cdot,t_n) - I_N\psi^{\langle n\rangle}\|_{L^2} \lesssim \tau + h^2, \quad \|I_N\psi^{\langle n\rangle}\|_{H^2} \le C(M),\\ &\|\psi(\cdot,t_n) - I_N\psi^{\langle n\rangle}\|_{H^1} \lesssim \sqrt{\tau} + h, \qquad 0 \le n \le T/\tau.\end{aligned} \tag{4.24}$$

Moreover, if $V \in W^{1,4}(\Omega) \cap H^1_{\rm per}(\Omega)$; f *satisfies Assumptions* (B), (B'), *and* (C) *with* $\alpha = 3$; *and* $\psi \in C([0,T]; H^3_{\rm per}(\Omega)) \cap C^1([0,T]; H^1(\Omega))$, *then we have, for* $0 < \tau < \tau_0$ *and* $0 < h < h_0$,

$$\|\psi(\cdot,t_n) - I_N\psi^{\langle n\rangle}\|_{L^2} \lesssim \tau + h^3, \ \|\psi(\cdot,t_n) - I_N\psi^{\langle n\rangle}\|_{H^1} \lesssim \tau + h^2, \quad 0 \le n \le T/\tau. \tag{4.25}$$

For notational simplicity, we define $B_N : C_{\rm per}(\overline{\Omega}) \to X_N$ as

$$B_N(\phi) := P_N(V\phi) + I_N G(\phi), \quad \phi \in C_{\rm per}(\overline{\Omega}), \tag{4.26}$$

where $G(\phi)(x) = f(|\phi(x)|^2)\phi(x)$ for $x \in \overline{\Omega}$. Then we have the following.

LEMMA 4.5. *Let* $v, w \in X_N$. *Assume that* $V \in L^\infty(\Omega)$ *and* f *satisfies* (A) *and* (C) *with* $\alpha = 2$. *If* $\|v\|_{H^2} \le M_0$ *and* $\|w\|_{L^\infty} \le M_1$, *then we have*

$$\|P_N B(v) - B_N(w)\|_{L^2} \le C(\|V\|_{L^\infty}, M_0, M_1)\|v - w\|_{L^2} + C(M_0)h^2. \tag{4.27}$$

Moreover, if $V \in W^{1,4}(\Omega) \cap H^1_{\rm per}(\Omega)$, f *satisfies Assumptions* (B') *and* (C) *with* $\alpha = 3$, *and* $\|v\|_{H^3} \le M_2$ *and* $\|w\|_{H^2} \le M_3$, *we have*

$$\|P_N B(v) - B_N(w)\|_{H^1} \le C(\|V\|_{W^{1,4}}, M_2, M_3)\|v - w\|_{H^1} + C(M_2)h^2. \tag{4.28}$$

Proof. Recalling (3.4) and (4.26), we have

$$\begin{aligned}P_N B(v) - B_N(w) &= P_N(V(v-w)) + P_N G(v) - I_N G(w)\\ &= P_N(V(v-w)) + (P_N - I_N)G(v) + I_N G(v) - I_N G(w).\end{aligned} \tag{4.29}$$

From (4.29), using assumption (C) with $\alpha = 2$, we have

$$\begin{aligned}\|P_N B(v) - B_N(w)\|_{L^2} &\lesssim \|V\|_{L^\infty}\|v - w\|_{L^2} + C(M_0)h^2 + \|I_N G(v) - I_N G(w)\|_{L^2}\\ &\le \|V\|_{L^\infty}\|v - w\|_{L^2} + C(M_0)h^2 + C(M_0, M_1)\|v - w\|_{L^2},\end{aligned} \tag{4.30}$$

where we use $\|I_N G(\phi)\|^2_{L^2} = h\sum_{j=0}^{N-1} |G(\phi(x_j))|^2$ and I_N is an identity on X_N in the last line, and we prove (4.27).

To prove (4.28), using (C) with $\alpha = 3$ and (B'), from (4.29), we have

$$\|P_N B(v) - B_N(w)\|_{H^1} \lesssim \|V\|_{W^{1,4}}\|v - w\|_{H^1} + C(M_2)h^2 + C(M_2, M_3)\|v - w\|_{H^1},$$

which proves (4.28) and completes the proof. ∎

Proof of Corollary 4.4. The proof is similar to the proof of Theorem 4.1, and we sketch it here for the convenience of the reader. We start with the proof of (4.24). Define the error function $e^{\langle n\rangle} := P_N\psi^{[n]} - I_N\psi^{\langle n\rangle}$ for $0 \le n \le T/\tau$. Then

$e^{\langle 0\rangle} = P_N\psi_0 - I_N\psi_0$ satisfies $\|e^{\langle 0\rangle}\|_{L^2} \leq C(M)h^2$. Recalling (2.16), (4.26), and (4.3), we obtain, for $0 \leq n \leq T/\tau - 1$,

$$e^{\langle n+1\rangle} = e^{i\tau\Delta}e^{\langle n\rangle} - i\tau\varphi_1(i\tau\Delta)(P_N B(\psi^{[n]}) - B_N(I_N\psi^{\langle n\rangle})). \tag{4.31}$$

From (4.31), by the boundedness of $e^{i\tau\Delta}$, P_N, and $\varphi_1(i\tau\Delta)$; Lemma 3.4; the triangle inequality; the uniform H^2-bound of $\psi^{[n]}$ in (3.2); and (4.27), we get

$$\begin{aligned}\|e^{\langle n+1\rangle}\|_{L^2} &\leq \|e^{\langle n\rangle}\|_{L^2} + \tau\Big(\|P_N B(\psi^{[n]}) - P_N B(P_N\psi^{[n]})\|_{L^2} \\ &\qquad + \|P_N B(P_N\psi^{[n]}) - B_N(I_N\psi^{\langle n\rangle})\|_{L^2}\Big) \\ &\leq \|e^{\langle n\rangle}\|_{L^2} + C(M)\tau h^2 + (1 + C(M, \|I_N\psi^{\langle n\rangle}\|_{L^\infty})\tau)\|e^{\langle n\rangle}\|_{L^2}. \end{aligned} \tag{4.32}$$

From (4.32), by the discrete Gronwall's inequality and the same induction process as in the proof of Proposition 4.3, noting first step error $\|e^{\langle 0\rangle}\|_{L^2} \leq C(M)h^2$, we obtain

$$\|e^{\langle n\rangle}\|_{L^2} \leq C(M,T)h^2, \quad 0 \leq n \leq T/\tau. \tag{4.33}$$

The rest of the proof of (4.24) can be completed by following the proof of (4.1).

Then we outline the proof of (4.25). Define the numerical flow $\Phi_h^{\langle\tau\rangle} : X_N \to X_N$ associated with the EWI-EFP scheme (2.13) as

$$\Phi_h^{\langle\tau\rangle}(v) = e^{i\tau\Delta}v - i\tau\varphi_1(i\tau\Delta)B_N(v), \quad v \in X_N. \tag{4.34}$$

Recalling (2.16), we have $I_N\psi^{\langle n+1\rangle} = \Phi_h^{\langle\tau\rangle}(I_N\psi^{\langle n\rangle})$ for $n \geq 0$. Recalling (3.16) and (4.34), the local truncation error can be decomposed as

$$\begin{aligned} P_N\psi(t_{n+1}) - \Phi_h^{\langle\tau\rangle}(P_N\psi(t_n)) &= -i\int_0^\tau e^{i(\tau-s)\Delta}\big(P_N B(\psi(t_n+s)) - P_N B(\psi(t_n)) + \\ & P_N B(\psi(t_n)) - P_N B(P_N\psi(t_n)) + P_N B(P_N\psi(t_n)) - B_N(P_N\psi(t_n))\big)\mathrm{d}s, \end{aligned} \tag{4.35}$$

which implies, by the boundedness of $e^{it\Delta}$ and P_N and using (3.38) and (4.28), that

$$\|P_N\psi(t_{n+1}) - \Phi_h^{\langle\tau\rangle}(P_N\psi(t_n))\|_{H^1} \lesssim \tau^2 + \tau h^2. \tag{4.36}$$

Besides, recalling (4.34) and using (B'), we have H^1-stability estimate

$$\|\Phi_h^{\langle\tau\rangle}(P_N\psi(t_n)) - \Phi_h^{\langle\tau\rangle}(I_N\psi^{\langle n\rangle})\|_{H^1} \leq (1 + C_3\tau)\|P_N\psi(t_n) - I_N\psi^{\langle n\rangle}\|_{H^1}, \tag{4.37}$$

where C_3 depends on $\|V\|_{W^{1,4}}$, $\|\psi(t_n)\|_{H^3}$, and $\|I_N\psi^{\langle n\rangle}\|_{H^2}$ and thus is under control. The proof of the H^1-error bound in (4.25) can be completed by applying the standard Lady Windermere's fan argument with (4.36) and (4.37). The proof of the L^2-error bound in (4.25) can be obtained similarly. Then the proof is completed. ∎

5. Numerical results. In this section, we present some numerical examples for the NLSE with either low regularity potential or nonlinearity. In the following, we fix $\Omega = (-16, 16)$, $T = 1$, $d = 1$ and consider the power-type nonlinearity $f(\rho) = -\rho^\sigma$ $(\sigma > 0)$.

Let $\psi^n (0 \leq n \leq T/\tau)$ be the numerical solution obtained by the EWI-FS method (2.11) or the EWI-EFP method (2.13), which will be made clear in each case. Define the error functions

$$e^k_{L^2} = \|\psi(t_k) - I_N\psi^k\|_{L^2}, \quad e^k_{H^1} = \|\psi(t_k) - I_N\psi^k\|_{H^1}, \quad 0 \leq k \leq n := T/\tau.$$

5.1. For the NLSE with locally Lipschitz nonlinearity. In this subsection, we only consider the NLSE with the power-type nonlinearity and without potential,

$$i\partial_t \psi(x,t) = -\Delta\psi(x,t) - |\psi(x,t)|^{2\sigma}\psi(x,t), \quad x \in \Omega, \quad t > 0, \tag{5.1}$$

where $\sigma > 0$. Recall that Assumption (A) is satisfied for any $\sigma > 0$ and that Assumption (B) is satisfied for any $\sigma \geq 1/2$. Note that when there is no potential, the extended Fourier pseudospectral method collapses to the standard Fourier pseudospectral method.

Two types of initial data are considered:

(i) Type I. The H^2 initial datum:

$$\psi_0(x) = x|x|^{0.51} e^{-\frac{x^2}{2}}, \quad x \in \Omega. \tag{5.2}$$

(ii) Type II. The smooth initial datum:

$$\psi_0(x) = x e^{-\frac{x^2}{2}}, \quad x \in \Omega. \tag{5.3}$$

The two initial data are specially chosen to demonstrate the influence of the low regularity of f around the origin. Since both Type I and II initial data are odd functions, the corresponding solutions of the NLSE will satisfy $\psi(0,t) \equiv 0$ for all $t \geq 0$. The difference of these two initial data lies in the regularity.

We shall test the convergence order in both time and space for Types I and II initial data. For each initial datum, we choose $\sigma = 0.1, 0.2, 0.3, 0.4$. The "exact" solutions are computed by the Strang splitting Fourier pseudospectral method with $\tau = \tau_{\mathrm{e}} := 10^{-6}$ and $h = h_{\mathrm{e}} := 2^{-9}$. When testing the spatial errors, we fix the time step size $\tau = \tau_e$, and when testing the temporal errors, we fix the mesh size $h = h_e$.

We start with the Type I H^2 initial datum (5.2). Figure 5.1 exhibits the spatial error in L^2- and H^1-norms of the EWI-FS (solid lines) and the EWI-EFP (dotted lines) method for $\sigma = 0.1$ with the Type I initial datum. We can observe that the EWI-FS method is second-order convergent in L^2-norm and first-order convergent in H^1-norm. Moreover, we see that there is almost no difference between the spatial error of the EWI-FS method and the EWI-EFP method, which suggests that the Fourier pseudospectral method seems also suitable to discretize the low regularity nonlinearity.

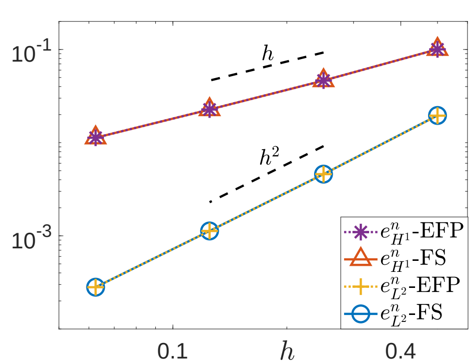

FIG. 5.1. *Comparison of the Fourier spectral and pseudospectral discretization of the nonlinear term in* (5.1) *with* $\sigma = 0.1$ *and Type* I *initial datum* (5.2).

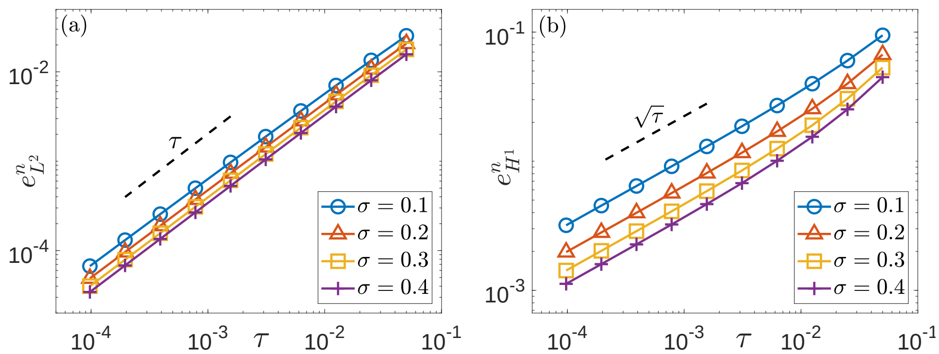

FIG. 5.2. *Temporal errors of the EWI for the NLSE* (5.1) *with Type* I *initial datum* (5.2)*:* (a) *L^2-norm errors and* (b) *H^1-norm errors.*

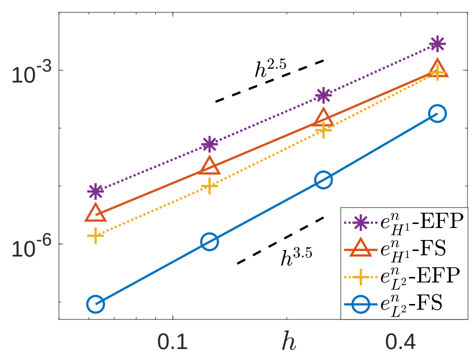

FIG. 5.3. *Comparison of the Fourier spectral and pseudospectral discretizations of the nonlinear term in* (5.1) *with $\sigma = 0.1$ and Type* II *initial datum* (5.3)*.*

Figure 5.2 plots the temporal error in L^2- and H^1-norms of the EWI for different $0 < \sigma < 1/2$ with Type I initial datum. Figure 5.2(a) shows that the temporal convergence is first order in L^2-norm for all the four σ's, and Figure 5.2 (b) shows that the temporal convergence is half order in H^1-norm for all the four σ's.

The results in Figures 5.1 and 5.2 confirm our optimal L^2-norm error bound for the NLSE with locally Lipschitz nonlinearity and demonstrate that it is sharp.

Then we consider the Type II smooth initial datum (5.3). Figure 5.3 shows the spatial error in L^2- and H^1-norms of the EWI-FS (solid lines) and the EWI-EFP (dotted lines) method for $\sigma = 0.1$ with the Type II initial datum. We can observe that the convergence orders in H^1-norm of the EWI-FS (solid lines) and the EWI-EFP (dashed lines) are almost the same (roughly 2.5), though the value of the error of the EWI-FS is smaller than the EWI-EFP. The convergence order in L^2-norm of the EWI-FS method is roughly 3.5, which is almost one order higher than that of the EWI-EFP method. This observation suggests that when the solution has better regularity, the Fourier spectral method outperforms the Fourier pseudospectral method for discretizing the low regularity nonlinearity.

Figure 5.4 displays the temporal error in L^2- and H^1-norms of the EWI for different $0 < \sigma < 1$ with the Type II initial datum. Figure 5.4 shows that the temporal convergence is first order in both L^2- and H^1-norms for all the four σ's. However, currently, we can only prove the first-order H^1-convergence in time under Assumption

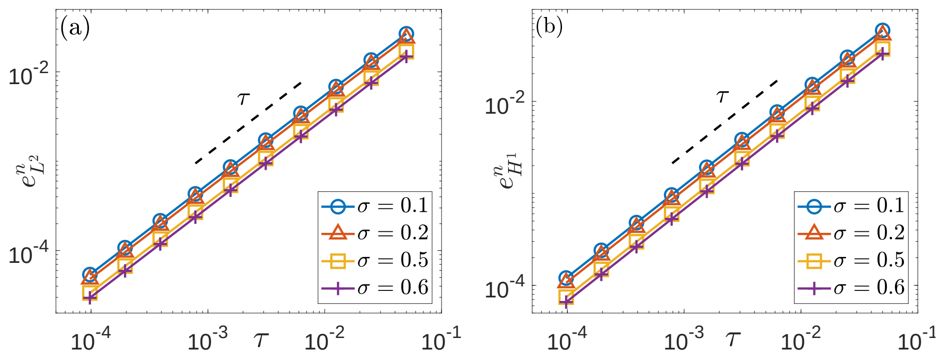

FIG. 5.4. *Temporal errors of the EWI for the NLSE* (5.1) *with Type* II *initial datum* (5.3)*:* (a) L^2*-norm errors and* (b) H^1*-norm errors.*

(B), which holds only when $\sigma \geq 1/2$. Besides, as shown in Figure 5.3 of [18], for the time-splitting methods, we can observe first-order convergence in H^1-norm only when $\sigma \geq 1/2$, which suggests that the EWI may be better than the time-splitting methods when the nonlinearity is of low regularity.

The results in Figures 5.3 and 5.4 confirm our optimal H^1-norm error bound for the NLSE with low regularity nonlinearity but also indicate that Assumption (B) may be relaxed.

5.2. For the NLSE with low regularity potential. In this subsection, we only consider the cubic NLSE with low regularity potential as

$$i\partial_t\psi(x,t) = -\Delta\psi(x,t) + V(x)\psi(x,t) - |\psi(x,t)|^2\psi(x,t), \quad \mathbf{x} \in \Omega, \quad t > 0, \tag{5.4}$$

where V is chosen as either $V_1 \in L^\infty(\Omega)$ or $V_2 \in W^{1,4}(\Omega)$ defined as

$$V_1(x) = \begin{cases} -4, & x \in (-2,2), \\ 0 & \text{otherwise}, \end{cases} \qquad V_2(x) = |x|^{0.76}, \qquad x \in \Omega. \tag{5.5}$$

We shall test the convergence orders for the NLSE (5.4) with $V = V_1$ and $\psi_0 \in H^2(\Omega)$ and $V = V_2$ and $\psi_0 \in H^3(\Omega)$, respectively. The "exact" solutions are computed by the EWI-EFP method with $\tau = \tau_{\mathrm{e}} := 10^{-6}$ and $h = h_{\mathrm{e}} := 2^{-9}$. When we test the spatial errors, we fix the time step size $\tau = \tau_e$, and when we test the temporal errors, we fix the mesh size $h = h_e$.

We start with the spatial error and compare the performance of the extended Fourier pseudospectral method and the standard Fourier pseudospectral (FP) method, which can be obtained by replacing $(\widehat{VI_N\psi^{\langle n\rangle}})_l$ with $(\widetilde{V\psi^{\langle n\rangle}})_l$ in (2.13). We remark here that, since the nonlinearity is smooth in (5.4), the results of the EWI-FS method are almost the same as those of the EWI-EFP method.

Figure 5.5(a) shows the spatial error in L^2- and H^1-norms of the EWI-EFP method (solid lines) and the EWI-FP method (dotted lines) with $V = V_1 \in L^\infty(\Omega)$ given in (5.5) and $\psi_0 \in H^2(\Omega)$ given in (5.2). We can observe that the EWI-EFP is second-order convergent in L^2-norm and first-order convergent in H^1-norm in space. However, the spatial convergence order of the EWI-FP method is only first order in both L^2- and H^1-norms, and the value of the error is much larger. This implies that when discretizing purely L^∞-potential, the extended Fourier pseudospectral method is much better than the standard Fourier pseudospectral method. Figure 5.5(b) plots

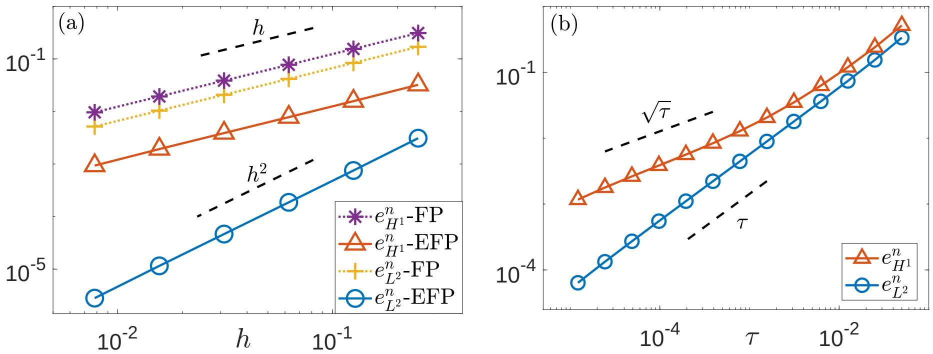

FIG. 5.5. *Convergence tests of the EWI for* (5.4) *with* $V = V_1 \in L^\infty(\Omega)$ *and* $\psi_0 \in H^2(\Omega)$*:* (a) *spatial errors of the Fourier spectral and pseudospectral discretizations for the linear potential and* (b) *temporal errors in* L^2*-norm and* H^1*-norm.*

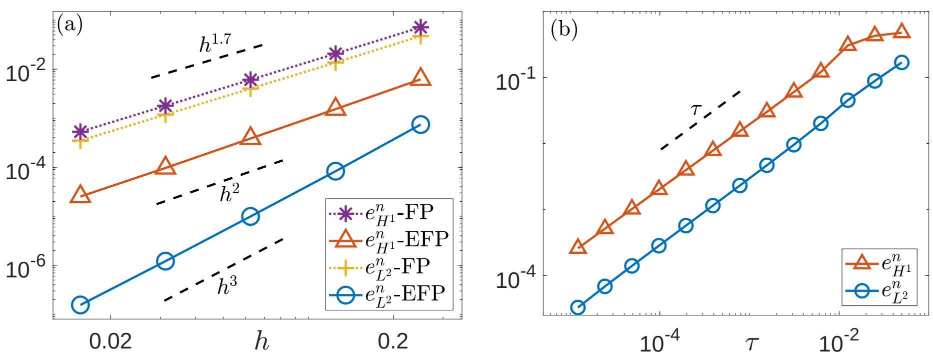

FIG. 5.6. *Convergence tests of the EWI for* (5.4) *with* $V = V_2 \in W^{1,4}(\Omega)$ *and* $\psi_0 \in H^3(\Omega)$*:* (a) *spatial errors of the Fourier spectral and pseudospectral discretizations for the linear potential and* (b) *temporal errors in* L^2*-norm and* H^1*-norm.*

the temporal convergence of the EWI in L^2- and H^1-norms with the Type I initial datum. We can observe that the EWI is first-order convergent in L^2-norm and half-order convergent in H^1-norm in time.

The results in Figure 5.5 validate our optimal L^2-norm error bound for the NLSE with L^∞-potential and demonstrate that it is sharp.

Figure 5.6(a) shows the spatial error in L^2- and H^1-norms of the EWI-EFP method (solid lines) and the EWI-FP method (dotted lines) with $V = V_2 \in W^{1,4}(\Omega)$ given in (5.5) and $\psi_0 \in H^3(\Omega)$ given by $\psi_0(x) = (1 + |x|^{2.51})e^{-x^2/2}$. We can observe that the EWI-EFP is third-order convergent in L^2-norm and second-order convergent in H^1-norm in space. However, the spatial convergence order of the EWI-FP method is only 1.7 orders in both L^2- and H^1-norms, and the value of the error is much larger. This implies again that the extended Fourier pseudospectral method is much better than the standard Fourier pseudospectral method when the potential is of low regularity. Figure 5.6(b) plots the temporal convergence of the EWI in L^2- and H^1-norms with the H^3 initial datum. We can observe that the EWI is first-order convergent in H^1-norm in time for $V \in W^{1,4}(\Omega)$.

The results in Figure 5.6 validate our optimal H^1-norm error bound for the NLSE with $W^{1,4}$-potential and demonstrate that it is sharp.

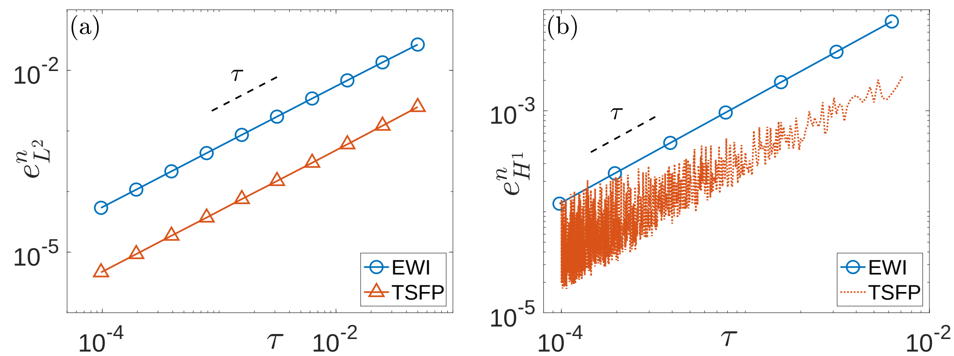

FIG. 5.7. *Comparison of EWI and LTFP for the NLSE* (5.1) *with* $\sigma = 0.1$*:* (a) *temporal errors in* L^2*-norm and* (b) *temporal errors in* H^1*-norm.*

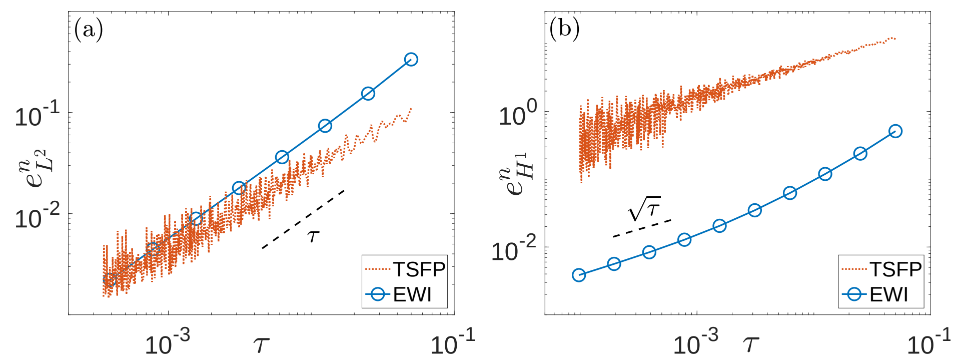

FIG. 5.8. *Comparison of EWI and LTFP for the NLSE* (5.4) *with* $V = V_1 \in L^\infty(\Omega)$ *in* (5.5)*:* (a) *temporal errors in* L^2*-norm and* (b) *temporal errors in* H^1*-norm.*

5.3. Comparison with the time-splitting method. In this subsection, we present some numerical results to compare the performance of the EWI and the time-splitting method applied to the NLSE with low regularity potential and nonlinearity. To be precise, we compare the EWI with the first-order Lie–Trotter time-splitting method with the standard Fourier pseudospectral method for spatial discretization (abbreviated as TSFP in the following). Here, we fix $h = h_e$ and compare the temporal errors; roughly speaking, this is equivalent to doing a comparison for semidiscretization in time by different time integrators.

First, we consider the NLSE (5.1) with low regularity nonlinearity $\sigma = 0.1$ and the smooth initial datum (5.3). In Figure 5.7, we can observe that both the EWI and the TSFP are first-order convergent in L^2-norm, although the value of the error of the TSFP method is smaller than the EWI. However, when measured in H^1-norm, the EWI is still first-order convergent (although this is not covered by our error estimates, as already mentioned in the discussion of Figure 5.4), but the error of the TSFP method fluctuates a lot and leads to order reduction.

Then we consider the NLSE (5.4) with low regularity potential $V = V_1 \in L^\infty(\Omega)$ in (5.5) and an H^2-initial datum given in (5.2). In Figure 5.8, we can observe that the EWI is first-order and half-order convergent in L^2- and H^1-norms, respectively. However, both the L^2- and H^1-errors of the TSFP method fluctuate drastically and suffer from severe order reduction.

Based on the discussion above, we can conclude that, in general, the EWI is better than the TSFP method when approximating the NLSE with low regularity potential and nonlinearity. However, the numerical results also necessitate the design and analysis of higher-order and structure-preserving (e.g., time-symmetric) EWIs for better error constant. This will be considered in our future work.

6. Conclusions. We established optimal error bounds for the first-order Gautschi-type EWI applied to the NLSE with L^∞-potential and/or locally Lipschitz nonlinearity under the assumption of H^2-solution. For the semidiscretization in time by the first-order Gautschi-type EWI, we proved an optimal L^2-norm error bound at $O(\tau)$ and a uniform H^2-bound of the numerical solution. For the full discretization obtained from the semidiscretization by using the Fourier spectral method in space, we proved an optimal L^2-norm error bound at $O(\tau + h^2)$ without any coupling condition between τ and h. For $W^{1,4}$-potential and a little more regular nonlinearity, under the assumption of H^3-solution of the NLSE, we proved optimal H^1-norm error bounds for both the semidiscrete and fully discrete schemes. As a by-product, we proposed an extended Fourier pseudospectral method to implement the full discretization when the potential is of low regularity and the nonlinearity is smooth, in which the potential and nonlinearity were discretized by the Fourier spectral method and the Fourier pseudospectral method, respectively. The proposed numerical implementation has similar computational cost as the standard Fourier pseudospectral method, but we can establish rigorous error bounds for this method. On the contrary, one cannot establish optimal error bounds for the standard Fourier pseudospectral method for the NLSE when the potential is of low regularity, e.g., $V \in L^\infty$. In the future, we will consider even weaker potential, e.g., $V \in L^1$, including Coulomb potential and/or spatial/temporal Dirac delta potential.

REFERENCES

[1] G. D. Akrivis, *Finite difference discretization of the cubic Schrödinger equation*, IMA J. Numer. Anal., 13 (1993), pp. 115–124.

[2] G. D. Akrivis, V. A. Dougalis, and O. A. Karakashian, *On fully discrete Galerkin methods of second-order temporal accuracy for the nonlinear Schrödinger equation*, Numer. Math., 59 (1991), pp. 31–53.

[3] Y. Alama Bronsard, *Error analysis of a class of semi-discrete schemes for solving the Gross-Pitaevskii equation at low regularity*, J. Comput. Appl. Math., 418 (2023), 114632.

[4] Y. Alama Bronsard, Y. Bruned, and K. Schratz, *Low Regularity Integrators via Decorated Trees*, preprint, arXiv:2211.09402, 2022.

[5] Y. Bruned and K. Schratz, *Resonance-based schemes for dispersive equations via decorated trees*, Forum Math. Pi, 10 (2022), pp. 1–76.

[6] X. Antoine, W. Bao, and C. Besse, *Computational methods for the dynamics of the nonlinear Schrödinger/Gross-Pitaevskii equations*, Comput. Phys. Commun., 184 (2013), pp. 2621–2633.

[7] G. E. Astrakharchik and B. A. Malomed, *Dynamics of one-dimensional quantum droplets*, Phys. Rev. A, 98 (2018), 013631.

[8] W. Bao and Y. Cai, *Mathematical theory and numerical methods for Bose-Einstein condensation*, Kinet. Relat. Models, 6 (2013), pp. 1–135.

[9] W. Bao and Y. Cai, *Optimal error estimates of finite difference methods for the Gross-Pitaevskii equation with angular momentum rotation*, Math. Comp., 82 (2013), pp. 99–128.

[10] W. Bao and Y. Cai, *Uniform and optimal error estimates of an exponential wave integrator sine pseudospectral method for the nonlinear Schrödinger equation with wave operator*, SIAM J. Numer. Anal., 52 (2014), pp. 1103–1127.

[11] W. Bao, Y. Cai, and Y. Feng, *Improved uniform error bounds of the time-splitting methods for the long-time (nonlinear) Schrödinger equation*, Math. Comp., 92 (2023), pp. 1109–1139.

[12] W. Bao, R. Carles, C. Su, and Q. Tang, *Error estimates of a regularized finite difference method for the logarithmic Schrödinger equation*, SIAM J. Numer. Anal., 57 (2019), pp. 657–680.

[13] W. Bao, R. Carles, C. Su, and Q. Tang, *Regularized numerical methods for the logarithmic Schrödinger equation*, Numer. Math., 143 (2019), pp. 461–487.

[14] W. Bao, R. Carles, C. Su, and Q. Tang, *Error estimates of local energy regularization for the logarithmic Schrödinger equation*, Math. Models Methods Appl. Sci., 32 (2022), pp. 101–136.

[15] W. Bao, Y. Feng, and Y. Ma, *Regularized numerical methods for the nonlinear Schrödinger equation with singular nonlinearity*, East Asian J. Appl. Math., 13 (2023), pp. 646–670.

[16] W. Bao, D. Jaksch, and P. A. Markowich, *Numerical solution of the Gross-Pitaevskii equation for Bose-Einstein condensation*, J. Comput. Phys., 187 (2003), pp. 318–342.

[17] W. Bao, N. J. Mauser, and H. P. Stimming, *Effective one particle quantum dynamics of electrons: A numerical study of the Schrödinger-Poisson-Xα model*, Commun. Math. Sci., 1 (2003), pp. 809–828.

[18] W. Bao and C. Wang, *Error estimates of the time-splitting methods for the nonlinear Schrödinger equation with semi-smooth nonlinearity*, Math. Comp., (2023), https://doi.org/10.1090/mcom/3900.

[19] M. Bayindir, B. Tanatar, and Z. Gedik, *Bose-Einstein condensation in a one-dimensional interacting system due to power-law trapping potentials*, Phys. Rev. A, 59 (1999), pp. 1468–1472.

[20] C. Besse, B. Bidégaray, and S. Descombes, *Order estimates in time of splitting methods for the nonlinear Schrödinger equation*, SIAM J. Numer. Anal., 40 (2002), pp. 26–40.

[21] O. Bokanowski and N. J. Mauser, *Local approximation for the Hartree-Fock exchange potential: A deformation approach*, Math. Models Methods Appl. Sci., 9 (1999), pp. 941–961.

[22] C. R. Cabrera, L. Tanzi, J. Sanz, B. Naylor, P. Thomas, P. Cheiney, and L. Tarruell, *Quantum liquid droplets in a mixture of Bose-Einstein condensates*, Science, 359 (2018), pp. 301–304.

[23] Y. Cai and H. Wang, *Analysis and computation for ground state solutions of Bose-Fermi mixtures at zero temperature*, SIAM J. Appl. Math., 73 (2013), pp. 757–779.

[24] T. Cazenave, *Semilinear Schrödinger Equations*, Courant Lecture Notes in Mathematics 10, American Mathematical Society, Providence, RI, 2003.

[25] E. Celledoni, D. Cohen, and B. Owren, *Symmetric exponential integrators with an application to the cubic Schrödinger equation*, Found. Comput. Math., 8 (2008), pp. 303–317.

[26] W. Choi and Y. Koh, *On the splitting method for the nonlinear Schrödinger equation with initial data in $H1$*, Discrete Contin. Dyn. Syst., 41 (2021), pp. 3837–3867.

[27] J. Eilinghoff, R. Schnaubelt, and K. Schratz, *Fractional error estimates of splitting schemes for the nonlinear Schrödinger equation*, J. Math. Anal. Appl., 442 (2016), pp. 740–760.

[28] L. Erdős, B. Schlein, and H.-T. Yau, *Derivation of the cubic non-linear Schrödinger equation from quantum dynamics of many-body systems*, Invent. Math., 167 (2007), pp. 515–614.

[29] Y. Feng and K. Schratz, *Improved Uniform Error Bounds on a Lawson-Type Exponential Integrator for the Long-Time Dynamics of Sine-Gordon Equation*, preprint, arXiv:2211.09402, 2022.

[30] B.-Y. Guo, *Spectral Methods and Their Applications*, World Scientific, River Edge, NJ, 1998.

[31] Z. Hadzibabic, C. A. Stan, K. Dieckmann, S. Gupta, M. W. Zwierlein, A. Görlitz, and W. Ketterle, *Two-species mixture of quantum degenerate Bose and Fermi gases*, Phys. Rev. Lett., 88 (2002), 160401.

[32] P. Henning and D. Peterseim, *Crank-Nicolson Galerkin approximations to nonlinear Schrödinger equations with rough potentials*, Math. Models Methods Appl. Sci., 27 (2017), pp. 2147–2184.

[33] M. Hochbruck and A. Ostermann, *Exponential integrators*, Acta Numer., 19 (2010), pp. 209–286.

[34] L. I. Ignat, *A splitting method for the nonlinear Schrödinger equation*, J. Differential Equations, 250 (2011), pp. 3022–3046.

[35] H. Kadau, M. Schmitt, M. Wenzel, C. Wink, T. Maier, I. Ferrier-Barbut, and T. Pfau, *Observing the rosensweig instability of a quantum ferrofluid*, Nature, 530 (2016), pp. 194–197.

[36] T. Kato, *On nonlinear Schrödinger equations*, Ann. Inst. H. Poincaré Phys. Théor., 46 (1987), pp. 113–129.

[37] M. Knöller, A. Ostermann, and K. Schratz, *A Fourier integrator for the cubic nonlinear Schrödinger equation with rough initial data*, SIAM J. Numer. Anal., 57 (2019), pp. 1967–1986.
[38] T. D. Lee, K. Huang, and C. N. Yang, *Eigenvalues and eigenfunctions of a Bose system of hard spheres and its low-temperature properties*, Phys. Rev., 106 (1957), pp. 1135–1145.
[39] C. Lubich, *On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations*, Math. Comp., 77 (2008), pp. 2141–2153.
[40] A. Ostermann, F. Rousset, and K. Schratz, *Error estimates at low regularity of splitting schemes for NLS*, Math. Comp., 91 (2021), pp. 169–182.
[41] A. Ostermann, F. Rousset, and K. Schratz, *Error estimates of a Fourier integrator for the cubic Schrödinger equation at low regularity*, Found. Comput. Math., 21 (2021), pp. 725–765.
[42] A. Ostermann and K. Schratz, *Low regularity exponential-type integrators for semilinear Schrödinger equations*, Found. Comput. Math., 18 (2018), pp. 731–755.
[43] A. Ostermann, Y. Wu, and F. Yao, *A second-order low-regularity integrator for the nonlinear Schrödinger equation*, Adv. Contin. Discrete Models, (2022), 23.
[44] A. Ostermann and F. Yao, *A fully discrete low-regularity integrator for the nonlinear Schrödinger equation*, J. Sci. Comput., 91 (2022), 9.
[45] D. S. Petrov and G. E. Astrakharchik, *Ultradilute low-dimensional liquids*, Phys. Rev. Lett., 117 (2016), 100401.
[46] P. W. H. Pinkse, A. Mosk, M. Weidemüller, M. W. Reynolds, T. W. Hijmans, and J. T. M. Walraven, *Adiabatically changing the phase-space density of a trapped Bose gas*, Phys. Rev. Lett., 78 (1997), pp. 990–993.
[47] F. Rousset and K. Schratz, *A general framework of low regularity integrators*, SIAM J. Numer. Anal., 59 (2021), pp. 1735–1768.
[48] L. Sanchez-Palencia, D. Clément, P. Lugan, P. Bouyer, G. V. Shlyapnikov, and A. Aspect, *Anderson localization of expanding Bose-Einstein condensates in random potentials*, Phys. Rev. Lett., 98 (2007), 210401.
[49] J. M. Sanz-Serna, *Methods for the numerical solution of the nonlinear Schrödinger equation*, Math. Comp., 43 (1984), pp. 21–27.
[50] J. Shen, T. Tang, and L.-L. Wang, *Spectral Methods: Algorithms, Analysis and Applications*, Springer Series in Computational Mathematics 41, Springer-Verlag, Berlin, 2011.
[51] C. Sulem and P.-L. Sulem, *The Nonlinear Schrödinger Equation: Self-Focusing and Wave Collapse*, Applied Mathematical Sciences, Springer-Verlag, Berlin, 1999.
[52] Y. Tourigny, *Optimal H^1 estimates for two time-discrete Galerkin approximations of a nonlinear Schrödinger equation*, IMA J. Numer. Anal., 11 (1991), pp. 509–523.
[53] J. Wang, *A new error analysis of Crank-Nicolson Galerkin FEMs for a generalized nonlinear Schrödinger equation*, J. Sci. Comput., 60 (2014), pp. 390–407.
[54] I. Zapata, F. Sols, and A. J. Leggett, *Josephson effect between trapped Bose-Einstein condensates*, Phys. Rev. A, 57 (1998), pp. R28–R31.
[55] X. Zhao, *Numerical integrators for continuous disordered nonlinear Schrödinger equation*, J. Sci. Comput., 89 (2021), 40.